THE NEXT GENERATION WIMS LATTICE CODE : WIMS9

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ABSTRACT

The WIMS8 lattice cell and burnup code[1] was issued in 1999 and is continuously under development to meet the needs of its users and the increasing accuracy demands of the nuclear industry in general. As part of this development programme, a series of detailed studies have been undertaken to compare the results from the deterministic WIMS modular code system with results from Monte Carlo calculations performed using the MONK8 code[2], a companion code in the ANSWERS code suite. These inter-comparisons have allowed the identification of the most significant method approximations remaining in WIMS8, in particular, in the resonance self shielding treatment, and method improvements have been developed and incorporated in WIMS for its next issue as WIMS9.

This paper describes the results from the inter-comparison of WIMS8 and the MONK code for a range of reactor types and the method improvements introduced to remove the main discrepancies. Following these code and method developments the accuracy on reactivity predictions is within the ± 200 pcm target set as an objective for all main reactor types independent of whether light, heavy or mixed moderators are utilised.

A brief history of the WIMS code scheme is also given and the paper is concluded with a general overview of the validation status of WIMS.

1. INTRODUCTION

WIMS is a major software package containing a wide range of lattice cell and burnup methods for the design and development of all types of thermal reactor systems including experimental low power facilities as well as commercially operating power reactors. The modular code system is designed for use by all levels of user expertise to solve problems ranging from simple homogeneous systems through to the most complex 3D whole core geometries. Central to the aim of WIMS is to use a single physics model treatment of the resonance region that is capable of representing all types of reactor within a common framework. It is still one of the few codes capable of dealing with graphite, heavy water and light water moderated systems as well as problems involving more than one moderator in the reactor. Current developments are strongly focused on the improvement of methods within WIMS and on the usability of the system for design and reference applications.

In today's world, and possibly increasingly in the future, operators and safety regulators need to seek improved accuracies from reactor calculations to allow more efficient reactor operation while maintaining high safety case standards. This in turn requires improvements in the accuracy of lattice cell codes. It is with this recognition that, during the three years since the release of WIMS8, a series of fundamental studies have been performed to improve the physics methods employed within the WIMS code to meet the accuracy requirements of the next generation of lattice codes.

Although Monte Carlo methods, implemented for example in the MONK8 code, are recognised for providing accurate reference solutions for specific configurations, they are still too computer intensive to provide a full range of solutions for reactor performance or transient analyses where variations in many parameters such as temperatures, densities and pressures must be considered. There is still a central role in these types of analyses for deterministic methods such as those applied in WIMS.

For the development of the next generation of WIMS, WIMS9, the approach taken has been to review the fundamentals of the physics models it contains and their affect on accuracy. This has been achieved by performing a series of detailed inter-comparisons of the results from Monte Carlo calculations with those of the deterministic WIMS methods. This approach is possible due to the extensive development work performed on the nuclear data library generation routes to give consistency between Monte Carlo format libraries and the 172 broad group library format of WIMS. A careful choice of a series of cases, increasing in complexity, allows the examination of individual approximations in the WIMS theory to isolate those contributing the most significant inaccuracies. The inter-comparisons are not restricted to integral values such as the system k-effective alone but also include nuclide reaction rates in individual neutron energy groups. Through these types of studies a physical insight is gained into the nature of individual deterministic method approximations and improved, more accurate methods can be developed.

This paper presents an outline of the results from these investigations and identifies areas that have benefited from an improvement in the methods applied to broad group cross-section generation methods for WIMS9. It should also be noted, however, that other significant advances, not discussed in this paper, will also be included with the issue of WIMS9. Finally, an overview of the status of WIMS validation is given. No direct validation is included for the MONK8 Monte Carlo code as extensive validation has been reported elsewhere[3].

2. WIMS HISTORY

The origins of WIMS can be traced back well over 35 years; as long ago as 1964, a first version of the WIMS code was being developed by Winfrith's reactor physicists[4]. Because of its sound theoretical basis, and its free availability, the reference version of that early code, WIMSD, is still probably the most widely used lattice physics code in the world. However, in 1969, limitations in WIMSD, specifically for the double heterogeneity of HTR fuels, led to the development of the WIMSE modular scheme[5], which has been developed into the present sequence of codes that started with WIMS6[6] in 1992 followed by WIMS7[7] in 1996 and WIMS8[1], the current production version, in 1998, WIMS9 will be issued later this year. In the early 1970's, a parallel development known as LWRWIMS[8] was introduced for square assembly LWR geometries; this too was based on the modular concept of WIMSE. The features of LWRWIMS were unified and incorporated into the general WIMS code sequence from the issue of WIMS7 onwards. Lately this approach has also been extended to treat VVER type geometries. In addition, a development of a companion ANSWERS code, the point energy Monte Carlo Code MONK8[2], has also been integrated into WIMS to run with the broad group cross-section data generated using WIMS. This code also had its initial origins over 35 years ago since when it has been under continuous development. Finally, recent work has been carried out to update the features in WIMS that deal with HTR type fuel and in particular with the PBMR variant of the reactor design.

3. CHOICE OF DEVELOPMENT VALIDATION CASES

For the treatment of the resonance region, the methodology employed in WIMS is to derive effective broad energy group cross-sections using a set of broad group library resonance integrals, calculated from a detailed solution of the slowing down equations by the NJOY code. Resonance integrals are

calculated for individual resonance nuclides in a homogeneous mix with a hydrogen like scattering nuclide. The library resonance integrals are tabulated as functions of temperature and the amount of hydrogen like scattering in the problem per atom of the resonant nuclide. The scattering is measured in terms of the 'sigmap' value, defined as :

$$\sigma_p = \frac{N_h \sigma^h_{pot} + N_i \lambda_i \sigma^i_{pot}}{N_i}$$

Here, σ_p = sigmap, N_h = hydrogen atomic number density, N_i = resonant nuclide atomic number density, σ^h_{pot} = hydrogen potential scattering cross-section, σ^i_{pot} = resonant nuclide potential scattering cross-section, λ_l = resonant nuclide Goldstein/Cohen intermediate resonance factor.

The theory in WIMS that employs these data needs to introduce corrections for the effects of :

- The presence of heavy scattering nuclides.
- Interactions between resonances of the different resonance nuclides.
- The heterogeneous nature of the geometry being considered.

From the definition of the library resonance integrals, WIMS will reproduce the NJOY solution in the simplest case of a homogeneous mixture of a single resonance nuclide with a hydrogen moderator, where the temperature and amount of hydrogen moderator (sigmap value) match library reference values. The first series of cases studied were therefore for homogeneous systems and included :

- Single resonance nuclides moderated by hydrogen.
  These cases test the reproduction of NJOY solutions and interpolation of sigmap values.
- Combinations of resonance nuclides moderated by hydrogen.
  These cases form the simplest test of the interaction model between nuclide resonances.
- Single resonance nuclides moderated by carbon moderator.
  These cases form the simplest test of the treatment of heavy moderators.
- Combinations of resonance nuclides moderated by carbon moderator.
  These cases test the combination of resonance interaction in the presence of heavy moderators.
- Combinations of resonant nuclides moderated by combinations of moderators.
  These cases represent the most complex form of homogeneous geometries.

Following the study of the homogeneous cases, studies were performed for heterogeneous geometries representing Magnox (natural uranium fuelled gas cooled reactor), AGR (advanced gas cooled reactor) and PWR (pressurised water reactor) reactor types. Where appropriate cases with different pin sizes, pin to pitch ratios (fuel to moderator ratios) and fuel enrichment were studied.

The inter comparison of Monte Carlo results and deterministic results was not restricted to just the integral k-effective values alone. Reaction rates were compared in 14 different broad group energy bands in the resonance region as well as in the fast and thermal energy regions. A particularly useful breakdown for identifying the origin of differences between the calculations was obtained from the use of a five factor formula decomposition of the k-effective. In this formulation the k-effective is represented as:

$$K_{eff} = \frac{P_{fast}}{A_{tot}} + \frac{(A_{res} + A_{therm})}{A_{tot}} \left[\frac{P_{res}}{(A_{res} + A_{therm})} + \frac{A_{therm}}{(A_{res} + A_{therm})} \left\{ \frac{P_{therm}}{A_{therm}} \right\} \right]$$

Here: P_{fast} = productions in the fast energy range, P_{res} = productions in the resonance energy range, P_{therm} = productions in the thermal energy range, A_{tot} = total absorptions, A_{res} = absorptions in the resonance energy range and A_{res} = absorptions in the thermal energy range.

The above formula can then be cast into the form given below where each term is given by inspection between the two formulae:

$$K_{eff} = \nu_{fast} + \eta_{fast}[\nu_{res} + \eta_{res}\nu_{therm}]$$

These five factors are : ν_{fast} = productions per fast neutron, η_{fast} = fast escape probability, ν_{res} = productions per resonance neutron, η_{res} = resonance escape probability, ν_{therm} = productions per thermal neutron.

In particular, differences in k-effective can be resolved into contributions from production and absorption in each of the three energy ranges and the different test cases could be classified by their resonance escape probability.

It should also be noted that the possibility of detailed comparisons between the MONK and WIMS codes results from a significant investment and development of the nuclear data generation methods to give processing consistency between the different nuclear data libraries. The MONK Monte Carlo code uses a point energy group scheme nuclear data library, in practice 13,193 fine groups together with a four group sub-group pre-shielding treatment. The reference WIMS nuclear data library uses 172 broad groups the structure of which resulted from collaborative studies with CEA France in the early 1990s.

4. SELECTED CASE STUDY RESULTS

In this section some selected results from individual case studies are given to illustrate areas where method improvements have been incorporated in WIMS9. Presentation of the results from all studies would be too lengthy and detailed. A summary of typical results is given in Section 5 for reactivity values.

For the homogeneous mixtures of U238 with a hydrogen moderator, it is important that the resonance escape probability is well predicted as this is fundamental to k-effective predictions. This comparison is shown in Figure 1 where a good agreement between WIMS and MONK is seen.

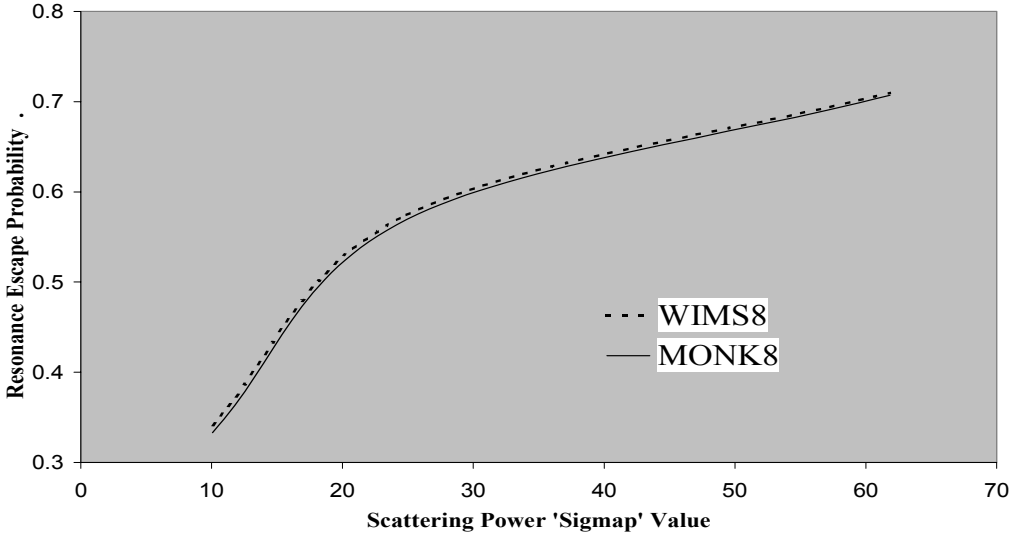

Figure 1. Resonance Escape Probability Comparisons Between WIMS and MONK for U238/Hydrogen Mixtures

However, although there is a good agreement for the resonance escape probabilities the K-effective values predicted by MONK were significantly higher than those predicted by WIMS8. This is due to the use of a single fission spectrum in WIMS8 for all nuclides and incident neutron energies; the U235

fission spectrum at 1MeV is used. For WIMS9 nuclide dependent fission spectra are introduced although no incident neutron energy dependence is currently planned. The results for cases 0 to 2 in Section 5 illustrate the improved agreement for k-effective values using a U238 rather than U235 fission spectrum.

Cases 7 to 10 of Section 5 represent homogeneous mixtures of U238, U235 and Hydrogen forming a rectangle in scattering space encompassing most reactor types. Several additional modifications were introduced to the WIMS8 theory to improve agreement between MONK and WIMS for these cases:

- Extension of the energy range treated as the resonance region by WIMS into the unresolved energy region with an upper energy of 183 KeV.
- Modelling of the interactions between resonances at lower resonance energies.
- Derivation of the correction factor for the broad group out-scatter cross-sections due to the presence of resonances.
- Introduction of resonance scattering theory in addition to the resonance absorption theory for both equivalence theory and sub-group theory calculations.

As an illustration of these modelling changes, the interactions between resonances is considered below. When modelling the interactions between different resonance nuclides, WIMS8 treats each resonance nuclide in turn and assumes the absorption due to all other resonance nuclides is equally distributed in the resonances of the nuclide being treated. This, effectively, assumes a random or statistical overlap of the resonances. At high resonance region energies this approximation is sound as there are many small narrow resonances present. At low energies in the resonance region this is a relatively poor approximation, the resonances here are broad and well separated. Interaction effects do not have a large effect on the U238 broad group cross-sections, however, the presence of U238 has a significant effect on the cross-sections of other resonance nuclides. This situation is illustrated in Figure 2 where a simple mixture of U235, U238 and Hydrogen is considered for the broad group containing the U238 6.7 eV resonance. Figure 2 shows the infinite dilution U235 absorption cross-section and part of the U238 infinite dilution absorption cross-section which peaks at about 7,086 barns. Fine group flux solutions are also shown for two different cases, with and without the presence of U238. Broad group average cross-sections are summarised in Table 1.

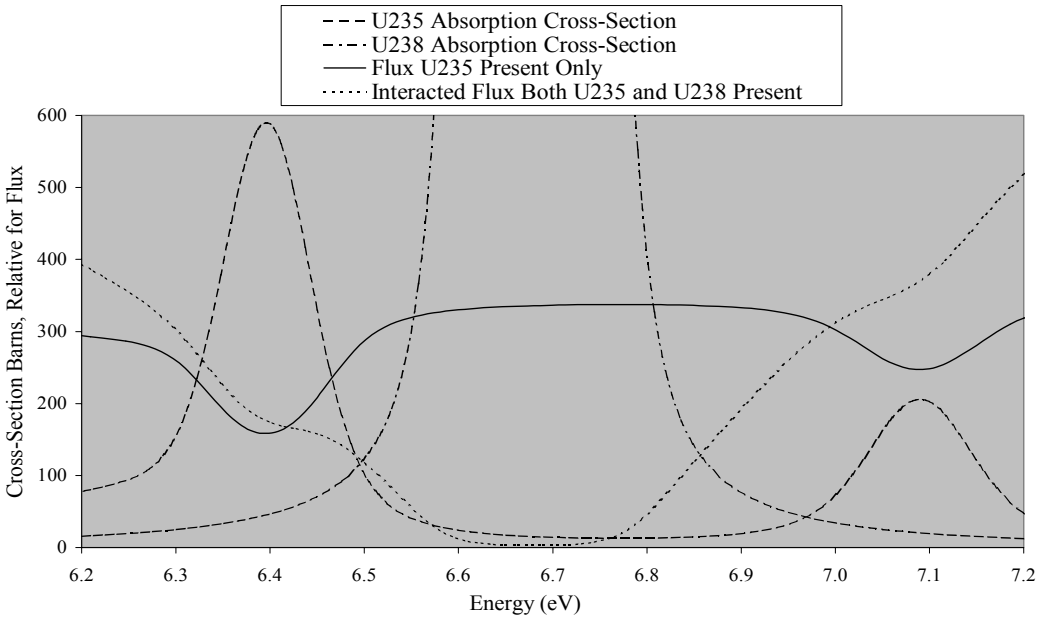

Figure 2. U238 and U235 infinite dilution cross-sections and un-interacted and interacted flux solutions in the broad group containing the U238 6.7 eV resonance.

The presence of the U238 does not introduce a situation which can be represented as a random overlap of resonances. In WIMS9, a cell calculation is performed to evaluate the resonance interaction effect rather than assuming random overlap. The results in Table 1 show that errors of 5% to 7% are present in the U235 absorption cross-section using the WIMS8 model and that these are significantly reduced using the WIMS9 model.

Table 1. Broad group average U235 absorption cross-sections in interaction with the 6.7 eV U238 absorption cross-section, calculated by MONK, WIMS8 and WIMS9.

Interaction effect due to U238 on the U235 absorption cross-section, Sigmap U238=62 barns						
Sigmap	MONK		WIMS8		WIMS9	
U235 barns	U235 only	U235+U238	U235+U238	Error %	U235+U238	Error %
500	77.0	89.1	84.3	-5.4	90.3	+1.3
1900	90.9	99.5	92.4	-7.1	99.4	-0.1

In the case of heterogeneous geometries treatment of the transport cross-section needs consideration. In WIMS8, flux rather than current weighting of both the transport and P1 scatter cross-section is employed. In WIMS9 current weighting is used for both of these cross-sections. In groups containing large resonances this can have a significant effect on the magnitude of the transport cross-section as illustrated in Figure 3.

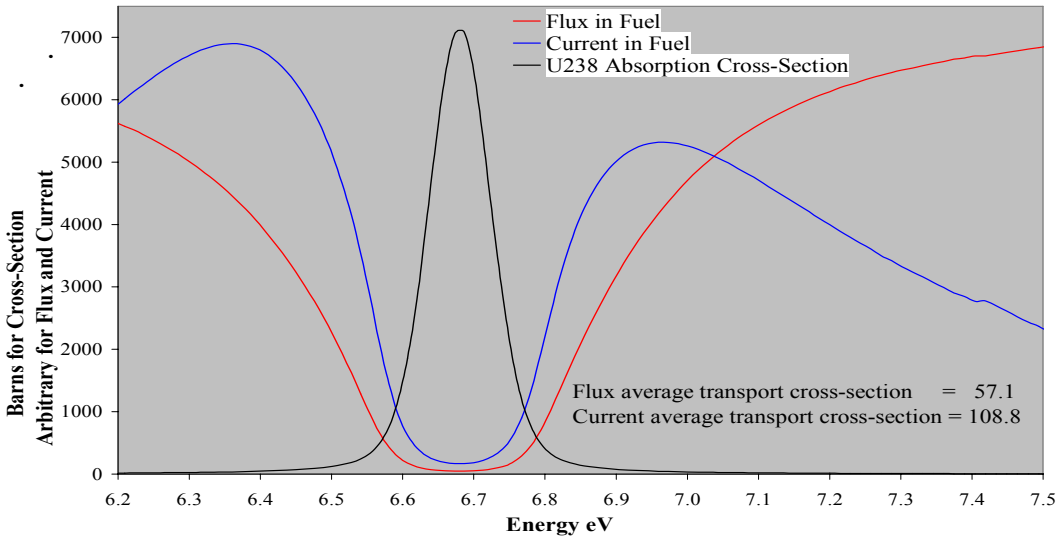

Figure 3. Flux and Current solutions in the broad group containing the U238 6.7 eV absorption resonance.

The case considered in Figure 3 is a PWR pin cell with a 2:1 moderator to fuel ratio. Although neutron currents are relatively small between the moderator and the fuel, most of the neutron transfer takes place in the wings of the resonance leading to a much larger contribution from the absorption cross-section to the transport cross-section when using current rather than flux weighting.

5. SUMMARY OF CASE STUDY RESULTS

Figure 4 gives a summary of k-effective differences between MONK8 and WIMS for a series of test cases illustrating a range of problem and reactor types. A key to the different cases is given in Table 2. The homogeneous cases cover a wide range of examples with single and combinations of resonance nuclides, U238, U235 and Pu239 moderated by hydrogen, carbon or a mixture of moderators. The results for WIMS9 show a mean closer to unity than those of WIMS8 and a reduced variance.

Results for AGRs, Magnox reactors and PWRs also show improvement. The trend with pin pitch for the Magnox reactors seen with WIMS8 (first 3 Magnox points in Figure 4) is eliminated in WIMS9. Although there remains about a –200 pcm offset in k-effective for PWR cases using WIMS9, this can easily be accounted for using a bias factor. It is also of note that there is little variance between the different PWR cases, the bias is independent of enrichment and moderator to fuel ratio.

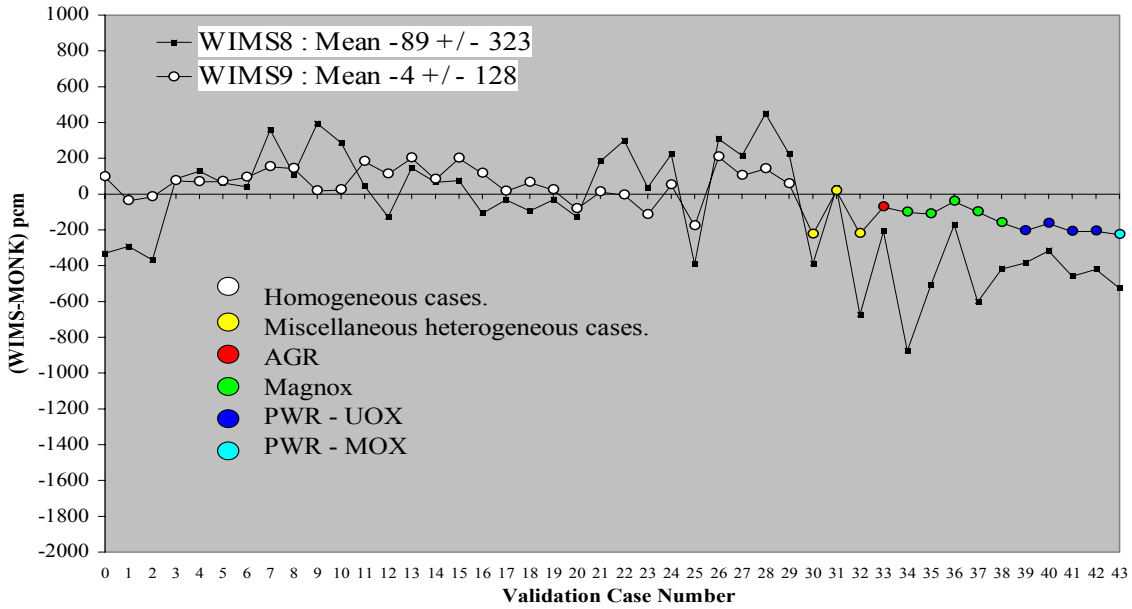

Figure 4. Summary Results for K-effective Differences between MONK and WIMS Illustrating Typical Homogeneous and Heterogeneous Cases.

The philosophy of WIMS has always been to use a single model for resonance self shielding for all reactor types and to use a generally applicable nuclear data library rather than one specifically generated for a given reactor type. The above results show that the application of this philosophy in WIMS9 can yield sufficient accuracy for the next generation of reactors.

Table 2. Key to the cases in Figure 4

Case	Description
0 to 6	Homogeneous : cases 0 to 2 U238/Hydrogen Mixtures, cases 3 and 4 U235/Hydrogen Mixtures, cases 5 and 6 Pu239/Hydrogen Mixtures
7 to 10	Homogeneous U238/U235/Hydrogen Mixtures
11 and 12	Homogeneous U238/Pu239/Hydrogen Mixtures
13 to 16	Homogeneous U238/U235/Pu239/Hydrogen Mixtures
17 and 18	Homogeneous U238/Carbon Mixtures
19 and 20	Homogeneous U235/Carbon Mixtures
21 to 25	Homogeneous U238/U235/Carbon Mixtures
26 to 29	Homogeneous U238/U235/Hydrogen/Carbon Mixtures
30 to 32	Heterogeneous 0.4 cm fuel pin, 3:1 hydrogen moderator:fuel ratio, case 30 with U238 fuel, case 31 with U235 fuel, case 32 U235 and U238 fuel 5% enrichment.
33	AGR 0.7 cm pin diameter, CO_2 cooled.
34 to 38	Magnox cases, natural uranium assembly pitches 6.35 cm to 10.0 cm, 1.16% U235 enriched fuel and depleted uranium fuel.
39 to 43	PWR UOX fuel enrichments 3% to 5%, moderator:fuel ratios 1:1 and 2:1,case 43 MOX fuel at 3.4% Pu enrichment.

6. STATUS OF WIMS VALIDATION

The earlier versions of WIMS have been extensively validated against both a range of experimental benchmarks and a series of different thermal power reactors. In Table 3 a list of some of the experiments used to validate WIMS is given.

Table 3. List of Experimental Validation Experiments used for WIMS.

Experiment/Reactor	Fuel Type	Moderator	Comments
DIMPLE	UO_2	Light Water	Standard Lattice Experiment
TRX	UO_2	Light Water	Standard Lattice Experiment
BROOKHAVEN	UO_2	Light water	Standard Lattice experiments with soluble Boron
KRITZ	UO_2 and MOX	Light water	Temperature Coefficient Measurement
ZR-6	UO_2	Light water	VVER Lattices
ORNL	Uranium Solutions	Light Water	Simple Critical Measurements
ESADA	MOX	Light Water	Variable MOX compositions
DUNGENESS B	UO_2	Graphite	AGR Geometry – Power reactor Commissioning experiments
BICEP	Uranium Metal	Graphite	Wide range of Lattices
Babcock and Wilcox	UO_2 with Gd poison	Light water	Simulation of LWR assemblies with poisoned fuel

The results of this validation are summarised in Table 4 below.

Table 4. Results of Validation of WIMS.

Parameter	Reactor Type	Results	Comments
Reactivity	UO_2 in light water	0.9967 ± 0.002	
	Solutions	0.9952 ± 0.002	
	MOX	0.9992 ± 0.006	Pu 2% enrichment
	Graphite moderated	0.9985 ± 0.007	
Reactivity with pitch	UO_2 in light water	No significant trend in KRITZ/TRX Small trend in DIMPLE/Brookhaven	
	MOX	Small trend with pitch	Based on ESADA results
	Graphite	Significant trend with pitch for BICEP	
Boron	UO_2 in light water	No significant trend	
	MOX	No significant trend	
Gd Poison	UO_2 in light water	Assembly powers to ~1%	
Temperature	UO_2 in light water	0.35 ± 0.4 pcm/^{o}C	Error in temperature coefficient from analysis of KRITZ
	MOX	-1.3 ± 0.4pcm/^{o}C	

The validation of the WIMS/PANTHER route for analysing power reactors was presented in Reference [9]. The reactors analysed in that work are given in Table 5 and the results are summarised in Tables 6 and 7.

Table 5. Reactors Analysed in Tables 6 and 7.

Reactor	Power MWth	No of Cycles Analysed	No. of Assemblies	Assembly type	Core Height (feet)
Callaway	3411	3	193	17x17	12’
Wolf Creek	3411	1	193	17x17	12’
Sizewell B	3411	3	193	17x17	12’
Tihange1	2652 (1)	20	157	15x15	12’
Tihange2	2775	11	157	17x17	12’
Tihange3	2988	12	157	17x17	14’
Doel1	1192	15	121	14x14	8’
Doel2	1192	14	121	14x14	8’
Doel3	2775(2)	13	157	17x17	12’
Doel4	2988	14	157	17x17	14’

(1) comparison covers cycles uprated to 2867 MWth
(2) comparison covers cycles uprated to 3054 MWth

Table 6. PANTHER Comparison with Measurement
Hot Zero Power Parameters at the Beginning of Cycle.

Parameter	Units	Predicted – Measured		Sample size
		Mean	1 sigma	
Critical boron conc. all rodded config's	[ppm]	8	21	38
Rod bank worths	Δ_r[%]	4.2	5.8	96
Moderator temperature coefficient	[pcm/°C]	-2.2	0.9	29
Boron worth	[pcm/ppm]	0	0.35	15

where Δ_r denotes a (PANTHER/Measured -1) difference.

Table 7. PANTHER Comparison with Measurement
Hot Full Power Parameters

Parameter	Units	Predicted – Measured		Sample
		Mean	1s	size
Critical boron conc.	[ppm]	-2	22	193
Axially averaged reaction rates unfiltered population	Δ_r [%]	0.0	1.3	13398
Axial form factor Fz (det)	Δ_r [%]	-0.9	1.5	13398
Axial offset (det)	Δ_r [%]	0.0	1.3	231

where Δ_r denotes a (PANTHER/Measured -1) difference.
Det denotes relative to detectors.

In addition to the analysis of the PWR reactors there has also been analysis carried out for VVER, AGR and Magnox reactors. The results of these analyses are consistent with the values quoted for the reactivity benchmarks for these systems given in Table 2.

7. CONCLUSION

During the course of the investigations outlined, improvements have been introduced to WIMS9 in the methods applied in several different areas :

- Extension of the energy range treated as the resonance region by WIMS into the unresolved energy region with an upper energy of 183 KeV.
- Modification of the single nuclide independent fission spectrum used in WIMS8 to include nuclide dependence.
- Modelling of the interactions between resonances at lower resonance energies.
- Derivation of the correction factor for the broad group out-scatter cross-sections due to the presence of resonances.
- Introduction of resonance scattering theory in addition to the resonance absorption theory currently used in WIMS8.
- Current rather than flux energy weighting for the condensation of the transport and P1 moment of the scatter cross-section.

WIMS9 is now a code package which is designed to meet the requirements of workers on all types of thermal reactors, for benchmarking, for analysis of unusual experimental configurations, for standard reactor operational fuel management, and for criticality survey work. This flexibility has been achieved by building on the original WIMSE modular concept, and also providing graphical aids for both standard and special specific applications. This flexibility has now been enhanced by the improved accuracy and reliability of the code which results from, amongst others, the improvements outlined in this paper.

8. REFERENCES

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