

Serco Assurance

NEW FEATURES

A Guide to the New Features of
WIMS Version 9A

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Executive Summary

Version 9A is the latest release of the WIMS reactor physics code package. This new version incorporates a range of additional features. In addition, WIMS9A is accompanied by the new version of WIMSBUILDER, a utility code for preparing input data. This report provides an introduction to the use of each of the additional features of the new code and is directed at existing WIMS8 code users. Further information on all the features introduced here can be found in the WIMS9 and WIMSBUILDER User Guides

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1 Introduction

The development and subsequent release of WIMS7 [1] was the culmination of a major unification programme for the WIMS reactor physics codes, with the combination of the capabilities of WIMSE and LWRWIMS in a single package. Additional changes were also made to improve CACTUS and BURNUP and include the new modules EDIT and TWOTRAN.

WIMS8A [2] released in 1998 contained several new features to improve the reactor physics package in terms of user image, speed and modelling flexibility.

WIMS9A [3] released in December 2004 builds on these developments to give a more comprehensive range of code features and includes a fundamental review of the resonance self-shielding methods as well as a new interface structure and an updated implementation of many of the modules to modern FORTRAN standards.

This report provides an introduction to the use of the new features and is directed at existing WIMS8 code users. Further information for all the features introduced here can be found in the WIMS9 User Guide.

The main new features of WIMS9A are:

- Changes to the user image.
- New interface structure and data storage policy.
- Inclusion of AGR geometry in WIMSBUILDER.
- New resonance treatment included in the modules HEAD, PRES and RES:
 - Extended resonance energy range treated,
 - Fine group calculation at low resonance range energies including current weighting of the transport and P1 cross-section, new resonance overlap model and calculation of the $f(p)$ correction to broad group out scatter,
 - Inclusion of resonance scattering theory as well as resonance absorption theory,
 - Change of the default fission spectrum from U235 at 1MeV incident energy to U235 at thermal energy.
- Collision probability flux solution module PIP, new convergence criteria, inclusion of adjoint solutions. There are also so additional minor options for the treatment of directional diffusion coefficients and the use of cell average D with bucklings.
- New beta effective and prompt neutron lifetime edit, BETA module.
- New FSPEC module to calculate the problem average fission spectrum.
- Extension of the PROCOL module to include a geometry with particles within pebbles as well as particles within annular geometry. Also, improvements to the input data options to aid in specifying refined mesh geometry.
- Inclusion of slab and spherical geometry options in addition to annular geometry within the FLURIG module.
- Inclusion of perturbation and prompt neutron lifetime edits in SNAP.
- Inclusion of the new MAX route.
- New edits with the EDIT module for the inclusion of leakage in the neutron balance option and a five factor formula edit.
- The INTER module has some enhance features which support the copying of parts of one interface to another.

The data library for WIMS9A is available in 172 broad energy groups and is based on the JEF2.2, 1997 library, as issued with WIMS8, extended to include data for the high energy resonance range and to include delayed neutron data previously only available as fixed data within the LED module.

The following section describes each of the new main new features in WIMS9A.

2 New Features Guide

2.1 User Image

WIMS9 has undergone major software re-engineering to ensure ageing code is brought up to date and to ensure its maintainability on many rapidly developing computer platforms well in to the future. During this development the opportunity has been taken to update a certain number of features, the W which stood for Winfrith, prefixing the name of each of the modules has been removed and the old numeric nuclide identifiers have been dropped in favour of nuclide names.

An additional major change is in the storage of interfaces. WIMS9 interfaces are now data structures held in memory and are only written to disk at the request of the user. The new ARCHIVE module has been provided with store and retrieve options facilitate this feature. In addition, there is a STORE keyword which can be given in the user input to set a storage policy for interfaces independent of the use of the ARCHIVE module. This keyword allows all interfaces or a named selection of interfaces, by interface number, to be automatically stored to disc whenever they are written or updated. One consequence of holding all interfaces in core memory is that memory management can become an issue. To aid with this the INTER module has been provided with an EMPTY option which clears interfaces that are no longer required.

2.2 WIMSBUILDER

WIMSBUILDER is a family of utility tools, which simplify the preparation of input to WIMS for specific geometries. The WIMS8 geometries were PWR single assembly, and a 60 degree sector of a VVER assembly. In WIMS 9, AGR geometry has been added, principally to support MAX perturbation calculations.

The main application of WIMSBUILDER is the generation of few-group cross section libraries for the whole-reactor code PANTHER. In these cases, many cycles are run, preparing cross sections, finding the reactivity and neutron flux, then solving the fuel burnup equations to form new material compositions. At some stages of burnup, many 'branches' are created, determining the neutron flux, reactivity and few group cross sections when the standard irradiation conditions (fuel or coolant temperature, coolant density, boron concentration, xenon concentration etc. WIMSBUILDER is also used in preparing cross section data for nuclide inventory calculations.

A new, more powerful version of the MAX module has been incorporated into WIMS9. MAX solves the multi-group neutron transport equations by a hybrid deterministic/ Monte Carlo method, based on exact perturbation theory. It is a general method, although it is particularly suited to the complex geometry of Advanced Gas cooled Reactors (AGR), which has axial gaps between fuel stringers and gadolinium poison toroids in the graphite sleeve.

A WIMS9/MAX AGR calculation consists of a series of perturbations from an unperturbed geometry. The solution for the unperturbed model is calculated by either a deterministic method such as CRITIC or CACTUS, or a previous run of MAX. Successive perturbations can then be used to increase the complexity of the model to 3D, with or without poisons, or to model a change to material properties such as temperature.

The input to a WIMS9 case involving MAX can be lengthy and complex if prepared by hand, the new WIMSBUILDER family member, AGRBUILDER, is now available to simplify this process.

2.3 HEAD Equivalence Resonance Treatment

The HEAD, PRES and RES modules treat resonance self shielding. Modifications to these modules have been introduced following an extensive comparison of the approximations used in deterministic theory relative to Monte Carlo methods. Significant improvements in the accuracy of the resonance self shielding method have resulted as illustrated in Reference 4 for example.

The HEAD module applies equivalence theory to shield the cross sections, see Reference 5. The theory has been extended to cover resonance scattering as well as resonance absorption. The resonance range has been extended to cover energies from 18,315.64 eV to 4.0 eV (groups 32 to 92 of the 172 group XMAS library) rather than 911.882 eV to 4.0 eV in WIMS8. In addition, at the energies of the distinct well separated resonances, between the energies of 55.59513 eV and 4.0 eV, a fine group calculation is performed for each pin or plate to derive correction factors for the overlap of resonances, the correction to the broad group out-scatter cross section and to derive the current at the surface of the fuel. This current is then used to weight the fine group transport and P1 cross sections rather than using the flux as in WIMS8.

It should be noted that in some cases HEAD does not have a full description of the geometry. In particulate fuel geometry for instance the geometry description is only approximate and the PRES, PROCOL and RES modules must be used to derive the cross sections using sub-group theory. In these cases the keywords NOFINE and NOFP should be included in the HEAD input to prevent the application of inappropriate correction factors.

2.4 PRES and RES Sub-group Resonance Treatment

The sub-group treatment of resonance self shielding can be applied by following the HEAD module by the sequence PRES/CACTUS/RES or PRES/collision probability module/RES. The cross sections output by HEAD for the nuclides selected in the user input are over written by cross sections derived by sub-group theory, Reference 5. The PRES and RES modules in WIMS9 include a treatment of resonance scatter as well as maintaining consistence with HEAD by applying current weighting of the transport and P1 cross sections.

2.5 PIP Collision Probability Flux Solution

The solution algorithm applied in PIP has been re-written allowing convergence tolerances for the k-effective, default 10^{-4} , and the flux, default 10^{-5} , to be specified following the keyword TOLERANCE. In addition, an adjoint solution can be obtained by specifying the ADJOINT keyword, the default is to perform a NORMAL flux solution.

There are also some additions to the buckling treatment. The keyword TRANSPORT specifies that, for materials that have both radial and axial transport cross sections, the mean transport cross section should be formed before deriving the diffusion coefficients for application in the DB^2 buckling leakage term. Note that the default is to use the radial transport cross section and to ignore the axial transport cross section.

Another minor option, indicated by the keywords PROBLEM AVERAGE, specifies that the problem average transport cross section should be used in the calculation of the DB^2 buckling leakage term. This option is useful if the problem contains a low density region where application of the region dependant transport cross section in the buckling term would lead to unphysical results.

2.6 BETA Delayed Neutron Fraction and Prompt Neutron Lifetime Edit

This is a new module allowing the calculation of the delayed neutron fraction and prompt neutron lifetime. The module takes both a flux and adjoint flux as input as well as a default set of delayed neutron data from the nuclear data library. Breakdowns of the delayed neutron fraction by delayed neutron group, nuclide and material are printed and optionally as a table by material/delayed neutron group/nuclide. The default delayed neutron library data can optionally be over written by user specified values.

2.7 FSPEC Problem Average Fission Spectrum

This is a new module that allows the calculation of a problem average fission spectrum. The default fission spectrum used in WIMS8 was the U235 fission spectrum at an incident neutron energy of 1 MeV. In WIMS9 this has been changed to the thermal U235 fission spectrum. In some

cases the user may wish to over write the default spectrum by a fission spectrum specific to the given problem. To do this the user first solves the problem using the default fission spectrum to create a flux on the interface. A call to the FSPEC module calculates the fission rates in the different problem nuclides and uses these data to combine the nuclide dependent fission spectra to form a problem dependent spectrum which over writes the default spectrum held in the microscopic and macroscopic cross sections. The flux solution can then simply be re-solved using the problem fission spectrum.

2.8 PROCOL Particulate Fuel Collision Probability Module

Procol calculates collision probabilities for a system of particulate fuel within a containing geometry. The main additional feature in PROCOL is to include a spherical as well as annular geometry as the containing geometry for the particulate fuel. In place of the ANNULUS keyword the SPHERE keyword can be used to specify spherical geometry.

In addition, there are some enhancements to the user input data to improve the ease of use of PROCOL. The sphere/annulus number following the SPHERE/ANNULUS keyword need not be one greater than the previous SPHERE/ANNULUS directive. If the sphere/annulus number on the previous SPHERE/ANNULUS directive was m and on the current SPHERE/ANNULUS directive is n then $(n-m)$ meshes of equal width are automatically inserted. This is also true for the SHELL directive specifying the meshing within the particulate fuel. In addition, a list of annulus/sphere numbers, rather than a single annulus/sphere number can be specified following the FUEL keyword. The particulate fuel type specified in the following SHELL directives is allocated to each of the meshes of the containing specified in the list.

2.9 FLURIG One Dimensional Geometry Collision Probabilities

FLURIG calculates collision probabilities for one dimensional geometry using the method of Carlvik which integrates the probabilities along a set of parallel lines through the geometry. In WIMS8 only annular geometry was treated. In WIMS9 this has been extended to include both spherical and slab geometry. FLURIG uses the volumes on the input interface and by default assumes a cylindrical geometry, this can now be specified as spherical or slab geometry using the keywords SLAB or SPHERICAL. The keyword CYLINDRICAL can be specified for completeness but this is assumed as the default.

2.10 SNAP

In addition to the SOLVE and ADJ SOLVE keywords to solve for the normal and adjoint flux respectively there is also an option NORMAL ADJ SOLVE or OPTIMISE NORMAL ADJOINT SOLVE. OPTIMISE requests the calculation of optimised acceleration parameters. A calculation of the system k -effective and solutions for both the flux and adjoint flux which are written to the WIMS interface. This option is more efficient than requesting separate solutions for the normal and adjoint fluxes and is recommended for use when a beta effective edit, using the BETA module, is to be run following SNAP.

In addition to the PRINT PHI option there is also a PRINT AD PHI option listing the adjoint flux.

Edits can be performed for the leakage per unit volume, radial buckling and axial buckling using the keywords LEAK, BR and BZ respectively.

There is a new edit for the prompt neutron lifetime invoked by the keywords PRINT LIFETIME this should be preceded with solutions of both the flux and adjoint flux, it gives good agreement with the prompt neutron lifetime edit in the BETA module.

Currents across a given surface can be printed using the PRINT CURRENTS keywords.

Finally, there is a perturbation edit available using the keywords PERT dk.

2.11 New MAX Module

The MAX code has been upgraded and improved. In particular, a version has been developed that can be used in conjunction with the CACTUS module. This option has been adapted for use with AGR's to carry out a range of perturbations for use when generating a PANTHER library.

The modifications to MAX have been:

1. The code can input a CACTUS flux and adjoint solution in addition to using CRITIC,
2. The code can also treat an irradiation as a perturbation relative to the previous irradiated solution. This option inputs the MAX solution at the last irradiation as the unperturbed state. In this way the running time for a case with many irradiation steps is greatly reduced.
3. The input options for describing the geometry have been simplified. Thus the input of tracking zones is now more user friendly. The code will generate the tracking zones from the other geometry input.

The convergence of the code has been upgraded and improved. The previous version did not ensure that the converged solution was orthogonal to the unperturbed solution. The procedure used by MAX has been extended to include this constraint.

As noted elsewhere, the MAX input has been incorporated in a new option in WIMSBUILDER. This option allows the user to limit the input to details of the geometry and the required perturbations. WIMSBUILDER then generates the WIMS9 input for both MAX and the other modules linked to the route (CACTUS, SMEAR etc.).

With these changes AGR 3D calculations with temperature perturbations and irradiation can be accurately carried out within 1 day on current UNIX or PC based machines.

2.12 EDIT Module

The EDIT module has two additional options.

The LEAKAGE keyword calculates the leakage from the set of selected meshes or materials in the selected energy group structure from a neutron balance. If there is a buckling on the input interface this is included in the report leakage calculation.

The keyword FIVEFACTOR produces a breakdown of the k-effective of the problem in terms of the fast, resonance and thermal energy regions as specified by the user. The five factors are a generalisation of the well known four factor formula which only holds for exactly critical systems. The five factors are:

- The number of productions per fast energy neutron.
- The number of productions per resonance energy neutron.
- The number of productions per thermal energy neutron.
- The fast energy escape probability.
- The resonance energy escape probability.

This edit is useful in examining the difference between two systems or for identifying the "hardness" of the neutron spectrum in the problem.

2.13 INTER Interface Operations Module

In WIMS8 the INTER module allowed the user to perform certain operations on an interface such as copy, print or build an interface from user input. The mode of operation reflected the form of the interface which was stored as five separate files. In WIMS9 the interface is a single entity held in core storage. This changes the image of INTER slightly, however, a similar but more comprehensive set of interface operations are available. There are main options to empty, print,

copy, list and build an interface. The list and build options perform inverse functions, list lists an interface to a named file while build takes data in the form output by list to build a new interface. This allows the user to amend specific data items on the interface. There are also options to copy part of an interface from one interface to another following a number of checks for consistency between the interfaces. Items that can be copied are the flux, the adjoint flux, collision probabilities, microscopic cross sections, compositions and the geometry.

The TRAIL option is no longer supported by INTER. Instead a separate TRAIL module is provided to perform this function, see section on TRAIL below.

There are also options associated with the MAX module described in Section 2.11 above.

2.14 TRAIL

This new module replaces the TRAIL option which was implemented as an option within the INTER module of WIMS8.

3 Summary

We are always very keen to learn of developments that the users of WIMS would like to see in the scheme. Please send any suggestions to the ANSWERS hotline.

4 References

- [1] The ANSWERS Software Service, WIMS7 User Guide, ANSWERS/WIMS(95)4
- [2] The ANSWERS Software Service, WIMS8 User Guide, ANSWERS/WIMS(98)9
- [3] The ANSWERS Software Service, WIMS9 User Guide, ANSWERS/WIMS(99)9
- [4] J L Hutton, T D Newton R J Perry and D J Powney , Validation of WIMS9, PHYSOR 2004 -The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments, Chicago, Illinois, April 25-29, 2004, on CD-ROM, American Nuclear Society, Lagrange Park, IL. (2004)
- [5] D J Powney and T D Newton, Overview of The WIMS 9 Resonance Treatment, ANSWERS/WIMS/TR.26, September 2004.