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Developments within the WIMS Reactor Physics Code for Whole Core Calculations

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Abstract - *The WIMS reactor physics code is traditionally used to perform 2D lattice calculations, typically to generate homogenized reactor physics parameters for whole core codes. Lattices of essentially all types can be treated, including square and hexagonal assemblies and large guide tubes/water rods. WIMS now includes support for 3D transport calculations, up to whole core size calculations, which can be performed on models of varying size and complexity. This paper described the development and application of whole core transport methodologies within WIMS. The CACTUSOT 3D method of characteristics transport solver is applied to a variant of the C5G7 benchmark, with good results. Application of these methodologies to SFR, HTR and MSR Generation IV concepts is also demonstrated through benchmarking. Recent developments for the purposes of uncertainty quantification are also discussed, including treatment of nuclear data uncertainties through sampling of the underlying nuclear data libraries, and derivation of sensitivity coefficients of reactor physics parameters to group-dependent cross-sections, with consistent treatment of resonance shielding.*

I. INTRODUCTION

The WIMS modular reactor physics code has been under continuous development for over fifty years [1]. In its traditional mode of operation, WIMS is used to perform 2D lattice calculations, typically to generate homogenized reactor physics parameters for a whole core code such as PANTHER [2]. Together, WIMS and PANTHER can be used to model reactor types including large PWRs, SMRs, BWRs, AGRs, VVERs and RBMKs. Through its fractal geometry capability, WIMS has the capability to handle 2D (including lattice) and 3D geometries of essentially arbitrary complexity, including square and hexagonal assemblies, treatment of non-regular lattices and large and/or off-centred guide tubes/ water rods.

Additionally, WIMS now includes support for 3D transport calculations up to whole core size calculations, which can be performed on models of varying size and complexity.

WIMS can perform equivalence and subgroup theory resonance shielding treatments for thermal spectrum reactors with light water, heavy water and graphite moderators, mixed moderator systems. WIMS can also be used to perform fast reactor calculations.

WIMS primarily utilizes nuclear data in the 172-group XMAS scheme which has been selected to give a balance between accuracy and computational efficiency. In addition to the standard 172-group libraries, fine group libraries containing 1968 groups are also provided for use with the ECCO cell code [3] which is available as a module within WIMS, primarily for fast spectrum systems. JEF-2.2, JEFF-3.x, ENDF and CENDL libraries are available, with the latest evaluations regularly being made available.

The current release version of WIMS is WIMS10. This paper gives an overview of developments in WIMS11, covering new features within the code and their application to small modular reactors and Generation IV systems.

II. NEW CAPABILITIES

1. 3D Method of Characteristics with Once-Through Tracking

The CACTUS method of characteristics in the WIMS reactor physics code was extended in WIMS10 to the modelling of 3D lattice geometries. In WIMS11, the CACTUSOT solver has been developed to improve spatial coverage of the model being considered. The CACTUSOT solver is described in more detail in a separate paper at this conference [4].

CACTUSOT instead uses a "once-through" tracking algorithm. Here, a set of parallel tracks is defined at each tracking angle. The starting points of the tracks at a given angle are uniformly distributed on the external surfaces of a model. Each track is followed from its starting point until the point at which it next intercepts an external surface; the track is then terminated. Due to the uniformity of the track distribution, it has been shown that uniformity of spatial coverage for 3D reactor-scale models can be assured.

CACTUSOT has been developed for use in the HPC environment and includes MPI parallelization of the track generation process and flux solution algorithm.

Here, the CACTUSOT solver is applied to the OECD Nuclear Energy Agency (NEA) Benchmark on Deterministic Transport Calculations Without Spatial Homogenisation: MOX Fuel Assembly 3-D Extension Case [5], a variant of the C5G7 benchmarks. This consists of a 3D mini core of UO_2 and MOX assemblies surrounded by a water reflector in all directions (Fig. 1). The mini core has octant in-plane symmetry and reflective symmetry in the axial direction. There are three cases, with control rods progressively inserted into some of the fuel assemblies. Both fuel pins and guide tubes (rodded and unrodded) are treated as a single cylinder inside of a square pincell. For example for the fuel pins the clad, gap and fuel are smeared together. Seven-group cross sections are supplied as part of the benchmark specification.

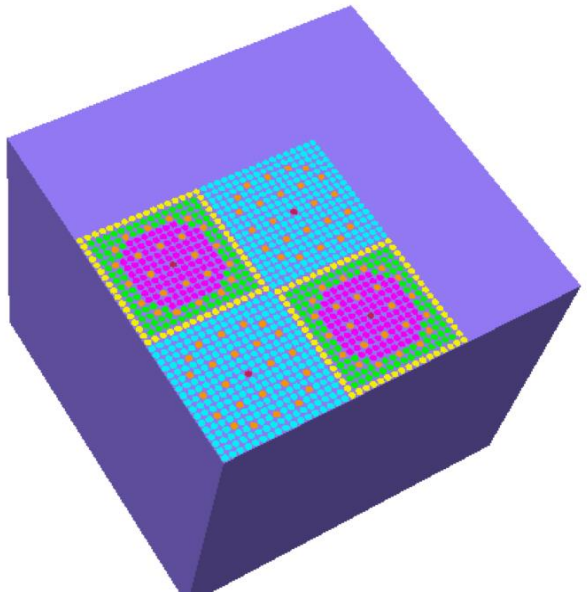

Fig. 1. MOX Fuel Assembly 3D Extension Case Mini-Core Model

The CACTUSOT solution utilized an angular discretization using an S_{16} quadrature set, with track spacing of 0.1 cm. Doubling the track spacing from 0.1 cm to 0.2 cm was found to give a difference of 7 pcm (Table I), implying sufficient track coverage, and the solution also converged with increasing quadrature order. The CACTUSOT model was prepared using a 'slice' geometry approach, where the tracks are generated for planar slices of the model, and these slices and synthesized to form a full 3D solution. This approach is described further in Ref. [4]. A substantial part of the remaining discrepancy with the MCNP reference solution is likely attributable to discretization in this 'slice method', and hence could likely be resolved through further refinement of the mesh used in the synthesis of the slices.

The CACTUSOT results are compared to reference MCNP [5] results from Ref. [6]. Table II gives results for the unrodded case with 0.1 cm track spacing, with rodded cases displaying similar magnitude and trends. While the discrepancy between CACTUSOT and the reference MCNP results falls outside of the 98% confidence interval for the MCNP statistical error in virtually all cases, the agreement for distributed parameters is within 1% in virtually all cases and the discrepancy between MCNP and CACTUSOT is in general consistent with discrepancies between deterministic and Monte Carlo codes for this benchmark reported in Ref. [6].

Track Spacing (cm)	**Unrodded**	**Rodded A**	**Rodded B**
0.2	-97	-98	-130
0.1	-90		

TABLE I. Discrepancy (pcm) between reactivity calculated by CACTUS and MCNP reference results [6] for MOX Fuel Assembly 3-D Extension Case Benchmark for Unrodded and Rodded Configurations, for different track spacing values in CACTUSOT.

2. 3D Discrete Ordinates Solver

The MDLTRAN flux solver, which uses the discrete ordinates (Sn) method in full 3D Cartesian geometry, is currently being benchmarked and integrated within WIMS. MDLTRAN can use both diamond difference and linear discontinuous difference methods to solve the discrete ordinates transport equation. It employs a multi-grid acceleration technique based on discontinuity factors and an equivalence theory diffusion solver, both within the inner iterations as a form of diffusion synthetic acceleration and within the outer iterations as a form of CMFD acceleration [7]. MDLTRAN has been developed for use in the HPC environment and includes parallelisation by both energy group and axial domain, and domain decomposition by axial slice.

3. Flux Solver Utilizing SP3 method

A 1D, 2D and 3D flux solution capability utilising diffusion theory and the SP3 method has been added to WIMS11, with application to design, group condensation and pincell homogenized core calculations.

A transient solution capability is being added to this solver, and a subchannel thermal-hydraulic solver is also being added to allow temperature feedback to be included in steady-state and transient neutronics calculations. Thermal-hydraulic calculations can be performed for fuel bundles of arbitrary geometry using the subchannel analysis. Neutronic feedback can be performed with re-shielding of cross sections at each neutronic calculation, including utilizing

subgroup theory to consider shielding effects arising through spatial variation in temperature within a fuel pin.

	MCNP Reference [6]	CACTUSOT	MCNP statistical error (98% CI) [6]	Discrepancy between CACTUSOT and MCNP
Max pin power slice 1	1.108	1.101	-0.60%	0.21%
Max pin power slice 2	0.882	0.877	-0.60%	0.23%
Max pin power slice 3	0.491	0.489	-0.43%	0.30%
Inner UO2 assembly power slice 1	2.481	2.467	-0.57%	0.14%
MOX assembly power slice 1	219	2178	-0.54%	0.19%
Outer UO2 assembly power slice 1	94.5	94.6	0.13%	0.14%
Inner UO2 assembly power slice 2	62.1	62.3	0.39%	0.10%
MOX assembly power slice 2	174.2	173.4	-0.45%	0.17%
Outer UO2 assembly power slice 2	75.2	75.4	0.24%	0.13%
Inner UO2 assembly power slice 3	49.5	49.7	0.33%	0.09%
MOX assembly power slice 3	97.9	98.0	0.14%	0.13%
Outer UO2 assembly power slice 3	42.9	43.3	1.01%	0.10%
Inner UO2 assembly power	27.8	28.1	0.96%	0.07%
MOX assembly power	491.2	489.3	-0.40%	0.29%
Outer UO2 assembly power	212.7	213.3	0.30%	0.21%

TABLE II. CACTUSOT results for MOX Fuel Assembly 3-D Extension Case Benchmark, Unrodded Configuration.

4. Uncertainty Analysis

To address a growing need to determine through life uncertainties in reactor core calculations, WIMS11 contains additional features to quantify nuclear data uncertainties.

A nuclear data covariance library has been produced, primarily based on the best available covariance data from JEFF-3.2, ENDF/B-VII.1, JENDL4.0 and TENDL-2011. In WIMS this can be utilized in two ways:

- Direct perturbation of the nuclear data libraries based on the covariances during the production of WIMS nuclear data libraries from the underlying nuclear data evaluations. Monte Carlo and Latin Hypercube sampling methods have been utilized to generate sets of perturbed data libraries. This involves simultaneous treatment of all nuclear data uncertainties to get a total response.
- Through derivation of sensitivity coefficients of reactor physics parameters to group and nuclide dependent cross sections, and combination with the covariance library to generate overall uncertainty. A methodology has been added to WIMS to calculate sensitivity coefficients through consistent perturbation of the group-dependent cross sections during the equivalence theory calculation. It is intended to propagate this to the subgroup theory treatment in WIMS in the near future. Combination with the covariance matrix can be performed within WIMS11.

Efforts are ongoing to propagate this methodology through to two stage assembly/core calculations. In the first instance, it is straightforward to utilize perturbed nuclear data libraries to generate nuclear data for a core calculation, and then perform core calculations with multiple sets of nuclear data. In the second case, a key challenge is to combine a large number of sensitivity coefficients, which are burn-up and reactor-state dependent, to produce perturbed nuclear data libraries for core calculations – to evaluate the relative impact of different uncertainties on core-level reactor physics parameters. A methodology to perform this task with a strong degree of automation is under development, with the goal of making the problem tractable by calculating a limited set of sensitivity coefficients that encompass the major contributors to uncertainty within the problem.

In addition to nuclear data uncertainties, automated features are being developed to determine sensitivities to manufacturing tolerances (fuel composition, geometry). These features are integrated within Visual Workshop, the graphical user interface for WIMS and other ANSWERS codes, which is further described in Section IV.2.

5. Method of Characteristics

The CACTUS solver has been extended to include an explicit treatment of P1 scatter.

III. NEW APPLICATIONS

WIMS is now capable of performing reactor physics calculations for essentially all reactor types. Previous versions of WIMS have been used to perform lattice calculations for PWRs, gas-cooled reactors VVERs, RBMKs and CANDUs; experimental reactors; and core calculations for pebble bed HTRs and fast reactors.

This section discusses the development of core calculation methodologies within WIMS for additional reactor types. In all cases, these methodologies are supported by benchmarking activities.

1. Boiling Water Reactors

Due to the strong possibility of ABWR new build in the UK, the application of WIMS and PANTHER to BWR analysis is currently being benchmarked and validated. This includes the following developments:

- Benchmarking a calculation route with WIMS11 for BWR lattices (e.g. Fig. 2) against continuous energy Monte Carlo calculations. As with PWRs, equivalence and/or subgroup theory is used to generate 172 group cross sections; a multicell collision probability method is used to condense to a smaller number of groups (22 in this case), and the CACTUS is used for the main transport solution. Good agreement between deterministic and Monte Carlo calculations was achieved.
- Benchmark of full core WIMS/PANTHER calculations using a continuous energy Monte Carlo code.
- Validation against plant data is planned.

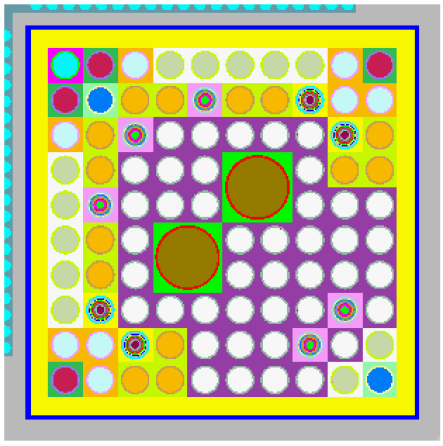

Fig. 2. Typical BWR lattice problem

2. Fast Reactors

An improved calculation route has been developed within WIMS11 to perform calculations for fast reactors with liquid metal and gas coolants. This is facilitated by the new 3D transport solvers within WIMS11. The calculation steps are:

- Heterogeneous calculation with the ECCO cell code to generate 172-group microscopic cross sections
- 2D lattice calculation to generate assembly-average cross sections.
- For the homogenisation of the control rod cells, a heterogeneous supercell model is used, with fuel assemblies surrounding each side of the control rod (see Fig. 3). The flux solution from this heterogeneous case is then used to refine the homogenized cross sections of the control rod cell such that the k-infinity and the flux solution of the heterogeneous problem are reproduced (the SPH method).
- An RZ model of the core is solved using the SP3 method to produce cross sections in a broader group scheme. When used to condense to the standard fast reactor 33 group scheme, this has been found to introduce an error of around 200 pcm relative to a full solution in 172 groups.
- The core solution is performed in hexagonal-Z geometry using CACTUSOT, diffusion theory or the multigroup Monte Carlo method (use of MONK as a module within WIMS). A hexagonal-Z geometry option is also currently being added to the WIMS SP3 solver, to be available within WIMS11, which will allow relatively quick core design calculations to be performed with a low order transport method.

In previous work, the above WIMS methodology with CACTUSOT 3D transport solution has been applied to the OECD/NEA Sodium Fast Reactor benchmark [8] (Fig. 4). Results [9] were in excellent agreement with reported benchmark solutions [10], and selected results are presented in Table III.

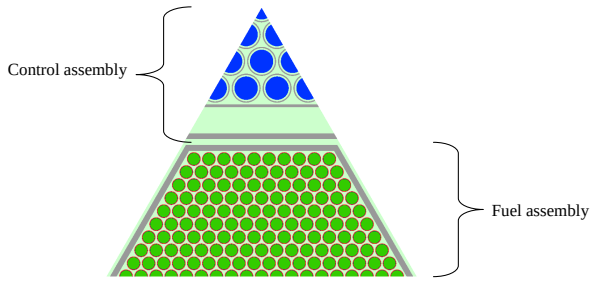

Fig. 3. Supercell calculation for fast reactor control rod cell calculation (from [8], implemented in [9])

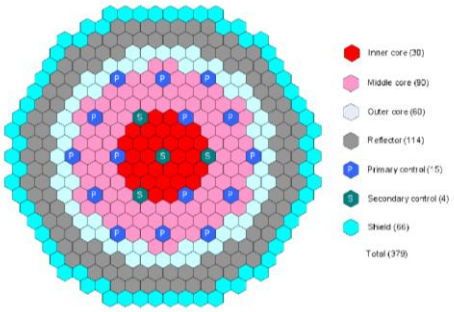

Fig. 4. Medium Oxide-fuelled Core from OECD/NEA SFR Benchmark (reproduced from [8])

	WIMS	**Benchmark (±sd)**
Beginning of Cycle		
k-eff	1.0328	1.0286 (0.0062)
β-eff (pcm)	336	333 (15)
Δρ Sodium Void (pcm)	1972	1831 (228)
Δρ Doppler (pcm)	-825	-730 (70)
Δρ Control Rods (pcm)	21230	21605 (2021)
End of Cycle		
k-eff	1.0154	1.0135
β-eff (pcm)	332	334 (13)
Δρ Sodium Void (pcm)	2187	1922 (220)
Δρ Doppler (pcm)	-781	-718 (74)
Δρ Control Rods (pcm)	21999	22226 (2157)

TABLE III. Results from OECD/NEA SFR benchmark for Medium Oxide-fuelled Core using WIMS [9], compared to reported benchmark solutions [10]

3. Prismatic HTRs

WIMS has the capability to evaluate geometries exhibiting 'double heterogeneity' in cylindrical, pebble and plate geometries, in particular for analysis of TRISO particulate fuel systems. While WIMS has a long-existing capability to perform pebble bed reactor core analysis, current work focuses on developing a full core analysis methodology for 'prismatic' high temperature reactors (HTRs), typically consisting of a hexagonal lattice of fuel compact and graphite moderator blocks, which balances speed and accuracy. Prismatic HTR concepts have been proposed of varying sizes, ranging from gigawatt scale concepts to micro-modular reactors.

Within WIMS, the first stage of a HTR calculation is performed in a simplified version of the 'double heterogeneity' geometry. In both the subgroup treatment and the transport solution, the collision probabilities between different shells of the TRISO particle are first evaluated, followed by the cross particle transmission probability. Surface collision probabilities are then used to combine region-to-region collision probabilities for one or more fuel compact types, moderator fuel pins, coolant holes (if present) and moderator blocks. This collision probability solution is used first to derive shielded multigroup cross sections, and then to solve for the flux.

The current work focuses on developing this 'multi-cell' flux solution towards a full core calculation for a small HTR. This has been performed through a series of computational benchmarks against Monte Carlo calculations. The development calculation route consists of:

- Use of the multi-cell calculation to homogenize the particle/matrix fuel compact.
- Group condensation based on the multi-cell flux solution for the fuel regions + group condensation for the reflector based on a reactor RZ calculation in diffusion theory or the SP3 method.
- Alternatively, method of characteristics calculation for a core slice. Use of flux solution to condense to a smaller number of groups (~10-30)
- 3D transport calculation in a reduced number of groups.

WIMS was been applied to the modelling of the Small Advanced High Temperaturee Reactor (SmAHTR). The AHTR is being developed by ORNL, Sandia National Laboratory and UCB [11]. The reactor concept is similar to the conventional gas-cooled HTR, except that it is filled with liquid salt coolant instead of gaseous coolant. The proposed salt is a mixture of lithium fluoride and beryllium fluoride ('FLiBe'). SmAHTR is a small modular version of the AHTR developed by ORNL [12]. It has a thermal power of 125 MW. It is envisaged to have 19 fuel assembly columns in a hexagonal layout.

The configuration considered here contains annular fuel pins with a graphite tie rod and both internal and external coolant. There are 15 fuel compacts per assembly and 4 graphite rods, arranged in a hexagonal lattice, inside of a circular coolant channel, with 19 coolant channels in the core. A sixth of core model is shown in Fig. 4.

Results from WIMS are compared to a Monte Carlo solution from [13] performed using the Serpent-2 code [14] developed by VTT Technical Research Centre of Finland. In both cases, the ENDF/BVII.0 nuclear data library was used. The results are given in Table IV. Initial k-infinity and discharge burn-up are in excellent agreement, with the fuel temperature coefficient and graphite temperature coefficient also predicted consistently in both analyses. The coolant temperature coefficient predictions differ, although both have the same sign and are of low magnitude.

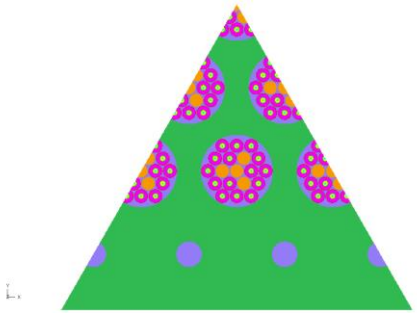

Fig. 4. HTR core slice model used for benchmarking the calculation scheme, based on a small HTR concept with a fluoride salt coolant from Ref. [13].

	WIMS	**Serpent-2 [14]**
k-infinity (fresh fuel)	1.35681	1.36059
Discharge burnup (GWd/t)	98.4	100.2
Fuel temperature coefficient (pcm/K)	-2.04	-1.82
Coolant temperature coefficient (pcm/K)	-0.16	-0.81
Graphite temperature coefficient (pcm/K)	-0.038	-0.024

TABLE IV. 2D core slice calculations for Prismatic HTR

4. Molten Salt Reactors

A calculation methodology has been developed for Molten Salt Reactors (MSRs), with an emphasis on performing rapid neutronics calculations for design studies.

The calculation steps are:

- For thermal MSRs, an equivalence theory calculation is performed for the fuel salt + graphite moderator geometry. For fast MSRs, a homogeneous fine group calculation is performed using the ECCO cell code.
- For thermal MSRs, unit cell calculation using method of characteristics (e.g. Fig. 5), followed by homogenization over fuel and moderator regions.
- The core calculation can be performed in 2D RZ or 3D RTZ geometry using the SP3 (design) or method of characteristics (reference) methods
- A facility has been added to WIMS to allow the user to specify flexibly additional terms in the depletion equations to model online refuelling and chemical processes as continuous processes. A 'batch' refuelling method is also available, and it is possible to adjust the fuel composition automatically and continuously in order to maintain k-effective of unity.

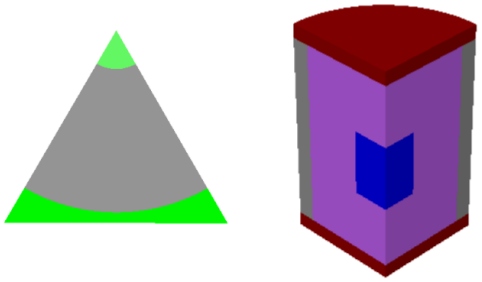

Fig. 5. Unit cell (left) and simplified core geometry (right) for a thermal MSR based on the Oak Ridge MSR [15].

The MSR modelling capability in WIMS is benchmarked here for the case of a fast spectrum MSR with a fluoride fuel salt based on Ref. [16]. The geometry for this design is shown in Fig. 6. This work was principally performed by the UK's National Nuclear Laboratory (NNL).

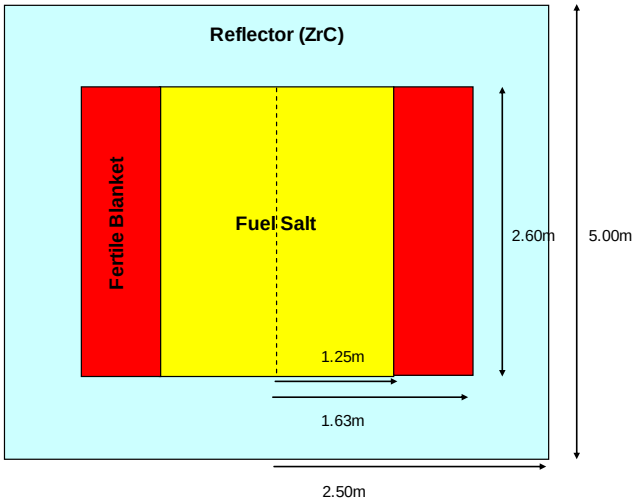

Fig. 6. Fast MSR geometry

The MSR was modelled with two fuel cycle variants: a core initially fuelled with a mixture of Th-232 and U-233, and a core initially fuelled with a mixture of Th-232, Pu and minor actinides (Am, Cm and Np, collectively MAs). In each case, the reactor was refuelled with Th-232 and a period of 200 years was modelled, giving a gradual transition towards an equilibrium cycle. The reactor was modelled with fuel and blanket regions, with the blanket containing a thorium fuel salt. The blanket was replaced annually with fresh thorium fuel salt, hence removing the bred U-233 (and heavier isotopes) from the system. The reactor is therefore a breeder. The fuel salt density is set to 4.3 g/cm^3 in each case, and the reflector density is 6.73 g/cm^3. The core power is 2500 MWth. The loop containing the heat exchangers through which the salt is pumped is considered as an additional out-of-core volume of 6.5 m^3. The beginning of life actinide inventories are given in Table V.

	Th-U	Th-Pu-MA	Blanket
Li-7	6.0760	6.0790	6.0649
F	35.5633	35.5940	35.5828
Th-232	51.8124	39.7799	58.3523
U-233	6.5484		
Np-237		1.1187	
Pu-238		0.1031	
Pu-239		11.0635	
Pu-240		4.2395	
Pu-241		0.2725	
Pu-242		0.5292	
Am-241		0.9948	
Cm-244		0.2259	

TABLE V. Beginning of life actinide inventories (wt%)

The nuclide inventories for the fast MSR over 200 years of operation are of importance when evaluating the system's sustainability with regards to use of nuclear fuel, decay heat and radiotoxicity for geological disposal, etc. To address these issues, NNL have previously developed a model of the fast MSR in the ERANOS fast reactor code [17], and benchmarked this against MCNP, with good results. Assessment of these systems with respect to short and long term implications for waste disposal were discussed in [18].

In the present work, the ERANOS model is itself benchmarked against WIMS under a consistent set of modelling assumptions, namely:

- Use of 1968 group calculation in ECCO cell code to generate 33 group cross sections for homogenous medium
- 3D RZ model with diffusion approximation
- Replacement of all fission products with an equivalent mass of Th-232 on an annual basis. The functionality to perform this refuelling exists within WIMS.

The ERANOS calculations were performed using ERALIB1, which is an adjusted version of JEF-2.2 based on integral experiments [17]. The WIMS calculations were performed using JEF-2.2.

Beginning of life k-infinity results are given in Table VI. There is reasonably good agreement for the Th-U startup core, but a substantial discrepancy for the Th-Pu-MA startup core. This is likely attributable to data library differences. In particular, ERALIB1 contains adjusted data for Pu nuclides (aimed at enhancing its accuracy for fast reactors), but not for Th-232 and U-233, and hence results may be expected to diverge more from JEF-2.2 for the startup core containing Pu. ERALIB1 also contains adjusted data for Zr and C, both of which are present in the reflector. Over the 200 years of operation, the difference in beginning of cycle k-effective rises to 1-2% as a result of slight long term deviations in the actinide inventories.

	Th-U startup core	Th-Pu-MA startup core
ERANOS	1.06069	1.02273
WIMS	1.06650	1.03949

TABLE VI. Beginning of life k-effective for different cores in WIMS and ERANOS

Actinide inventory results for this benchmark problem are given in Figs. 7 and 8 for the Th-U startup core and Figs. 9 and 10 for the Th-Pu-MA startup core. In general, excellent agreement in key nuclide inventories is observed. There are some discrepancies in nuclide inventories for MAs, which are likely attributable to nuclear data library differences. For the Th-U start-up core, the U-233 breeding rate in the blanket was used to calculate the doubling time for fissile fuel – this was calculated as 55 years and 54 years with ERANOS and WIMS respectively, and hence the codes were in good agreement.

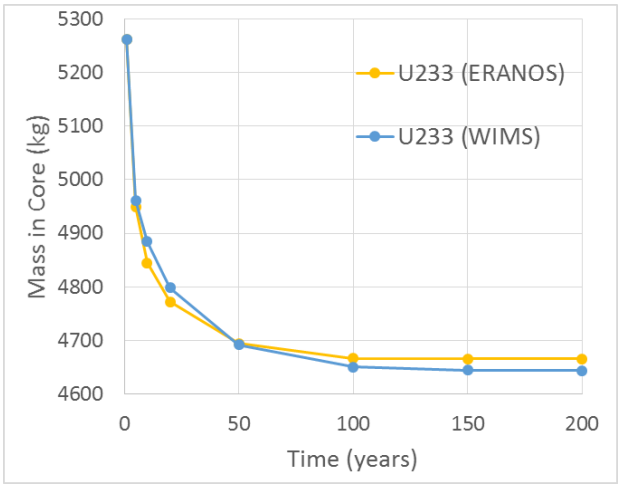

Fig. 7. U-233 inventory in Th-U startup core

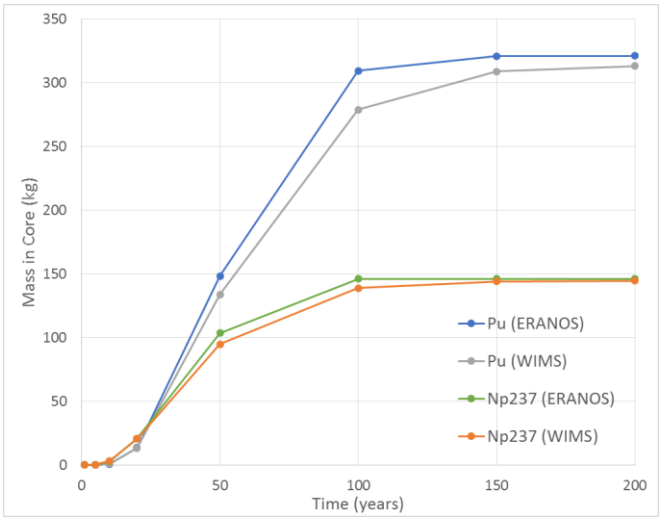

Fig. 8. Selected transuranic inventories for Th-U startup core

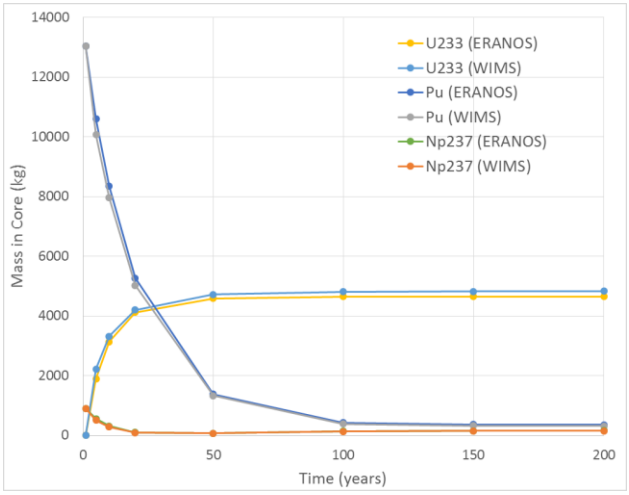

Fig. 9. Selected actinide inventories for Th-Pu-MA startup core

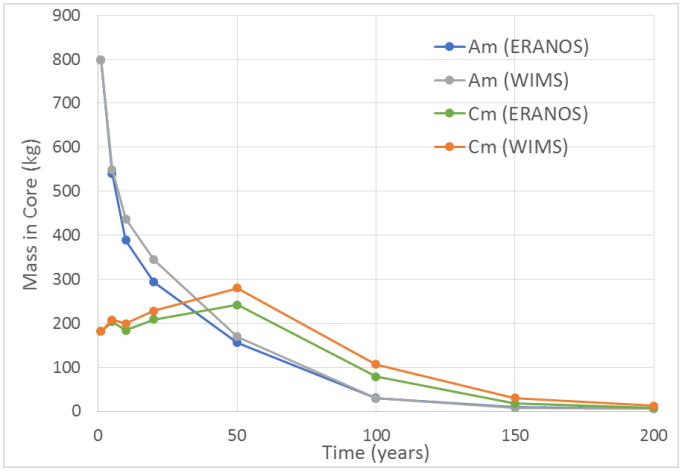

Fig. 10. Am and Cm inventories for Th-Pu-MA startup core

The refuelling scheme utilized in these calculations is an approximation to the online refuelling which is typically proposed for molten salt reactors. Within WIMS, online refuelling was modelled by two separate methods:

(1) Adding additional artificial decay terms to the Bateman Equations in the depletion solver

(2) Looping between the 'batch' refuelling process utilized previously and the depletion solver over a fine timestep during the depletion calculation.

As expected, use of either method results in some divergence from the WIMS and ERANOS solutions given in Figs. 7-10 as the refuelling scheme is different. However, the methods are in excellent agreement with each other, as shown in Table VII. Minor remaining differences, for example in the very small Am and Cm populations, are potentially caused by residual 'batch' effects for Method (2) above.

Years	Th-232	U-233	Pa-233	Np-237	Pu	Cm	Am
5	0.01	-0.09	-0.11	0.00	0.00	0.00	0.00
10	0.02	-0.13	-0.06	0.42	0.00	0.00	0.00
20	0.02	-0.15	-0.03	0.34	0.46	0.00	0.00
50	0.02	-0.13	-0.02	0.22	0.43	0.00	0.00
100	0.01	-0.09	-0.01	0.22	0.56	1.60	1.21
150	0.01	-0.04	0.00	0.35	0.79	1.79	1.40
200	0.00	0.00	0.01	0.52	1.11	2.29	2.00

TABLE VII: % Difference in actinide populations for continuous refuelling by (1) addition of artificial decay terms to the Bateman equations and (2) discrete fuelling every 0.1 years.

Finally, the effect of different core solution methodologies in WIMS was evaluated, through use of the SP3 method and, separately, increasing the number of groups used in the core solution from 33 to 172. The results of this study are shown in Table VIII for beginning of cycle 1 k-effective. The difference between the diffusion and SP3 methods is very small at around 15 pcm. Increasing the number of groups in the core calculation from 33 to 172 results in a difference in k-effective of ~200 pcm. This is not unexpected as condensation to a smaller number of groups at the cell level can be expected to incur some error due to the effect of leakage on the neutron spectrum that is typical for a fast reactor.

	Diffusion	**SP3**
33 groups	1.06650	1.06665
172 groups	1.06429	1.06446

TABLE VIII. Beginning of life k-effective for the Th-U fuelled MSR core, with different WIMS core calculation methodologies.

IV. ADDITIONAL IMPROVEMENTS

1. Support for Large Calculations

With increasing computational resources there has been a growing trend for performing transport calculations on larger problems, up to and including 3D full core models. As a result, it is becoming increasingly common for transport calculations to be performed in parallel on HPCs. A number of the WIMS modules have been parallelized to allow efficient performance for whole core calculations, including CACTUS, the 3D multicell collision probability calculation, and the depletion equation solver.

2. Visual Workshop

Visual Workshop is the ANSWERS tool for visualising and verifying model geometries using 2D and 3D ray-trace

views and a 3D wire-frame display. A particular benefit of this tool is that the ray tracing engine is built from the same geometry source code as the physics models giving maximum possible confidence that the model geometry as displayed is the same as that sampled by the physics codes.

Visual Workshop also contains an input file editor, and a tool for running calculations, thus forming a complete integrated development environment for WIMS and other ANSWERS products. A capability to display results graphically is under development.

WIMS is distributed with tools which facilitate input preparation for performing lattice calculations for whole core calculations for PWRs, VVERs and AGRs based on an engineering description of the fuel assembly. This is currently being extended to BWRs, with a view to consolidating these tools within Visual Workshop.

A major new feature in the next version of Visual Workshop (version 3C) will be a tool known as SPRUCE. This is designed for uncertainty analysis and allows multiple calculations to be run in serial or parallel, where parameters defining the model geometry and material compositions are sampled from statistical distributions. The uncertainty analysis capability described in Section II.4 is integrated within Visual Workshop, giving the user access to a range of uncertainty quantification methodologies.

3. Whole core model input preparation

The generation of whole core/ core slice models is facilitated by the inclusion of additional input preparation facilities through GEOM, a new module within WIMS. This allows an engineering description of the problem to be input, with calculation methodology handled internally. The calculation steps, described below, are similar to those used in a conventional lattice calculation in WIMS.

- Resonance shielding using equivalence and, optionally, subgroup methods.
- Generation of a condensation spectrum using a 3D multicell collision probability method.
- Condensation from 172 groups to a smaller number of groups (22 is typical)
- Main transport solution with CACTUS or SP3 (2D); CACTUSOT, MDLTRAN or SP3 (3D).

GEOM contains several capabilities designed to facilitate performing full core analysis, including handling of:

- Definition of control rods in single groups or banks
- Control rod movement
- Burn-up with automated reshielding for through-life calculations
- Capability to export data on a thermal mesh via HDF5 (see below) for use in an external thermal-hydraulic code to treat thermal feedback effects.
- Capability to link to the WIMS subchannel thermal-hydraulic solver under development
- Capability to perform critical searches on soluble boron, rod position and water height.

4. Improvements to Gamma transport solver

Power deposition in WIMS can be treated through following neutrons and/or photons to their point of interaction. Photon transport can be treated using a deterministic approach in CACTUS with an isotropic scatter assumption, or using a Monte Carlo approach with explicit treatment of anisotropic scatter. The Monte Carlo solver has the capability to treat PWR and cluster geometries.

Explicit treatment of energy deposited in gamma emission and deposition is necessary to calculate accurately the energy produced through fission. The simplest treatment available in WIMS is to use isotope specific 'Q values' for energy-per-fission and assume all energy (gamma + neutron) is deposited at the point of fission. A more accurate treatment is available using a coupled neutron and gamma transport calculation. This allows more accurate calculation of burn-up dependent assembly powers.

The improved heat deposition methodology has been applied to treatment of a part MOX-fuelled PWR core. With a neutron transport calculation, the calculated fission rate in the MOX assembly instrumentation tube fission chambers is generally calculated as being about 3% low on average compared to detector measurements. Coupled neutron-gamma transport calculations have been used to demonstrate that this is in large part attributable to gamma transport effects. While the neutron response of detectors placed within the core is typically larger for the UO_2 assemblies due to their more thermal spectrum, the gamma response in UO_2 and MOX assemblies is very similar. Supercell calculations have been used to demonstrate that the gamma response can account for most of the described discrepancy between predicted and measured detector response.

5. HDF5

The capability to store and export data via HDF5 has been added to WIMS, improving the capability to manage and transfer data and interface WIMS with other codes.

V. CONCLUSIONS

The WIMS reactor physics code is under continuous development. A current priority is development of a whole core transport capability based on:

- New and improved 3D transport solvers with support for large calculations, in particular the CACTUSOT 3D method of characteristics transport solver.
- Development of a thermal-hydraulic feedback capability within the code

- Developing whole core calculation methodologies within WIMS for a range of reactor types, including fast reactors, high temperature reactors and molten salt reactors.

Methodologies to assess uncertainties due to nuclear data and engineering tolerances are being developed for incorporation within WIMS11 and Visual Workshop. Uncertainty quantification capabilities include:

- Direct perturbation of the nuclear data libraries based on the covariances during the production of WIMS nuclear data libraries from the underlying nuclear data evaluations.
- Derivation of sensitivity coefficients of reactor physics parameters to group and nuclide dependent cross sections with consistent treatment of shielding, and combination with the covariance library to generate overall uncertainty.
- Tools to support sampling of uncertainties in a general sense, along with associated postprocessing.

In this paper, these capabilities are demonstrated through:

- Application of the CACTUSOT solver has been applied to an OECD/NEA benchmark variant of the C5G7 problem, with good results.
- Solution to an OECD/NEA SFR benchmark problem with WIMS
- Demonstration of a core slice calculation for a prismatic HTR concept
- Application of WIMS to the analysis of a fast-spectrum MSR core, including verification and benchmarking of the online refuelling methodologies that have been implemented within WIMS.

REFERENCES

1. J. R. ASKEW et al., "A general description of the lattice code WIMS," *Journal of the British Nuclear Energy Society,* Oct 1966.
2. P. HUTT et al., "The UK Core Performance Code Package," *Nuclear Energy, J. British Nuclear Energy Society,* vol. 30, p. 291, 1991.
3. G. RIMPAULT, "Algorithmic Features of the ECCO Cell Code for Treating Heterogeneous Fast Reactor Subassemblies," in *International Topical Meeting on Reactor Physics and Computations, Portland, Oregon*, May 1-5, 1995.
4. J. G HOSKING et al. "CACTUSOT: A 3D Method of Characteristics Solver in WIMS". *Submitted to M&C2017*
5. T. GORLEY et al., "Initial MCNP6 Release Overview - MCNP6 Version 1.0," LA-UR 13-22934, 2013.
6. OECD NUCLEAR ENERGY AGENCY "Benchmark on Deterministic Transport Calculations Without Spatial Homogenisation: MOX Fuel Assembly 3-D Extension Case" OECD Nuclear Energy Agency, Paris, France, 2011.
7. A. COPESTAKE, "A consistent diffusion synthetic accelration technique using discontinuity factors". *M&C2009, Saratoga Springs, NY, May 3-7 2009.*
8. D. BLANCHET et al. , "AEN - WPRS Sodium Fast Reactor Core Definitions (version 1.2 - September 19th)," OECD Nuclear Energy Agency, Paris, France, 2011.
9. B. STRAY et al., "Solution of the OECD/NEA SFR Neutronic Benchmark using WIMS and MONK," in *PHYSOR2016,* Sun Valley, ID, USA, May 1-5, 2016.
10. N. E. STAUFF et al., "Evaluation of the Medium 1000MWth Sodium-Cooled Fast Reactor OECD Neutronic Benchmarks," in *PHYSOR2014,* Kyoto, Japan, Sep 28 – Oct 3, 2014
11. C. W. FORSBERG, "The Advanced High-Temperature Reactor: High-Temperature Fuel, Molten Salt Coolant, and Liquid-Metal Reactor Plant," in *1st COE-INES Int Symp on Innovative Nuclear Energy Systems for Sustainable Development of the World*, Oct 31 - Nov 4, 2004.
12. D. ILAS et al., "SmAHTR-CTC Neutronic Design," in PHYSOR 2014, Kyoto, Japan, Sept 28 - Oct 3, 2014.
13. D. KOTLYAR, B. A. LINDLEY and H. MOHAMED, "Improving fuel utilization in SmAHTR with spectral shift control design: proof of concept," *Annals of Nuclear Energy In Press*
14. J. LEPPANEN, M. PUSA, T. VIITANEN, V. VALTAVIRTA and T. KALTIAISENAHO, "The Serpent Monte Carlo code: Status, development and applications in 2013," *Annals of Nuclear Energy,* vol. 82, pp. 142-150, 2015.
15. J.R. ENGEL et al., *Conceptual Design Characteristics of a Denatured Molten-Salt Reactor with Once-through Fuelling*, Technical Report. ORNL/TM-7207, Oak Ridge National Laboratory, Oak Ridge, TN, USA(1980)
16. S. DELPECH et al., *Reactor physic and reprocessing scheme for innovative molten salt reactor system,* Journal of Fluorine Chemistry 130 (2009) 11-17
17. G. RIMPAULT. *European ERANOS formulaire for fast reactor core analysis,* 4th RCM meeting on updating codes and methods to reduce the calculational uncertainties of the LMFR reactivity effects, IPPE, Obninsk, 19-23 May 2003.
18. K. HESKETH and M. THOMAS, *The Potential Role of the Thorium Fuel Cycle in Reducing the Radiotoxicity of Long-Lived Water – 13477*, WM2013 Conference, Feb 24-28 2013, Phoenix, Arizona, USA.