THE USE OF WIMS FOR GAS-COOLED REACTOR CALCULATIONS

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ABSTRACT

The Advanced Gas Cooled Reactors(AGR) operated in the UK are a design that has features that test the capability of reactor codes. The WIMS code is a general neutronics package that has the capability to model this type of reactor. This paper outlines some recent developments to the hybrid Monte Carlo package called MAX within WIMS. These improvements were designed to improve the speed and accuracy of calculations that mainly involve perturbations due to temperature or irradiation. The method adopted is outlined in the paper, in particular the linkage to the deterministic code CACTUS and the treatment of sequences of perturbations are described. The paper also outlines the developments to the WIMSBUILDER package that significantly eases the generation of input for WIMS calculations involving a sequence of perturbations to temperature and then cycles through a set of depletion steps.

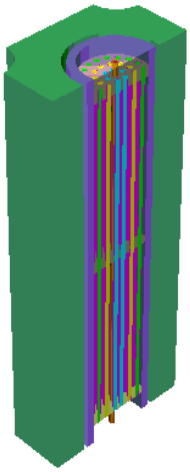
Finally the paper outlines a number of validation results that test the performance of this new package. Results are presented that show the package accurately predicts 3D effects, temperature coefficients, poison worth and irradiation effects. The resultant code is also shown to be ~ 2 orders of magnitude faster than both the older version of the code and conventional Monte Carlo calculations. Thus the paper concludes that this new method is capable of being used to accurately model complex situations and can be used in conjunction with the code PANTHER to apply these results to whole core situations.

1 INTRODUCTION

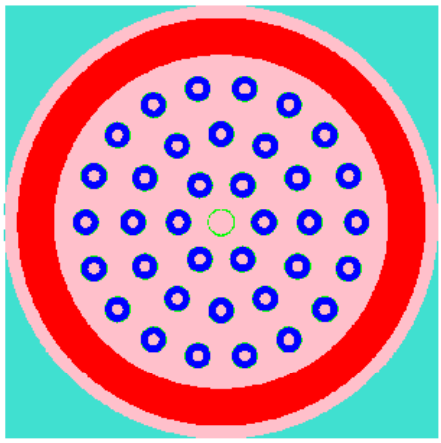
The Advanced Gas Cooled Reactors(AGR) that are currently operated in the UK have a cluster geometry with graphite moderation and carbon dioxide coolant. These reactors have a number of features that are difficult to model accurately in core physics studies, including:

1. Significant heterogeneous effects in both the radial and axial plane
2. Significant cross assembly tilts in power due to the proximity of either control rods or reflector.
3. Complex 3D effects, due to the presence of burnable poison, in the form of toroids of Gadolinium oxide encased in a steel sheath.

An outline of a typical AGR assembly is given in Fig 1.



Whole assembly



Slice through cluster

Fig 1 Geometry of AGR Cluster

The WIMS code is a general neutronics package that can accurately model a wide range of power reactors and other reactor assemblies. These include PWR, PBMR, AGR and natural uranium metal fuelled gas reactors (e.g. Magnox), as well as experimental reactors and MTR. Previous papers[1,2,3] have outlined the modelling capabilities of WIMS, that include:

1. Use of Subgroup theory for complex resonance shielding calculations
2. Use of the characteristics method (the CACTUS module of WIMS) to model both 2D and 3D features in AGR's
3. Use of a hybrid Monte Carlo method (the MAX module) based on perturbation theory to model poison and axial peaking effects.

There is currently a need to develop a fast but accurate method to treat the complex 3D features of the AGR fuel assembly identified above in order to generate accurate data for use in a whole core calculation using the PANTHER code [4]. This paper outlines the way in which the features of WIMS were both developed and adapted to meet this requirement.

2 METHOD OF CALCULATION

The developments were based on the MAX method, but also included extensions to the WIMS sub-group method and the development of links between the MAX module and CACTUS. The MAX method is based on perturbation theory where the unperturbed solution is a deterministic flux solution in a simplified geometry and the perturbation is calculated using a Monte Carlo based method. That is, the basic method is a hybrid of both deterministic and Monte Carlo techniques for solving the transport equation. The two techniques are combined using perturbation theory.

2.1 BASIC METHOD

Consider the Boltzmann Transport equation which can be written as:

$$\Omega.\nabla\phi(r,E,\Omega)+\Sigma_t(E).\phi(r,E,\Omega)=\int dE'd\Omega'\Sigma_s(r,E'\rightarrow E,\Omega'\rightarrow\Omega).\phi(r,E',\Omega')+\lambda)$$

$$+\lambda\chi(E)\int dE'd\Omega'\nu\Sigma_f(r,E')\phi(r,E',\Omega') \quad (1)$$

this equation can be rewritten using operator formalism as:

$$T\phi = S\phi + \lambda F\phi \quad (2)$$

Where T is the transport operator, S is the scattering operator, F is the fission(production) operator, λ is the eigenvalue and ϕ is the angular flux solution.

Now consider a situation with a solution of the transport equation for an unperturbed system being given by the equation:

$$T_0\phi_0 = S_0\phi_0 + \lambda_0 F_0\phi_0 \quad (3)$$

Then for the perturbed system where:

$$T = T_0 + \Delta T$$
$$S = S_0 + \Delta S$$
$$F = F_0 + \Delta F$$
$$\lambda = \lambda_0 + \Delta\lambda$$
$$\phi = \phi_0 + \Delta\phi$$

It can be shown that:

$$\Delta\phi = \frac{1}{T}\left[(S+\lambda_0 F)\Delta\phi + (\Delta S + \lambda_0\Delta F - \Delta T)\phi_0 + \Delta\lambda F(\phi_0+\Delta\phi)\right] \quad (4)$$

It is this equation that is solved in the MAX method in WIMS to obtain both the perturbation in the flux and the perturbation in the eigenvalue.

The equation has a fixed source term given by:

$$(\Delta S + \lambda_0\Delta F - \Delta T)\phi_0 \quad (5)$$

and the change in eigenvalue can be shown to be given by the standard expression

$$\Delta\lambda = \frac{\int \phi_0^*(\Delta T - \Delta S - \lambda_0\Delta F)(\phi_0+\Delta\phi)}{\int \phi_0^* F(\phi_0+\Delta\phi)} \quad (6)$$

where the adjoint flux ϕ_0^* is given by the equation:

$$T_0^*\phi_0^* = S_0^*\phi_0^* + \lambda_0 F_0^*\phi_0^* \quad (7)$$

where O^* is the adjoint operator of the general operator O

2.2 IMPLEMENTATION OF THE IMPROVED METHOD

The basic method above has been implemented in WIMS and some results were reported in [2]. In this form, the MAX method uses a homogeneous flux solution as the unperturbed case, and the flexibility of the code to treat different types of perturbation is limited. This results in relatively slow calculations when dealing with cases involving either temperature changes or depletion.

There is a current requirement for a fast but accurate implementation of this method. To meet this objective the following enhancements have been incorporated:

1. MAX has been linked to the deterministic transport code CACTUS within WIMS. Thus the unperturbed solution in the MAX method has been supplied by CACTUS.
2. The perturbations in temperature, density and due to irradiation are all treated explicitly by MAX so that estimates of temperature coefficient are not obtained by comparing two different MAX calculations but by treating the effect of temperature as a perturbation.
3. A special method for treating the resonance shielding of end pellets where the end surface is not shielded from incoming neutrons has been included in WIMS.

2.2.1 Link to CACTUS

The CACTUS code in WIMS[1] is a deterministic solution of the transport equation based on the characteristics methods. This code has been extended, as part of this development, so that there is an option in the code to estimate the adjoint flux in addition to the normal flux. This uses the same tracking technique but reverses the direction of the tracking and uses the adjoint operators for scatter and fission. Both the adjoint and normal flux are then read by MAX and used to determine both the fixed source and the initial eigenvalue for the tracking process.

Currently the CACTUS method is used to estimate the scalar flux and the higher components of the flux are not stored. This presents a problem for the MAX solution as the fixed source term will require higher components of the flux. The source term is given by:

$$(\Delta S + \lambda_0 \Delta F - \Delta T)\phi_0$$

where ϕ_0 is the angular flux from a deterministic calculation.

Even if we assume that scatter in a graphite reactor is isotropic, this source term has a component, related to the change in the transport operator i.e. ΔT, which requires the angular flux. Thus the total angular flux is required to calculate the source accurately.

In order to estimate the angular flux, when determining the source term, a ‘reverse tracking’ technique is used in MAX. If it is assumed that the scatter is isotropic, then the scatter and fission(yield) source is isotropic, and only the scalar flux is required to estimate that term. Thus to find the angular flux at a point in the problem, the assumption is made that this is given by the equation:

$$\phi_0 = \frac{1}{T}(S_0 + \lambda_0 F_0)\phi_0 \tag{8}$$

Note that while the flux on the left-hand side of the above equation is the total angular flux, the source term $(S_0 + \lambda_0 F_0)\phi_0$, with our assumptions, only requires the scalar flux. Thus at a given point the angular flux is obtained by tracking back to the previous collision and estimating the scattering and fission source terms at that point.

The solution method in MAX requires that the problem is subdivided into meshes where it is assumed that the flux is constant. For a mesh in the problem the scalar flux will be available from the CACTUS solution. This back tracking technique can then be used to obtain both the angular and the positional weighting of the total flux within the mesh. The sampling procedures are designed to conserve the scalar flux within each mesh so that it is consistent with the value from CACTUS.

That is

$$\int_{mesh} \phi_0(r,E,\Omega)d\Omega dr = \psi_{mesh}(E) \tag{9}$$

where $\psi_{mesh}(E)$ is the scalar flux for the mesh at energy E

2.2.2 Orthogonality to Unperturbed Flux

The above equations can be solved to give an estimate of the perturbed flux but an additional constraint must also be included in order to give accurate solutions. The perturbed flux must be orthogonal to the unperturbed flux in the sense that

$$\int \phi_0^*(r,E',\Omega')\chi(E')\nu\Sigma_f(r,E)\Delta\phi(r,E,\Omega)dE'dEd\Omega d\Omega' dr = \int \phi_0^* F_0 \phi_0 = 0 \tag{10}$$

where the integration is over all phase space.

This constraint is incorporated in the iteration process to generate the perturbed flux solution.

2.2.3 Sequences of Perturbation

The method has also been developed to treat a sequence of perturbations. Two situations have been allowed for:
(a) Parallel Perturbations. All perturbations refer to a common unperturbed state. Thus one perturbation does not interact with any subsequent perturbations. This is the case when generating data at different temperatures, at the same time point, for a PANTHER whole core calculation
(b) Series Perturbations. All perturbations refer to the previous perturbed state. Thus all perturbations in the sequence interact with the previous perturbations. This is the case when treating depletion as a sequence of perturbations.
Both types of sequences can be treated in MAX . The parallel perturbation sequence can be treated using the theory outlined in Section 2.1. For a series perturbation sequence the theory can readily be extended to give the following equations which calculate the change in flux and eigenvalue due to perturbation type 2 relative to perturbation type1:

$$\Delta\phi_{12} = \frac{1}{T_2}\left[(S_2 + \lambda_1 F_2)\Delta\phi_{12} + (\Delta S_{12} + \lambda_1 \Delta F_{12} - \Delta T_{12})\phi_1 + \Delta\lambda_{12} F_2(\phi_1 + \Delta\phi_{12})\right] \tag{11}$$

where $\Delta\phi_{12}$ is the flux perturbation of perturbation type 2 relative to perturbation type 1
and ΔO_{12} is the change from operator type 1 to operator type 2
and O_2 is the total operator for perturbation type 2

Thus the total perturbation due to perturbation type 2 is

$$\Delta\phi_2 = \Delta\phi_1 + \Delta\phi_{12} \tag{12}$$

and

$$\phi_1 = \phi_0 + \Delta\phi_1$$

Note also that for all the perturbations, the orthogonality relation in equation (10) must be satisfied.

2.2.4 Types of Perturbation

There are a number of possible perturbations that could be applied to a problem. They can be roughly categorised as follows

1. Perturbations due to changes in material conditions – e.g. temperature, density
2. Perturbations due to changes in geometry - e.g. rod insertions
3. Perturbations due to neutron interaction – e.g. depletion, fission
4. Changes due to modelling improvements – e.g. 2D to 3D, more energy groups, groups to point data, higher order scatter representations.

All these categories can be treated with the latest version of the MAX code presented in this paper. Thus as noted above in Section 2.2.3, the perturbations which involve changes in material conditions such as temperature are treated as parallel perturbations whilst depletion is treated as a series perturbation with each burnup step interacting with subsequent steps. The types of perturbation for a typical run are shown in Figure 2

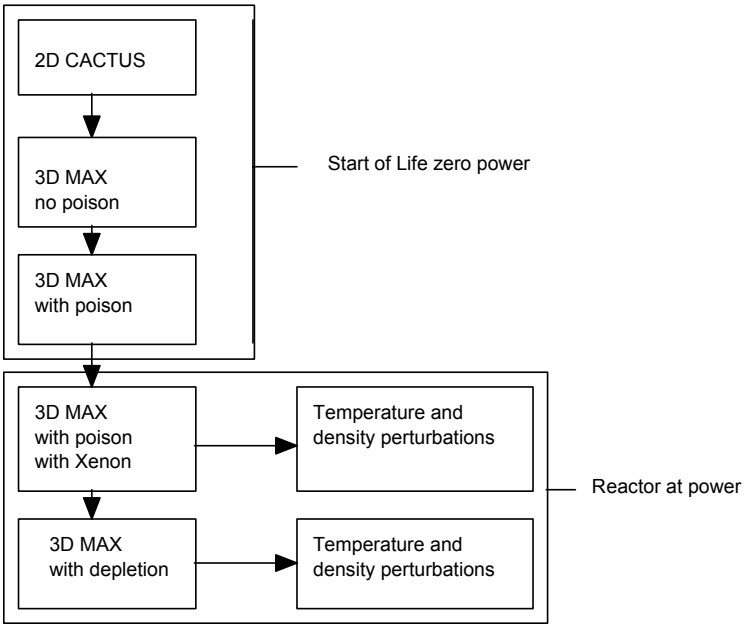


Fig 2 Sequences of Perturbations

Note in Figure 2 the vertical connecting arrows indicate series perturbations and the horizontal connecting arrows indicate parallel perturbations.

2.2.5 Resonance Treatment

A special model was used to generate the shielded cross sections for the fuel. The model was based on the sub-group treatment in WIMS[1] but was extended to treat the special modelling problems associated with the end pellet in the cluster. This pellet has an extra surface for neutron capture and hence the end pellet has more capture in U^{238} and consequently more Plutonium production than the

other pellets. This is modelled using an enhancement to the sub-group method that increases the effective resonance integral for this zone of the problem.

2.2.6 Link to PANTHER

A PANTHER whole core calculation requires a library of cell constants that are a function of a series of perturbations to the base conditions in the core. These perturbations include variations in temperature and power. Standard Monte Carlo calculations are not very effective in dealing with small perturbation due to the stochastic effects. However a perturbation method can overcome this shortcoming by reducing the variance associated with the perturbations and also reducing run times

A PANTHER library also tabulates the library of cell constants as a function of irradiation. Using the old MAX method this calculation is carried out in WIMS as a series of independent Monte Carlo calculations, and this can lead to significant statistical noise on the resultant library. To reduce these random effects, perturbation theory was employed as shown in Section 2.2.4

3 WIMSBUILDER

The series of developments above leads to a complex calculational route through WIMS. To assist the user by hiding the complexity, an extension to the WIMSBUILDER[5] tool has been developed for AGR application. This new option has been designed to input cluster geometry and treat 3D problems. This not only eases the input of data but also selects the appropriate calculational route for the geometry and model being considered. With this new facility input into WIMS is as straightforward as for the PWR cases shown in [5].

4 VALIDATION

The new method outlined above has been used to generate data for AGR systems. In the following sections a series of calculations, which are used to validate the method and quantify the resulting speed gains, are presented. The models used in these calculations consisted of a series of AGR clusters at varying enrichments, with and without poison. The results are then compared with a set of reference calculations using either other transport solutions or earlier versions of MAX. This results outlined in the following sections indicate that the new method is accurate and leads to a gain in speed of approximately two orders of magnitude.

4.1 PIE (POST IRRADIATION EXAMINATION)

A series of PIE measurements have been carried out on AGR fuel to estimate the axial peaking in power. These results were reported in References 2 and 3 and showed good agreement between prediction based on the WIMS/MAX method and measurement. The mean discrepancies are shown in Table 1.

Table 1 Mean (C-E)/E % for AGR Stage 1 Fuel –Variation with Enrichment
Hot Initial Dimensions

Position	Enrichment w/o				
	1.162	1.542	2.012	2.012 – 0.25" Bore	2.500
Top Pellet	-1.17	0.29	1.24	0.22	-0.60
Sdev	1.18	1.18	1.17	1.17	1.05
2nd Pellet	-1.40	-0.53	-0.67	-0.27	-0.14
Sdev	1.32	1.22	1.28	1.32	1.28
Mean	-0.28				
Sdev	1.22				

The values quoted in Table 1 are the ratio of axial power in a particular pellet relative to the mean over the whole fuel element.

4.2 TEMPERATURE EFFECTS

A series of calculations were carried out to validate the estimate of temperature coefficient using MAX. Initially a comparison was made between MAX, PIJ, and CACTUS for a 2D problem. PIJ and CACTUS are two deterministic codes used in WIMS. The results are shown in Table 2 and indicate good agreement between MAX, CACTUS and PIJ.

Table 2 Results of the AGR lattice cell calculations with MAX
and PIJ and CACTUS in 2D

Case	keff			dρ/dT (mN/°C)		
	PIJ	CACTUS	MAX	PIJ	CACTUS	MAX
Fuel 1100°K Moderator 644°K	1.05267	1.04864	1.050020±0.00080			
Fuel 1000°K	1.05397	1.05000	1.051386±0.00080	-1.18	-1.24	-1.27 ±0.02
Moderator 544°K	1.05174	1.04792	1.049389±0.00082	0.84	0.66	0.57 ± 0.17

A calculation was then carried out in full 3D but with data consistent with the 2D case used above. The results are shown in Table 3 and show temperature coefficients consistent with the 2D cases.

Table 3 Results of the AGR lattice cell calculations with MAX in 3D

Case		keff	dρ/dT (mN/°C)
Temperatures	Geom	MAX	MAX
Fuel 1100°K Moderator 644°K	2D	1.049703±0.00052	
As Above	3D	1.014505±0.00052	
Fuel 1000°K	3D	1.015804±0.00052	-1.26 ± 0.015
Moderator 544°K	3D	1.013824±0.00054	0.66 ± 0.10

Tables 1 and 2 also show that the variance associated with these calculations is of the order of 1-2% for the fuel coefficient and 15% for the moderator coefficient.

4.3 IRRADIATION EFFECTS

Using a case with strong poison loading, the WIMS/MAX model was run to estimate the variation of reactivity with depletion. The results are shown in Table 4.

Table 4 Estimates of reactivity for an irradiated case with poison

	New MAX		Old MAX	
Irradiation	K-eff	Stdv	K-eff	Diff with New MAX(pcm)
0	1.303747	0.00337	1.31692	-0.0100
50	1.273559	0.00005	1.28342	-0.0077
500	1.263592	0.0	1.28342	-0.0076
2000	1.252615	0.00014	1.26255	-0.0079
6000	1.235572	0.00040	1.24191	-0.0051
10000	1.228986	0.00029	1.21503	0.0114
15000	1.184801	0.00018	1.19100	-0.0052
20000	1.124981	0.00017	1.13282	-0.0069
25000	1.061392	0.00018	1.07052	-0.0086
30000	0.993827	0.00020	1.00099	-0.0072

The results illustrate that the variance associated with this type of calculation is generally less than 100 pcm and the results are in reasonable agreement with the old version of MAX, although there is an overall reduction in reactivity of ~700 pcm. The positive difference at 10000 MWD/Te is due to the poison burning out in the new version more quickly. The reduction in worth with the new version is shown to be in agreement with results from MONK in the next section.

4.4 COMPARISON WITH MONK FOR POISON WORTH

The MONK code[6] uses conventional Monte Carlo techniques to solve the transport equation. A MONK calculation was also carried out for the heavily poisoned case and the results are compared with those for MAX in Table 5. The agreement is within the uncertainties and illustrates that the reactivity estimated by the new version of MAX is in agreement with standard Monte Carlo predictions.

Table 5 Comparison of MONK and MAX for an unpoisoned and a poisoned AGR assembly

	Unpoisoned	Stdv	Poisoned	Stdv
MONK	1.4032	0.0005	1.3079	0.0005
MAX	1.4032	0.0005	1.3037	0.0034
Diff (pcm)	0.0	0.0007	-0.0032	0.0034

4.5 SPEED GAINS

The speed of the new MAX calculation can be compared with a conventional Monte Carlo calculation for the unpoisoned and the poisoned cases. The MAX calculation took 162 secs cpu on a SUN ULTRA workstation for each case whereas the MONK cases took 42900 secs cpu. Thus for this case the MAX is ~250 times as quick as the MONK calculation. In addition the MAX is a factor of ~1000 faster for the estimate of temperature coefficients, because in conventional Monte Carlo temperature coefficients are obtained by taking the difference between two separate calculations . Thus it can be concluded that the new method gives between 2 and 3 orders of magnitude increase in speed relative to conventional Monte Carlo.

In addition, the new version of MAX can be compared with the old version for generating a PANTHER library. For a single fuel type in a PANTHER library there are approximately 10 depletion steps and at each depletion step there are 8 temperature perturbations. This gives 80 calculations. Each calculation with new MAX will take ~160 secs cpu giving about a 4hour cpu run on a SUN ULTRA for the library. It was estimated that the old MAX would take ~ 2-4 weeks to generate a library. This means that new MAX is about 2 orders of magnitude faster for this type of calculation.

5 CONCLUSIONS

This paper outlines a significant development of the WIMS computational scheme. This development allies characteristics methods with perturbation Monte Carlo to produce a fast accurate method of dealing with the difficult features of a reactor model. The results illustrate that the method is a viable option for use with whole core calculations such as PANTHER. Whilst currently used for AGR calculations, the paper shows that the generality of the method can lead to the use of these techniques on other reactor problems.

6 REFERENCES

1. M. J. Halsall, “WIMS8 – Speed with Accuracy”, Paper presented at International Conference on the Physics of Nuclear Science and Technology, Long Island Oct 1998.
2. J. L. Hutton, “New Capabilities of the WIMS Code”, Paper presented at International Conference on Advances in Reactor Physics and Mathematics and Computations into the Next Millenium – PHYSOR 2000, Pittsburgh, May 2000.
3. J. L. Hutton and N R Smith “Use of a Hybrid Monte Carlo Technique for Power Shape Calculations” MC2000, Lisbon, Portugal, 2000.
4. P. K. Hutt et al. “The UK Core Performance Code Package” ,Nuclear Energy, Journal of British Nuclear Energy Society, October 1991.
5. E. B. Webster. “WIMSBUILDER” Paper presented at International Conference on Advances in Reactor Physics and Mathematics and Computations into the Next Millenium – PHYSOR 2000, Pittsburgh, May 2000.
6. N. R. Smith and G. A. Morrell. “An Introduction to MONK7”, Proceedings of ICNC’95, Albuquerque, USA, 1995