NEW CAPABILITIES OF THE WIMS CODE

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ABSTRACT

The WIMS code has recently been extended to include new capabilities in the library and the flux solution modules. These extensions increase the range of the code both in the type of problem which can be solved and the detail of the solution. The library has been extended so that the resonance self shielding calculation is more accurate over a wider range of fuel to moderator ratios. This has been achieved by extending the resonance integral tabulations on the library and improving the interpolation procedure. In addition to this change, the code has had a significant improvement in its capability for modelling 3D problems and two new features are described: the CACTUS method has been extended to 3D and the hybrid perturbation Monte Carlo method MAX has been extended. These changes to the code are outlined and the basic approach presented. Results are presented to show the accuracy of these methods. The two methods are inter-compared and also compared with both a standard Monte Carlo code MONK and measurement. The problems chosen cover both LWR and gas cooled reactors. In the one case of a partially inserted rod in a PWR assembly, CACTUS is compared with MONK for the calculation of the variation of power at a rod tip. In the second case MAX is compared with CACTUS and measurement for the estimation of power peaking in a gas cooled fuel assembly. The results show that both methods give accurate results within a reasonable time on current computer hardware.

1. INTRODUCTION

WIMS has been established as a standard reactor physics code for a wide range of reactor types for the last 30 years. The latest version of the code, WIMS8[(1)], has established routes for calculations on LWR, heavy water moderated reactors and gas cooled reactors. The latest routes for all these types of reactor use the CACTUS transport solution, which is based on a characteristics method, as the main engine for the calculation.
Currently, typical calculations with WIMS are carried out using the standard 69 group WIMS library in 2D for a single lattice cell. This is the case for all reactor types. There are however a number of effects that require more complicated modelling. In this paper a review of a series of enhancements to the WIMS modelling capability is presented. These show the use of WIMS

with an extended library and the use of 3D methods. The paper includes validation evidence for these extensions to the WIMS capabilities.

2. LIBRARY EXTENSIONS

WIMS has traditionally employed a 69 energy group structure for its data library and recently a move towards the adoption of the JEF based data libraries has been taking place. As part of this exercise, a finer group library (172 groups) has been produced in order to better represent some of the resonance structure particularly for the Plutonium isotopes. In addition the resonance tabulations and other data have been improved. This new data library has the potential to improve the accuracy and extend the range of applicability of WIMS calculations.

2.1. RESONANCE TABULATIONS

The WIMS library contains a tabulation of resonance integral as a function of potential scatter which is used in the evaluation of self shielding. The code stores a set of tabulations of the resonance integral for a homogeneous mixture of the resonance nuclide and hydrogen. The tabulation covers the whole range of possibilities from highly shielded cases with little moderation to the infinitely dilute case with only a trace of resonance nuclide. WIMS tabulates the integral at up to 10 points and uses a piecewise interpolation procedure to evaluate the integral at a given value of the potential scatter. The variation of the resonance integral with potential scatter cross section is complex and the functionality of the integral varies with the value of the potential scatter. This whole procedure has recently been enhanced so that the accuracy of the WIMS method has been improved over the whole range. This has been achieved by increasing the number of tabulations to 30 and improving the interpolation procedure. The following table gives an outline of the new interpolation scheme

Interpolation Formulae	Value of R (ratio of actual resonance integral to infinitely dilute value)
$1/\sigma$	$R>0.95$
$1/\sqrt{s}$	$0.95>R>0.8$
$\mathrm{Log}(\sigma)$	$0.8>R.0.5$
$\sqrt{s}$	$0.5>R$

Comparisons with NJOY[2] calculations of resonance integral at very fine increments in potential scatter has shown this to give accuracies of <0.5% in resonance integral.

3. 3D METHODS

The standard flux solution methods in WIMS are based on 2D flux solutions. This is normally adequate for data generation for the thermal reactors to which WIMS is applied. However there are modelling situations where a full 3D solution would be of benefit. An example of this is in UK gas reactors where there are significant 3D effects associated with axial gaps in the fuel element, which cause significant perturbations to the flux and hence power. These power perturbations are important because they determine the peak pin rating in the fuel assembly. To date these effects have been evaluated by an approximate synthesis method. However recent developments in WIMS have led to the introduction of accurate 3D transport theory methods to model this situation.
Other reactors also exhibit 3D effects that are currently represented by synthesis methods. These include the effects of grids, partial insertion of control rods and axial reflector modelling. Again the recent WIMS developments can model these situations explicitly.

Four methods are currently available in WIMS to model 3D problems. These are:

- 3D diffusion theory (SNAP)
- Monte Carlo (MONK)
- an extension of the characteristics solution (CACTUS in 3D)
- a hybrid Monte Carlo method (MAX)

This section outlines the approaches used for the latter 2 methods in the above list. Results from the application of the 3D version of CACTUS and the hybrid Monte Carlo code MAX to the estimate of axial peaking in gas cooled reactor fuel and the effect of partial rod insertion in PWR fuel are outlined in the paper. Estimates of the accuracy and efficiency of these methods by either comparison with the standard Monte Carlo methods used in the MONK code or by comparison with experiment, are provided.

3.1. CACTUS 3D CALCULATIONS

The CACTUS option in WIMS is outlined in reference (3). The CACTUS method is a flux solution method using the characteristics formulation of the Boltzmann transport equation. With this method the transport equation is solved along the characteristics of the equation which are straight lines in 3D space. The method solves the following equation

$$\frac{dN}{dS} + \Sigma N = \frac{Q}{4p}$$

where N is the angular flux along a characteristic
S is the distance measured along the characteristic
Σ is the total macroscopic cross section

The original CACTUS solution was restricted to a 2D geometry, where the intersections of the characteristics are with surfaces parallel to the axial direction. This geometry can describe any 2D problem using planes and curved surfaces joining a set of user defined points. The tracking in CACTUS has now been extended so that zones in the 2D map can be further subdivided using planes perpendicular to the z-axis. Thus CACTUS geometry modelling has now been extended to a sub set of the full 3D situation. This geometry can now be used to model partially inserted

rods in a LWR and some gas cooled reactor geometries and thus significantly extends the modelling capability of WIMS.

3.2. MAX 3D CALCULATIONS

The WIMS code also has an option that allows users to use a hybrid Monte Carlo method to solve 3D problems. This method is based on perturbation theory where the unperturbed solution is obtained from a deterministic method and the perturbation in the flux is obtained using a Monte Carlo approach. This gives the final perturbed flux solution as a hybrid of the deterministic and Monte Carlo fluxes. The basic equations are

$$\Delta\Phi = \frac{1}{(T - S - lF)}\{(\Delta S + l_0\Delta F - \Delta T)\Phi_0 + \Delta l F\Phi_o\}$$

$$\Delta l = \frac{\int \Phi_0^* [\Delta S + l_0\Delta F - \Delta T](\Phi_0 + \Delta\Phi)}{\int \Phi_0^* F(\Phi_0 + \Delta\Phi)}$$

Where $T = T_0 + \Delta T$ is the transport operator

$S = S_0 + \Delta S$ is the scatter operator

$F = F_0 + \Delta F$ is the fission operator

$l = l_o + \Delta l$ is the eigenvalue

$\Phi = \Phi_0 + \Delta\Phi$ is the flux

Δ indicates a perturbed quantity

The unperturbed flux is obtained from a deterministic solution in WIMS. For this initial application of the method, the initial flux was taken to be the homogeneous flux solution for the problem, which is then used to determine the source for the Monte Carlo solution in MAX. The source generates both positive and negative weight particles which are tracked in the normal way but throughout the tracks these particles can annihilate each other to bring a pair of positive and negative tracks to an end.

This option has also been used recently to analyse 3D problems. In particular the method has been applied to gas reactor problems with axial gaps in the fuel. Using this method the tracks are concentrated at the perturbation and hence make the tracking process more efficient. Thus this approach is viable for dealing with 3D problems where the 3D geometry is a relatively small perturbation on the 2D geometry. This is the case for most LWR and gas cooled reactors.

4. COMPARISON OF MAX AND CACTUS

Two comparisons of CACTUS with Monte Carlo methods are presented in this paper. In the first case a partially inserted rod in a PWR assembly is modelled by CACTUS and these results are compared with values from the Monte Carlo code MONK. Secondly an idealised case, typical of a gas cooled assembly (AGR) with representations of both the axial gap in the fuel and the grids, is modelled. The geometry of this type of element is shown in Figure (1).

4.1. COMPARISON FOR RODDED PWR

In this case a CACTUS calculation was compared with the Monte Carlo method MONK, which is available as an option in WIMS. The case considered consisted of a standard 17x17 PWR cluster with axial length of 50cm. Into this assembly a control rod was inserted to the mid point so that the rod was inserted to 25cm. Reflective boundary conditions were used for all surfaces of the problem. For the purposes of this comparison, identical data were used in both the Monte Carlo and the CACTUS calculation. This was 6 group data condensed in WIMS using standard procedures available in the code. Thus 6 group data was produced using a 2D model representing the unrodded and the rodded region of the problem. These data were then used in either a CACTUS calculation or a MONK calculation. The results of the comparison are shown in Tables 1 and 2. The reactivity and the power variation for the average pin is compared. The CACTUS model could give the power variation on a pin by pin basis but to improve the statistics for the Monte Carlo results the total power for a given axial height was estimated and a comparison between the codes is based on that estimate.

Figure 1 Outline of Axial Dimension of AGR fuel Element

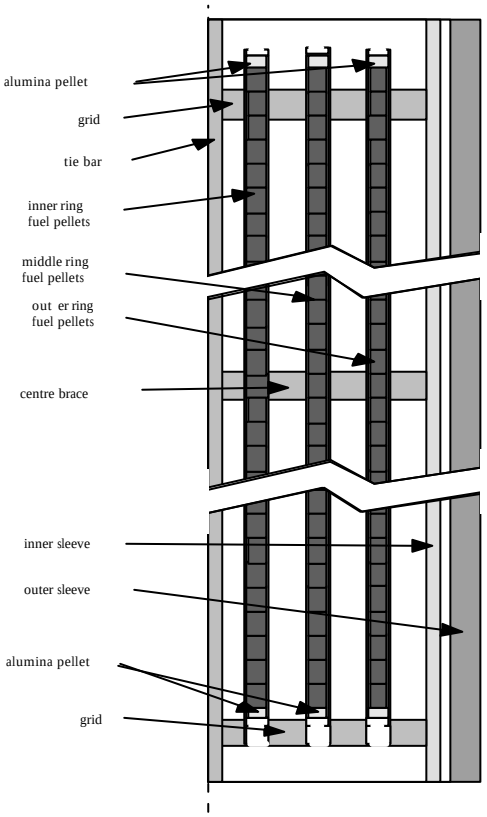


Table 1 Comparison of Reactivity from CACTUS and MONK

CACTUS	MONK	Difference pcm
1.15415	1.15911±0.001	370±100

It can be seen from Table 1 that there is good agreement between MONK and CACTUS on reactivity. The CACTUS result does depend on the axial and radial mesh structure, and refining the mesh structure does increase reactivity. It is estimated that some of the underestimate would be removed by a further refining of the CACTUS mesh. This was not pursued in this exercise because the main aim was to compare power and that was not as sensitive to mesh size.

Table 2 Comparison of average pin power from MONK and CACTUS

Axial Height	CACTUS	MONK	Difference %
5.0	0.245	0.242	1.2
15.0	0.365	0.363	0.6
21.0	0.529	0.535	-1.1
23.0	0.657	0.671	-2.1
24.5	0.795	0.794	0.1
25.5	0.930	0.908	2.4
27.0	1.103	1.086	1.6
29.0	1.298	1.262	2.8
35.0	1.604	1.582	1.4
45.0	1.896	1.890	0.3

It can be seen from table 2 that there is good agreement between MONK and CACTUS and the mean discrepancy is 0.72±0.5% . The uncertainty associated with the Monte Carlo result is ~ ±1% hence the agreement is within the uncertainties associated with the Monte Carlo. This indicates that for this problem CACTUS is giving the axial variation in pin powers at the rod tip to ~1% accuracy.

4.2. COMPARISON FOR AGR

In this case calculations were carried out using both the MAX code and CACTUS. The geometry was similar to that shown in Figure 1 but idealised for this comparison. Thus the problem was chosen to be axially symmetric. The case has reflective boundaries at the mid point of the fuel (height 51.5cm) and the mid point in the gap between fuel elements (height 0.0cm). The repeat length of the fuel is 95 cm and there is a 6 cm gas gap between fuel elements. The grids are 3cm in height and are positioned at the fuel mid point and at the end of the fuel.

The results of the MAX and CACTUS calculations are shown in Tables 3, 4, 5 and 6. Tables 4,5 and 6 give the results for the 3 rings in the AGR cluster.

Table 3 Comparison of reactivities of MAX and CACTUS for AGR problem

MAX	CACTUS	Discrepancy (pcm)
1.36457±0.00068	1.363721	-46

Table 3 shows that there is excellent agreement between the MAX and the CACTUS method for the AGR problem. The discrepancy between the methods is less than the uncertainty on the Monte Carlo result.

Table 4 Comparison of axial power profile for Inner ring pin

Axial Height cm	CACTUS	MAX	Discrepancy between MAX and CACTUS %	Uncertainty in MAX %
4.5	1.18	1.177	-0.24	1.68
6.0	1.087	1.093	0.59	0.68
11.0	1.035	1.034	-0.06	0.20
22.5	1.005	1.004	-0.14	0.18
35.0	0.989	0.990	0.08	0.15
45.0	0.957	0.959	0.16	0.31
50.75	0.878	0.878	0.02	0.35

Table 5 Comparison of axial power profile for Middle ring pin

Axial Height	CACTUS	MAX	Discrepancy between MAX and CACTUS %	Uncertainty in MAX %
4.5	1.152	1.141	-0.90	0.98
6.0	1.087	1.076	-0.97	0.67
11.0	1.035	1.032	-0.25	0.10
22.5	1.005	1.003	-0.20	0.20
35.0	0.9924	0.992	-0.07	0.13
45.0	0.964	0.965	0.14	0.16
50.75	0.873	0.888	1.68	0.59

Table 6 Comparison of axial power profile for Outer ring pin

Axial Height	CACTUS	MAX	Discrepancy between MAX and CACTUS %	Uncertainty in MAX %
4.5	1.116	1.105	-0.96	0.53
6.0	1.063	1.061	-0.15	0.34
11.0	1.029	1.028	-0.10	0.14
22.5	1.000	1.000	0.02	0.12
35.0	0.989	0.990	0.11	0.08
45.0	0.974	0.976	0.17	0.09
50.75	0.928	0.925	-0.30	0.60

The results shown in Tables 4, 5 and 6 show excellent agreement between CACTUS and MAX for this idealised fuel element. The stochastic errors for the MAX calculation are given in Tables 4,5 and 6 and do vary with ring and axial position. The maximum uncertainty is for the peak power in the inner ring where the uncertainty is ~1.6% this maximum reduces to about 0.5% for the outer ring. With the exception of those peak values the uncertainties are <0.5%. and the CACTUS results agree with MAX within these uncertainties. Thus CACTUS and MAX are generally consistent to an uncertainty of ~0.5% except at peak power at the end of the fuel where a value of ~1% is found. This is within the required accuracy for this type of calculation and certainly less than measurement errors for PIE as shown in the next section.

4.3. COMPARISON WITH MEASUREMENT

A series of PIE measurements have been carried out to examine the axial variation in power in an AGR element. The elements measured ranged in enrichment from 1.162w/o to 2.5 w/o and the irradiation at which measurements were taken varied from 0 to ~20GWd/Te. These results have been compared with values produced by WIMS using the MAX method. The comparison is illustrated in Figure 2. Table 7 shows the mean differences between experiment and MAX for a range of enrichments and irradiations. In general the agreement with MAX is very good and shows that MAX reproduces the variation with both enrichment and irradiation.

Table 7 – Mean (C-E)/E % for AGR Stage 1 Fuel

Position	Irradiation (GWd/te):				
	0	5	10	15	20
Top	0.87	0.65	2.04	1.50	1.01
Sdev	1.38	0.89	1.56	0.80	0.81
2nd	1.21	0.55	0.28	-0.07	-0.09
Sdev	1.17	0.65	1.17	0.71	0.92
Mean	0.94				
Sdev	0.68				

5. COST OF EXECUTION

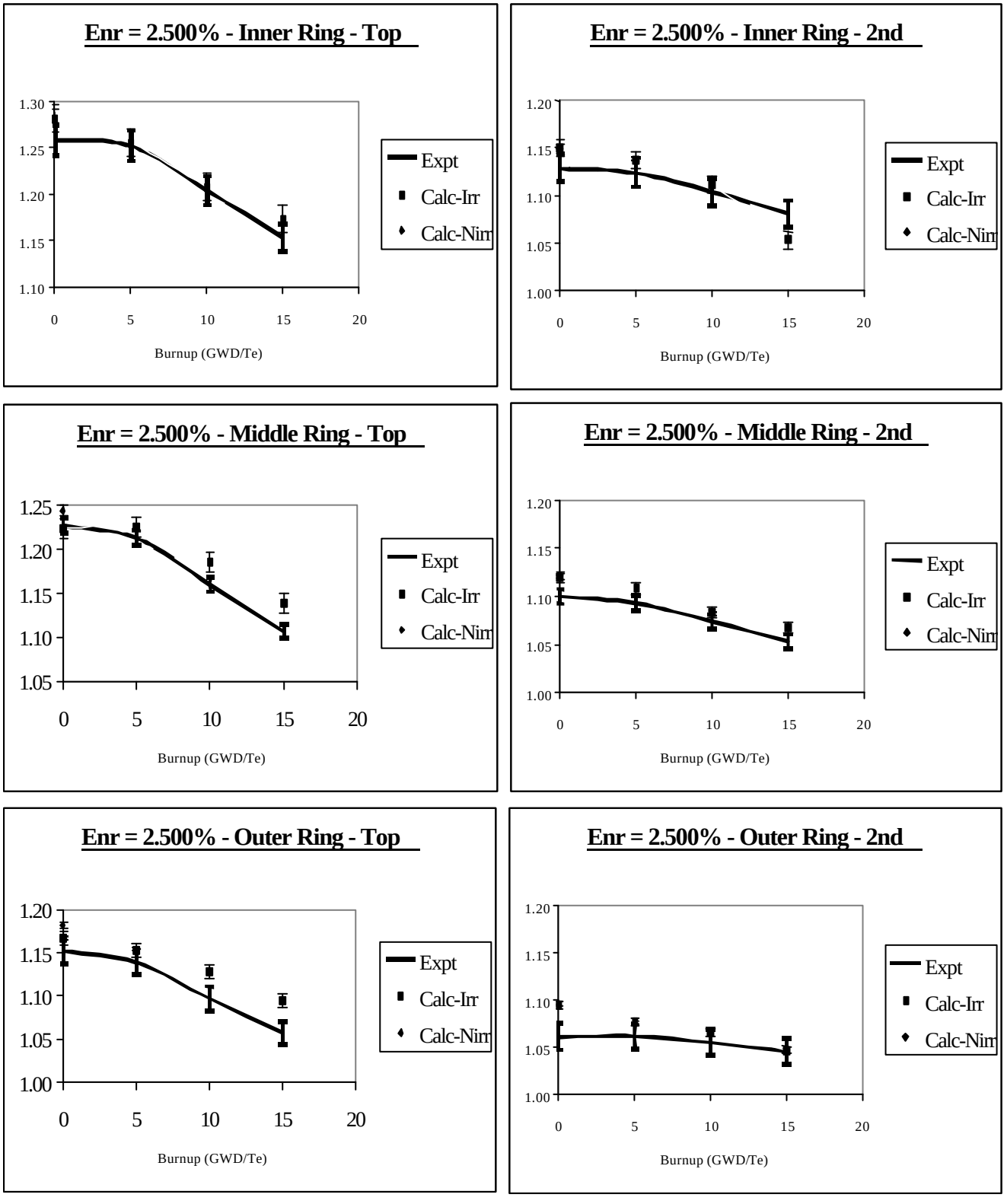
These calculations were carried out on an Ultrasparc5 Sun computer and gave the following run times to obtain results for the quoted accuracies

CACTUS cpu time (mins)	MAX cpu time (mins)
10 (PWR) 20(AGR)	60

6. SUMMARY

A range of new features has been added to the WIMS code to extend the range of the code and improve the overall accuracy. These features will allow the user to more accurately model complex features in a reactor and to improve the confidence in the results of such analysis. In particular the library has been improved so that the resonance shielding calculation is accurate over the whole range of the tabulation. This will lead to more accurate estimates when the code is used in a criticality mode to survey non standard assemblies.
The code now has a number of modules that enable the user to carry out 3D calculations. This paper has shown that for two problems typical of both LWRs and Gas Cooled Reactors the two methods give adequately accurate solutions and thus enable these effects to be modelled accurately. The validation presented show that both MAX and CACTUS give results that are consistent and agree with both a standard Monte Carlo calculation and measurement. These modules are now in a version of WIMS and so can be used with the depletion facility in WIMS. This enables the interaction of depletion and 3D effects to be estimated accurately as shown by the comparison with the PIE measurements presented in section 4.3.

Figure 2 Results of Comparison of Axial Fine Structure between MAX and Experiment



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