IMPROVEMENTS TO MONK & MCBEND ENABLING COUPLING & THE USE OF MONK CALCULATED ISOTOPIC COMPOSITIONS IN SHIELDING & CRITICALITY

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ABSTRACT

Isotopic composition through time can be derived for 3D reactor core configurations using the Monte Carlo Criticality and Reactor Physics code MONK. MONK can be coupled to thermal-hydraulics (TH) codes (e.g. RELAP5) to model temperature feedback and coupled to the Monte Carlo radiation transport code MCBEND for onward neutron and/or gamma calculations. MONK derived isotopic compositions can be directly and automatically transferred to another MONK or MCBEND model for either subsequent:

- burn-up steps or branching calculations with MONK using the same 3D whole core model;
- shielding calculations with the compositions transferred to MCBEND utilised as elemental compositions of reactor components or fuels (for example in the case of a fuel flask or waste storage facility);
- criticality calculations with the compositions transferred to another MONK model .

Results from a typical whole core PWR calculation with MONK are presented demonstrating MONK TH code coupling and generating burnt-up isotopic compositions. The compositions from three PWR fuel assemblies were automatically transferred to separate MCBEND and MONK models of a fictitious SNF facility performing shielding and criticality calculations respectively. Results are presented to demonstrate the reactivity differences and how burn-up credit may be used.

An innovative scheme for speeding up MONK and improving resolution of MONK burn-up/TH meshes utilising parallel computing architecture is described. This will enable refinement of isotopic composition variations even further. The parallelisation scheme utilises a novel domain decomposition method, enables optimisation for user controlled calculation speed adjustment and has the potential for adaptive meshing.

Key Words: MONK, MCBEND, criticality, shielding, thermal-hydraulics

1   INTRODUCTION

This paper is split into 4 parts

1. Description of the PWR whole core calculation with TH (thermal hydraulics) feedback

2. Description of a SNF storage facility model with compositions for SNF from either the PWR whole core calculation or using non-burnt-up fuel
3. Comparison of results between SNF compositions and non-burnt-up fuel using MONK [1] and findings from the MCBEND [2] calculation
4. An innovative solution utilising parallel computing architecture for speeding up MONK and improving the resolution of the burn-up and TH meshes in MONK

2   DESCRIPTION OF THE PWR WHOLE CORE CALCULATION WITH TH FEEDBACK

MONK has been enabled to couple to a TH code so that calculations of k-effective, spatial dependent fluxes, powers and isotopic compositions can be calculated at discrete times taking account of the feedback from the TH code model.

A detailed whole core model of a PWR based upon publicly available information (from the UK HSE website) was created. The geometry model used simple body geometry.

The basis of the coupling method is as follows. An XYZ mesh is overlaid over the MONK geometry. This XYZ mesh represents a mesh for linking to the Thermal-Hydraulics code (hence is called the TH-mesh) and within a given mesh element the power is calculated in MONK. This power distribution is then fed into a TH code which in turn returns the relevant temperatures and densities of the materials in the mesh element.

In addition to the TH-mesh another XYZ mesh is overlaid which is combined with the TH-mesh. This enables the user to define a finer mesh for burn-up. This is called the BU-mesh. The BU-mesh is combined with the TH-mesh to form a BUTH-mesh.

The materials for the MONK geometry are defined by the user in the usual way, however the code then recognises that the user defined material in a given BUTH-mesh element will (as time goes by) burn-up differently and have a different temperature and density to the same user defined material in another BUTH-mesh element. The code therefore converts every user defined material inside each BUTH mesh element to a new "Artificial Material" which as time goes by will have its own isotopic composition at each time step of the calculation.

The PWR MONK model created represents the largest number of mesh elements and Artificial Materials that can be utilised with this model running on a 32 bit Windows PC with a 4GB RAM. This used a 3 x 3 x 10 BUTH Mesh. The calculation of k-effective for each time step typically took 8 or 9 hours. These aspects of the method mean that using serial computing technology with a 32 bit version of MONK leads to limitations that restrict the resolution of the burn-up mesh and TH mesh in MONK. In addition the inherently long execution times (as with any Monte Carlo calculation) are increased by coupling to a TH code and performing time-dependent calculations to derive burnt-up fuel compositions.

A method currently being developed which could mitigate these limitations (in regard MONK execution times and the resolution of the MONK model) is discussed in the final section of this report. The method is an innovative solution utilising parallel computing architecture; a novel domain

decomposition and potential for optimisation of user controlled calculation speed adjustment and adaptive meshing.

The MONK model is nevertheless very detailed with every attempt to model individual pins in fuel elements with grid straps and absorber rods. The 157 fuel elements were modelled in an explicit layout inside a steel reactor pressure vessel. Pictures of the geometry (using Visual Workshop [3]) showing various aspects of the geometry model are shown below.
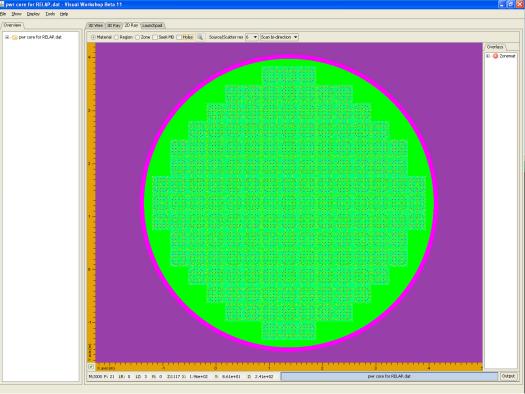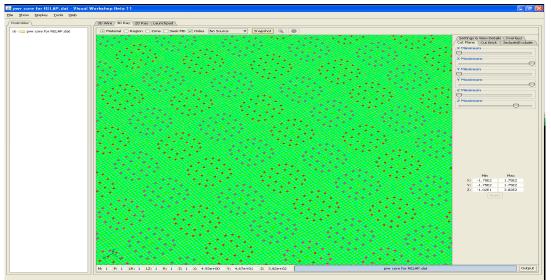

Figure 1. PWR Model Whole Core layout

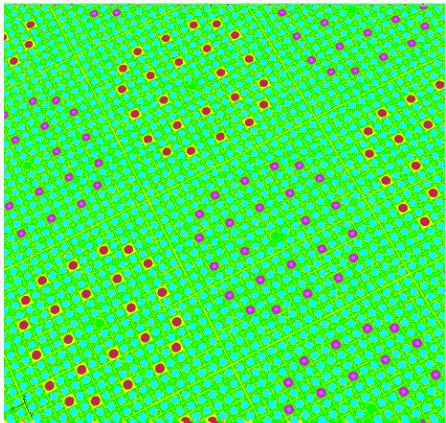**Figure 2. Close up of the core layout**

Figure 3. Core layout showing elements with RCCA, GRAY control rod assemblies and fuel assemblies with burnable absorber
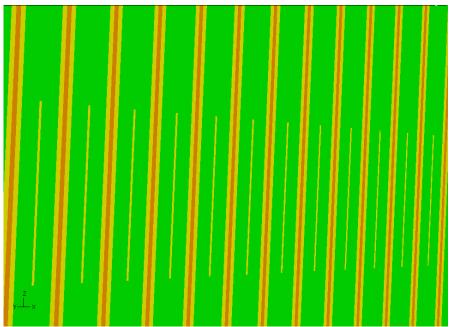

Figure 4. Rods and grid straps.

3   DESCRIPTION OF A SNF STORAGE FACILITY MODEL WITH COMPOSITIONS FOR SNF FROM EITHER THE PWR WHOLE CORE CALCULATION OR USING NON-BURNT-UP FUEL

The MONK model of the SNF facility (SNFF) is 3 fuel elements taken from 3 different parts of the PWR core after 360 days burn-up and 60 days cooling and stored in water surrounded by a steel vessel. The fuel elements are taken from the XY grid positions in the whole core PWR TH-mesh: (1,2), (2,2) and (3,2).

There are two calculations: one for burnt-up fuel and the second for fresh fuel. For the first calculation the material data is the Artificial Material composition for each fuel element extracted from the ARCHIVE file for the final time step of the whole core PWR calculation. The axial variation of fuel compositions is determined in the whole core calculation in 8 "z-slices". The geometry of the fuel elements is split into 8 "z-slice" sections and the appropriate material automatically extracted from the ARCHIVE file and allocated to the appropriate "z-slice". For the second calculation fresh fuel is used.

Visual Workshop [3] pictures of the geometry are shown below. Both models aim to calculate k-effective for each system with a view to comparing the resulting values.
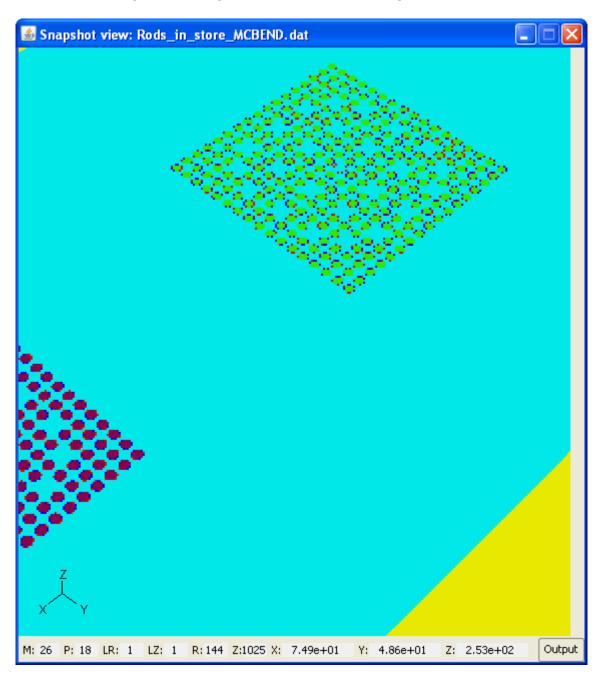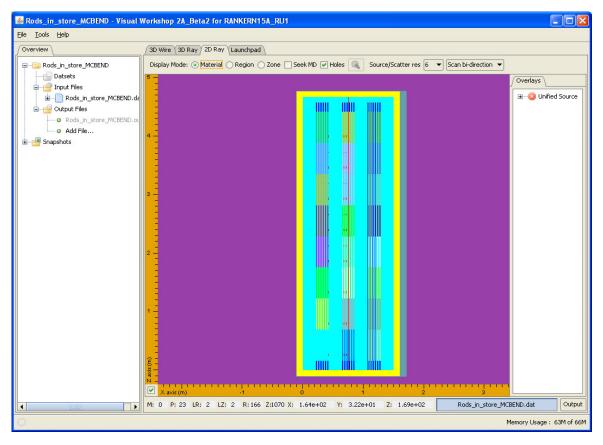
Figure 5. Showing 3 fuel elements in water through a z-slice view

Figure 6. Showing a magnified image of 2 of the fuel elements shown in Figure 5
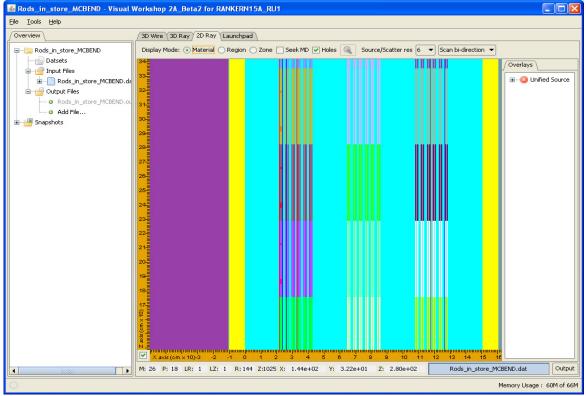
Figure 7. Axial variation of materials (bottom picture magnification of the top

The MCBEND geometry model of the SNFF is identical to that used for MONK. The gamma source used is based on an estimated source distribution. This is because (unlike the MONK-MCBEND-MONK burn-up calculation where the models are identical and the power distribution is identical) there is no source intensity or source spectrum available for such a model at present, although methods are being investigated.

The aim of the MCBEND calculation is to demonstrate that isotopic material compositions for spent fuel are successfully transferred from the whole core PWR model with MONK into the SNFF model MCBEND gamma shielding calculation. Nevertheless to demonstrate that the method can be used to calculate gamma dose rate, a nominal source distribution (with energy greater than 0.1 MeV) was used based upon an assessment of the isotopes in the compositions.

Dose rate contribution was calculated for energies greater than 0.1 MeV in a region on the outside of the steel vessel wall, in order to demonstrate the method.

4   RESULTS

4.1 MONK Whole Core Model

The figure below shows a histogram of the power distribution across the PWR core at z-mesh =5 (i.e. mid way axially) in the 3x3 XY variation of the TH Mesh.
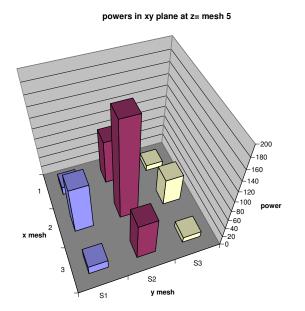

Figure 8. Power distribution mid axial plane

Neutron activation analysis of Nd148 is used as an indicator of burn-up in irradiated uranium fuel. Nd148 number density in the fuel increases as the fuel in the core burns up. The whole core PWR model has a burn-up mesh of 3x3 in the XY plane and the fuel is sliced into 8 axial meshes. This means that there are effectively 72 fuel materials (i.e. 3x3x8) in the core. The following figures show how the Nd148 and U235 vary over the first 4 burn-up steps in all the 72 fuel materials.
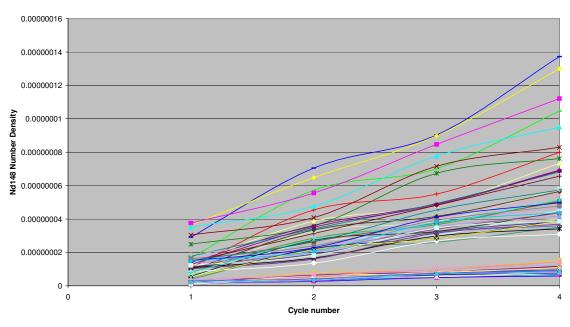
ND148 v BU Cycle

FIGURE 9. Nd148 variation over the first 4 burn-up steps in all the 72 fuel materials
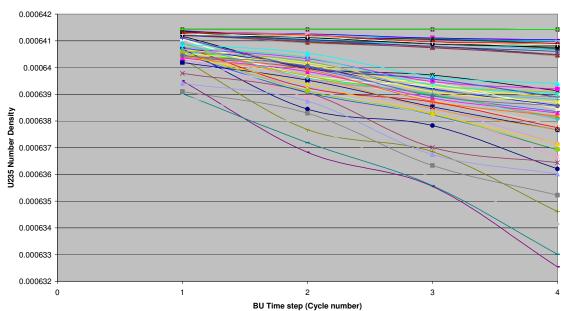
U235 Burnup

Figure 10. U235 variation over the first 4 burn-up steps in all the 72 fuel materials

4.2 MONK to MONK and MONK to MCBEND Findings

Material compositions were successfully transferred to the MONK model and checked to be identical to those in the ARCHIVE file. The results for k-effective below demonstrate that using the depleted fuel leads to a reduction in reactivity of 4% of the reactivity of fresh fuel.

- The k-effective for the burnt-up fuel case is 0.6975 (std. deviation = 0.0002)
- The k-effective for the fresh fuel case is 0.7254 (std. deviation = 0.0002)

Material compositions were successfully transferred to the MCBEND model and checked to be identical to those in the ARCHIVE file. The dose rate at the desired position was calculated.

5   AN INNOVATIVE SOLUTION UTILISING PARALLEL COMPUTING ARCHITECTURE FOR SPEEDING UP MONK AND IMPROVING THE RESOLUTION OF THE BURN-UP AND TH MESHES IN MONK

A Monte Carlo neutron tracking process can be broken down into individual processes. The Figure below demonstrates how this can be done for a Monte Carlo method that uses weighted tracking where the entire geometry model is defined as a HOLE (i.e. a region where all tracking uses Woodcock Tracking [4]).
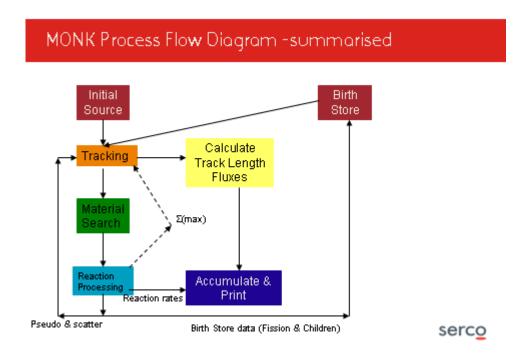

Figure 11. MONK Process flow diagram

This process flow diagram can be converted into a plan for using parallel processing as shown in Figure 12.
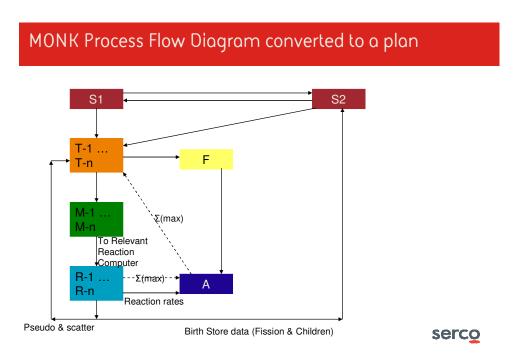
Figure 12. MONK Process flow diagram converted to a plan

Each of the individual boxes represents one or more cores. The function of each individual process running on an individual core is described as follows.

S1 = Generates the source particle data in the first stage and every alternate subsequent stage. In the second stage (and every alternate stage subsequent to the second stage) it acts as the birth store.

S2 = similar to S1 but only starts generating source in the second stage. This is because it acts as the birth store in the first stage.

T-1:T-n = These are the TRACKING computers. They receive data from S1/S2, calculate collision point data and pass this on to the next available MATERIAL SEARCH computer. (These can also pass track length data to the FLUX computer)

M-1:M1n = These are the MATERIAL SEARCH computers. They search for the material number at the collision point and pass the data on to the relevant REACTION computer. Very complex geometries can be defined using MONK and by utilising the MONK geometry tracking routines in the coding accessed by these computers the appropriate Artificial Material number can be obtained for whatever geometry model MONK is capable of modelling.

R-1:R-n = These are the REACTION computers. Each one processes collisions only in a given range of the Artificial Materials. This enables them to hold only a limited amount of the nuclear data (which is the main source of the large RAM requirement). They also send pseudo collision and real scattered particles back to the TRACKING computers; reaction rates to the ACCUMULATOR computer; and birth store data to the relevant SOURCE computer S1 or S2.

A and F = These are the ACCUMULATOR and FLUX computers respectively. These process reaction rates and fluxes and control when results are printed.

Only the REACTION computers need the nuclear data, the TRACKING computers require none of the nuclear data (only maximum cross sections) and none of the geometry data. Only the MATERIAL SEARCH computers need to know the geometry model. This aspect of the design enables a method of Domain Decomposition based upon Artificial Material number. Within the geometry model there could be thousands of Artificial Materials. By allocating a proportion of the total number of Artificial Materials to a single core and increasing the number of cores dealing only with nuclear data will enable significant improvement to the resolution of the burn-up and TH meshes in MONK. Utilising parallel computing will significantly reduce execution times required to run a single Monte Carlo calculation.

6   CONCLUSION

It has been demonstrated that it is possible to model a whole core reactor with MONK and include TH feedback by coupling MONK to a TH code. However there are currently some limitations that restrict the resolution of the burn-up mesh and TH mesh in MONK. In addition the inherently long execution times in any Monte Carlo calculation are increased by coupling to a TH code and performing time-dependent calculations to derive burnt-up fuel compositions.

It has further been demonstrated it is possible to automatically extract burnt-up material compositions from such a whole core reactor calculation and utilise in a storage facility model to perform either a criticality calculation (using MONK) or a shielding calculation (using MCBEND). By comparison with calculations using the same geometric model but fresh fuel compositions we have demonstrated the potential benefits of taking credit for burn-up.

Finally a method is currently being developed which could mitigate the limitations (referred to above) in regard MONK execution times and the resolution of the MONK model. This method is an innovative solution utilising parallel computing architecture; a novel domain decomposition and potential for optimisation of user controlled calculation speed adjustment and adaptive meshing.

7   REFERENCES

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