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Abstract

As nuclear fusion progresses towards a sustainable energy source and the power of tokamak devices increases, a greater understanding of the radiation fields will be required. As well as on-load radiation fields, off-load or shutdown radiation field are an important consideration for the safety and economic viability of a commercial fusion reactor. Previously codes such as MCR2S have been written in order to predict the shutdown dose rates within, and in regions surrounding, a fusion reactor. MCR2S utilises a Constructive Solid Geometry (CSG) model and a superimposed structured mesh to calculate 3-D maps of the shutdown dose rate. A new approach to MCR2S calculations is proposed and implemented using a single unstructured mesh to replace both the CSG model and the superimposed structured mesh.

This new MCR2S approach has been demonstrated on three models of increasing complexity. These models were: a sphere, the ITER computational shutdown dose rate benchmark and the DEMO computational shutdown dose rate benchmark. In each case the results were compared to MCR2S calculations performed using MCR2S with CSG geometry and a superimposed structured mesh. It was concluded that the results from the unstructured mesh implementation of MCR2S compared well to the CSG structured mesh calculations. It was found that the resolution of the unstructured mesh can significantly affect the results of the calculations, and therefore it is important to finely mesh components which contribute to the dose rate in the areas of interest. Although computationally more expensive it was found that there are some clear advantages when using unstructured meshes with MCR2S calculations which are outlined in this paper.

Keywords: MCR2S, Unstructured Mesh, Neutronics, Shutdown Dose

1. Introduction

Nuclear fusion is the process that powers the stars. If we could harness this process in a safe and sustainable way here on Earth it has the potential to fulfil a large portion of our energy needs. On the path to a commercial magnetic confinement fusion reactor will be a prototype DEMOnstration reactor (DEMO). It is predicted that devices such as DEMO will be capable of operating at fusion powers between 2.5 and 5 GW and produce more than 10^{21} neutrons per second. This is 1000 times greater than the neutron output from the current Joint European Torus (JET) and about 5-10 times greater than ITER, a fusion research reactor currently being built in the south of France.

Neutrons are one of the primary methods of transferring energy out of the plasma and also allow tritium, which makes up part of the fusion fuel, to be created in breeder blankets. However these neutrons also create large on-load neutron and prompt photon radiation fields which require evaluating in order to ascertain the dose rates to personnel.

During on-load operations the neutron flux causes significant material activation to occur in the reactor and surrounding structures. Activation products build up while the reactor is on-load and continue to decay during off-load periods. The decay of activation products creates a photon source which is present even when the reactor is shutdown. This source is known by many terms including ‘off-load’, ‘decay’, ‘activation’ and ‘shutdown’ photon source and can lead to radiation fields during shutdown in areas where personnel access is required for operations and maintenance purposes.

In order to meet the As Low As Reasonably Achievable (ALARA) requirements, stringent limits are placed on occupational exposure to radiation and it is therefore essential during the design and engineering of new fusion reactors to take these limits into account. As part of this process of demonstrating compliance with these limits it is necessary to have validated, robust, reliable and efficient computational codes to estimate the radiation fields both on- and off-load.

Estimating on-load neutron and prompt photon radiation fields can be carried out with a range of standard particle transport codes, such as MCNP [1]. In order to accurately calculate shutdown radiation fields, several methods requiring the coupling of radiation transport codes with an inventory code have been developed. These include the ‘advanced direct-one-step’ or Advanced D1S method [2] and the ‘rigorous-two-step’ or R2S method [3]. This report concerns the R2S method only.

The R2S method couples neutron flux and energy spectra results, from a particle transport code, with an activation code. At CCFE the R2S method has been implemented in the form of the Mesh Coupled Rigorous Two Step [4] (MCR2S) code. MCR2S couples neutron flux data from MCNP with the activation capabilities of FISPACT-II [5], currently via the use of a superimposed structured mesh tally. MCR2S can be used to produce 3-D maps of the activation, nuclear inventory and shutdown photon source, with the shutdown photon source being used in a subsequent MCNP calculation to determine shutdown dose fields.

A full description of the MCR2S process can be found in previous papers [4] but the process follows these basic steps:

1. A structured rectangular mesh superimposed onto a Constructive Solid Geometry (CSG) model is used in MCNP to track neutrons throughout regions of interest while the reactor is on-load. The structured rectangular mesh is used to record the neutron flux and energy spectrum during on-load operations.
2. Activation calculations are carried out for a given irradiation and decay schedule using the flux, energy spectrum and material in each structured mesh voxel. The results of these activation calculations are collated to create a shutdown photon source within the structured mesh.
3. The CSG model and the shutdown photon source are used in MCNP to track the shutdown photons and calculate the shutdown dose rate in the areas of interest.

Although the current MCR2S method can be used to produce reliable and accurate shutdown dose rate results, one issue with this approach is the superimposed structured mesh does not necessarily conform to the shape of the geometry. This can result in mesh voxels containing a mix of materials, large sections of void or regions of significantly different neutron flux, particularly where the geometry is complex. Depending on the mesh resolution, this can lead to some parts of the geometry having predicted levels of activation significantly higher or lower than the ‘true value’. The use of superimposed meshes also fails to resolve small features, such as streaming paths, where increased neutron fluxes are effectively homogenised into the neighbouring material regions.

With the addition of an unstructured mesh capability to MCNP6 it is now possible to describe geometry using a volumetric unstructured mesh. This mesh can be used not only to track particles but also to record the neutron flux and energy spectrum. Instead of superimposing a structured mesh, activation calculations can be carried out on each of the unstructured mesh elements and the results can be collated to create a shutdown photon source.

The main advantage of using an unstructured mesh, over a rectangular superimposed mesh, for MCR2S type calculations is the mesh is conforms to the geometry. This means the recorded neutron flux values are more realistic as there is no flux averaging between areas of void and material each element only has a single material. Additionally, the use of unstructured meshes allows for more complex shapes to be modelled as the user is not limited to analytical surfaces. It also has benifits for geometry creation time, with more geometrically complexity able to be modelled with less user effort when compared to CSG.

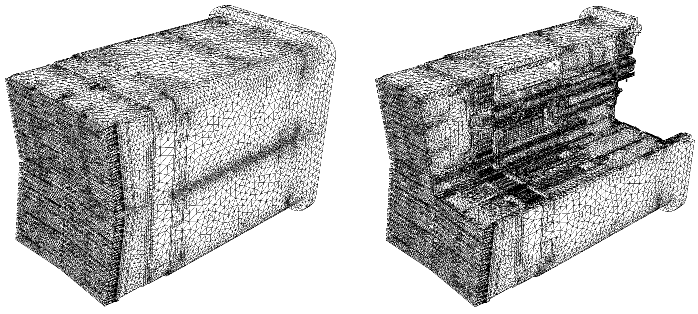
In order to investigate some of these advantages, as well as any potential disadvantages, the MCR2S code has been modified. The modifications allow MCR2S to read in neutron flux and energy spectrum results, as well as element material, density and volume from the MCNP6 unstructured mesh output file. MCR2S creates a gamma source file which is then read by a new MCNP6 unstructured mesh photon source routine.

This paper details the modifications made to the MCR2S code and presents the number of test cases. The results of the test cases are compared to results gained using the structured mesh approach and conclusions are drawn.

2. MCR2S Unstructured Mesh Implementation

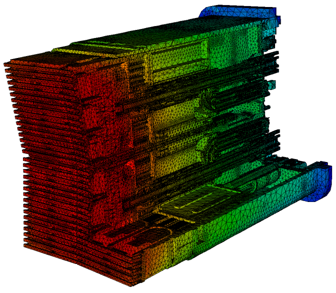
2.1. Unstructured Meshes

In order to carry out unstructured mesh shutdown dose rate calculations the on-load neutron flux needs to be calculated using an unstructured mesh model. Unlike CSG, where analytical surfaces and Boolean operations are used to define regions/cells, unstructured meshes allow the user to define geometry by splitting solids up into many small pieces known as elements. For a sufficient spatial resolution, these elements combine to give a good approximation of the original geometry. An example of an unstructured mesh geometry is given in Figure 1 where the ITER Ion Cyclotron Resonance Heating (ICRH) Antenna has been meshed.



(a) ICRH Mesh

(b) ICRH Mesh Internal Mesh



(c) ICRH Mesh with neutron flux results

Figure 1: An example of an unstructured mesh.

Unstructured meshes are constructed from 3-D CAD models using readily available meshing programs such as ABAQUS [6], ANSYS [7] or CUBIT [8]. The ICRH mesh has been made from approximately 3 million tetrahedral elements but it is possible to utilise other element types such as tetrahedral, pentahedral and hexahedral shaped elements.

The unstructured mesh routines implemented in MCNP6 use an Abaqus type unstructured mesh [9]. The Abaqus mesh file essentially contains information on the location of the nodes and their connectivity to form elements. The unstructured mesh utilises the universe structure in MCNP6. This allows the unstructured mesh to be defined in its own geometric space/universe and then embedded into a CSG model, thus both geometry types may be in the same model if required.

2.2. *MCR2S Modifications*

Modifications to implement shutdown dose rate calculations on unstructured meshes have been made to MCR2Sv2. This version of MCR2S uses FISPACT II [5] with the 175 'Vitamin J energy group EAF 2007 [10] and 2010 [11] libraries to carry out activation calculations.

The structured mesh version of MCR2S reads in both a mesh tally file, containing the neutron flux and energy spectrum data, and a seperate file containing data on the fraction of materials under each voxel. However, using unstructured mesh geometry in MCNP6 results in an output file which contains not only the flux and energy spectrum in each element but also the material, density and volume of the element. Thus, in the case of the unstructured mesh, the MCR2S calculation only requires a single file to be read and processed.

An unstructured mesh reading module has been added to MCR2S. As unstructured mesh elements only ever contain a single material, the material mixing step in MCR2S can be skipped. MCR2S then carries out FISPACT-II activation calculations on each mesh element and collates the activity, contact dose rate, decay heat and decay photon source results.

The modifications to MCR2S allow the same capabilities and limitations with unstructured mesh element types as MCNP6. Therefore, like MCNP6, MCR2S support first and second order: tetrahedral, pentahedral and hexahedral elements; however, only pentahedral and hexahedral elements are allowed in the same 'part'.

The resulting shutdown photon source files for the unstructured mesh contain, for each element; the element index, normalised photon source strength and a cumulative energy distribution. The normalised photon source strength (f) is computed out by MCR2S using Equation 1.

$$f = \frac{V_E \times N_{\gamma V}}{N_\gamma} \tag{1}$$

Where V_E is the volume of the element, $N_{\gamma V}$ is the number of photons per cm^3 per second for the mesh element and N_γ is the total number of photons per second across the entire unstructured mesh.

A VTK output routine, used for visualisation of the results, has also been modified to allow unstructured mesh output. The VTK output routine outputs the node coordinates, element-node relationships and activity, contact dose rate and decay heat data in a cell-based format; this can be plotted directly in visualisation programs such as VISIT or paraview.

2.3. *MCNP6 Unstructured Mesh Source Routine*

In order to be able to use the unstructured mesh shutdown photon source file for a shutdown dose rate calculation in MCNP6, an unstructured mesh source reader routine has been written. The source routine is compiled along with MCNP6 and is activated by the use of the IDUM card [1] in the MCNP input file.

A flow diagram showing the process carried out by the MCNP6 unstructured mesh source routine is shown in Figure 2.

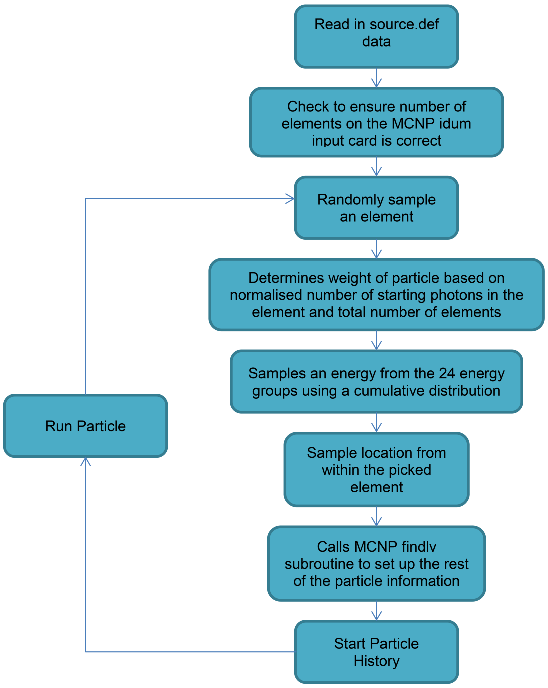


Figure 2: Flow Chart of MCNP6 Unstructured Mesh Source Routine

The new source routine reads in the data from the shutdown photon source file the first time MCNP creates a source particle. The data is then held in arrays for subsequent source particles.

In order to sample the starting location of a particle a random number is generated. This random number is used to pick a mesh element with equal probability. The MCNP6 routines for starting a particle in a given element are then utilised. These routines set up a bounding rectangular box around the element, and then randomly sample a point in the bounding box and perform a check to determine whether this location is inside the element. The position within the bounding box is randomly resampled until a point with the element is selected.

The weight of the particle is set based on the normalised number of source photons in the selected element multiplied by the number of elements, as shown in Equation 2. The multiplication by the number of mesh elements is required to renormalise the weight (w) to the number of mesh elements.

$$w = f \times N_E \tag{2}$$

Where N_E is the total number of elements in the unstructured mesh.

By normalising the weight of the particles by the number of elements, the average weight of the source particles is set to 1.

The energy of the starting photon is sampled using the cumulative distribution for the selected element in the source file. This distribution allows an energy bin from a 24 group energy structure to be selected. The energy is then picked randomly within this energy bin.

All particles are started with a random direction vector.

3. MCR2S Unstructured Mesh Testing

In order to ensure the new MCR2S unstructured mesh routines and gamma source reader perform correctly, comparisons were undertaken for three models of increasing complexity.

1. A model of a sphere has been created and meshed using tetrahedral elements. In order to compare results, an identical CSG model was created with a superimposed rectangular mesh.
2. A second, slightly more complex model, was then created of the 'ITER port plug benchmark'. This geometry was meshed using hexahedral elements. CSG results are already available from previous analysis [12] for comparison.
3. A third, more complex model, has also been meshed. This is based on the DEMO_HCLL CAD model created by KIT [13]. This model has previously been used as a shutdown dose rate benchmark and therefore already has CSG results available.

3.1. Sphere Model

A simple model of a sphere with a 14 MeV isotropic point neutron source was created. The sphere was made of 316L(N)-IG Stainless Steel with a density of 8 g/cm^3 and a radius of 200 mm. It was centred on the origin and surrounded by a void. The isotropic point source was placed on the x-axis at -400 mm. A layout of the model at z=0 mm can be seen in Figure 3.

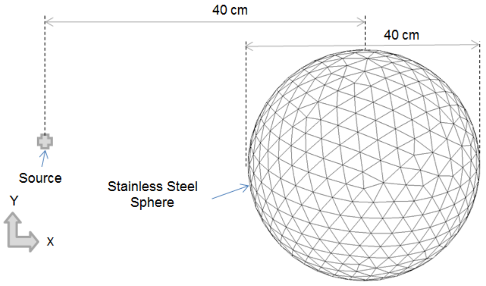


Figure 3: MCNP Tetrahedral Mesh Model Layout (xy slice at z=0 cm)

Figure 3 also contains an image of the meshed sphere. The sphere was meshed using tetrahedral shaped elements. The mesh contains 1698 nodes and 8294 elements. The comparative CSG model contained a structured rectangular mesh with 1000 voxels. This rectangular mesh covered the area -20 to 20 in all three dimensions. An MCNP6 neutron run was carried out and the neutron flux across the sphere was recorded in 175 energy groups. This neutron flux was used in an MCR2S calculation along with the irradiation schedule given in Table 1 and a decay time of 10^3 seconds. The source strength in Table 1 is given as a fraction of the source strength, 1×10^{10}n/s.

Source Strength	Duration	Repetitions
1	5 years	1
1	10 days	1

Table 1: Sphere Irradiation Scenario

Simulation results for the total neutron flux recorded for both the unstructured mesh model and the CSG model can be seen in Figures 4a and 4d respectively. The neutron flux has been normalised to source strength of 1×10^{10} n/s. The total activity of the sphere at a decay time of 10^3 seconds can be seen in Figures 4b and 4e for the unstructured mesh and CSG structured mesh models respectively. The total number of shutdown photons per second predicted for the unstructured mesh sphere is 7.48×10^7 p/s. The total number of shutdown photons per second for the CSG structured mesh sphere with a superimposed regular mesh is 7.72×10^7p/s, a difference of approximately 3%.

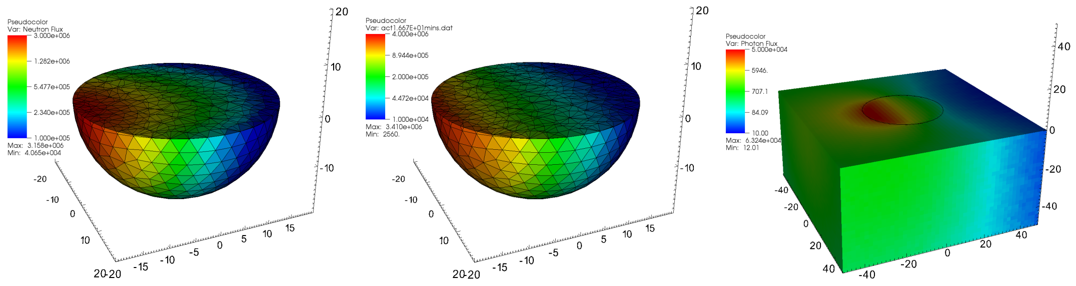
The higher total number of shutdown photons in the CSG structured mesh model can be explained by the structured nature of the superimposed regular mesh used to record the neutron flux. Rectangular voxels at the edge of the sphere clearly overlap both material and void regions. The averaging of higher flux from the void areas leads to an increased activation and subsequent shutdown source strength at the edge of the sphere.

The CSG structured mesh results, 4e, show that some activation of the void occurs around the edge of the sphere. However, this is taken into account when the photon run is carried out, as particles are only started in areas where there is a material, and thus MCNP will only start photons within the sphere. This means it will only start particles within the sphere. The unstructured mesh routine will only start particles within the activated material regions which should mean better agreement of shutdown flux results for the same spatial resolution.

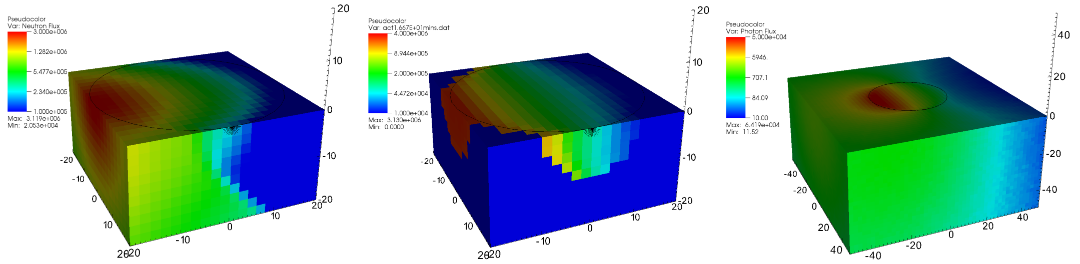
The resultant MCR2S shutdown photon sources were used to calculate the shutdown photon flux in and around the sphere. This shutdown photon flux was recorded on a rectangular structured mesh tally for both the unstructured mesh and CSG models. The shutdown photon flux results can be seen in Figures 4c and 4f.

Visually the results for the unstructured mesh and the CSG structured mesh look almost identical. In order to ascertain a quantitative measure of the difference in results the values from a line along the x-axis at y=0 and z=0 were extracted for both models, and the ratio of the results are presented in Figure 5.

The ratio of the unstructured mesh results and the CSG structured mesh results show very good agreement. The ratio is close to 1 for results across the sphere and void space with all results lying between 0.9 and 1.1.



(a) UM Neutron Flux (n/s/cm^2) (b) UM Activity (Bq/kg) (c) UM Shutdown Photon Flux (p/s/cm^2)



(d) CSG Neutron Flux (n/s/cm^2) (e) CSG Activity (Bq/kg) (f) CSG Shutdown Photon Flux (p/s/cm^2)

Figure 4: Comparison of UM and CSG Sphere Results, Top Row=Unstructured Mesh Model, Bottom Row=CSG Model

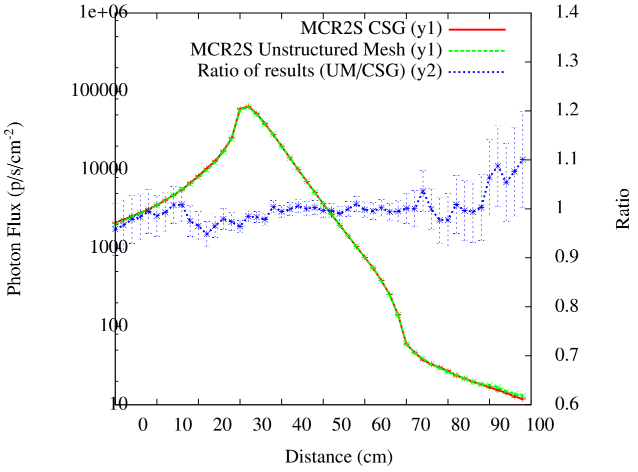


Figure 5: Sphere Results, Comparison between CSG and Unstructured Mesh, y1: Left Hand Scale, y2: Right Hand Scale

For the ratio plot the relative statistical errors of the CSG and unstructured mesh results have been added in quadrature. The errors plotted represent two standard deviations. 20% lie outside two standard deviations and it is therefore unlikely that the differences between the results are solely due to statistical errors in the shutdown photon calculation. The majority of these ten results occur between 20 cm and 40 cm. This is the area at the edge of the sphere closest to the neutron source. As previously mentioned, this area, due to the ill-fitting structured mesh, has artificially high neutron fluxes in the CSG model. This leads to higher activation in the CSG model and may explain some of the difference in shutdown dose rate in this area. This highlights the importance of having well fitting structured and unstructured meshes.

Although the errors were low (<10%) there are currently no processes in MCR2S for error propagation from the initial neutron transport calculations through to the activation calculations. Statistical errors in the original neutron runs and cross section data may also explain some of the differences in the shutdown dose rate.

3.2. *ITER Benchmark*

The ITER port plug computational benchmark has previously [12] been used to compare the results of a number of R2S codes using superimposed structured meshes. This included codes developed by CCFE, KIT and FDS.

The ITER port plug model made up of cylindrical layers containing both steel and, steel and water mixtures. The geometry specification can be seen in Figure 6. To better represent an ITER port plug the model has two streaming paths, one directly through the middle of the steel and water cylinder and one between the inner cylinder and outer cylinder.

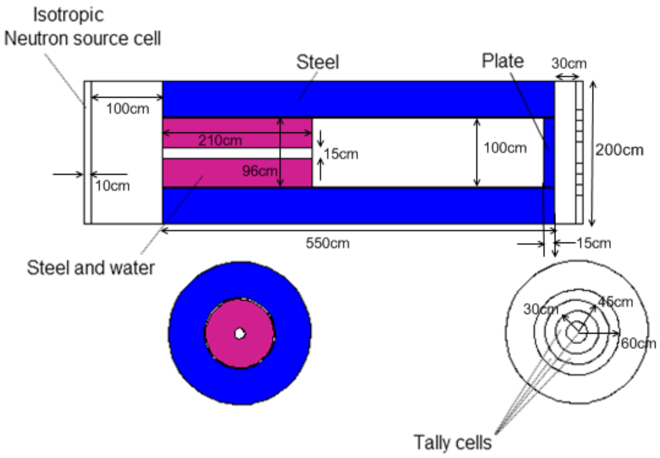


Figure 6: ITER Benchmark Configuration [12]

Material definitions used were as per those specified in the ITER port plug benchmark [12]. Cell tallies were defined in the void to record the resulting shutdown dose rate, consisting of concentric cylinders with radii of r<30 cm, 30 cm<r<45 cm and 45 cm<r<60 cm.

Since the benchmark geometry was defined only with an MCNP model, a matching CAD model of the solids meeting the requirements of the reference design was created in Cubit. The CAD model was meshed using hexahedral elements. An image of the unstructured mesh can be seen in Figure 7. The hexahedral mesh has 65520 nodes and 56757 elements. This results in a reasonably fine mesh with an approximate resolution of about 6cm, the streaming paths are still clearly visible and all have relatively smooth edges.

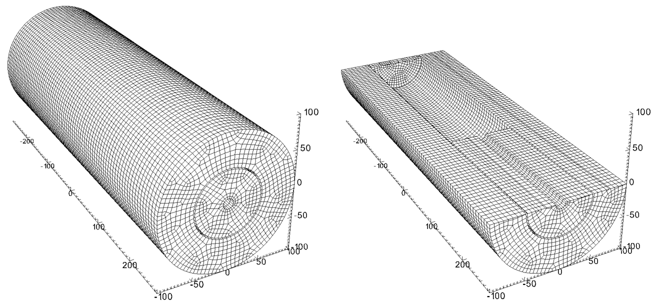

(a) Full mesh (b) Clip along the cylindrical axis

Figure 7: ITER Benchmark Hexahedral Mesh, scale in cm

An isotropic 14 MeV neutron source was defined with a radius of 100 cm and a thickness at 10 cm; located 100 cm from the front edge of the port plug and with a source strength of 2.0×10^{19} n/s.

A neutron transport calculation was performed to ascertain the neutron flux throughout the unstructured mesh in 175 energy groups. In order to improve computational efficiency, source biasing and particle splitting/rouletting [1] variance reduction techniques were employed. The results for the total neutron flux can be seen in Figure 8a.

Small streaming paths between the central steel-water cylinder and the outer steel cylinder can be seen to slightly increase the dose rate in the surrounding material. There is also a slight elevation in neutron flux in the centre of the rear plate due to the steaming path down the centre of the central steel and water cylinder.

MCR2S was used to calculate the activity and shutdown photon source. Along with the neutron flux, this calculation used the material information and irradiation schedule given in Table 2. The irradiation schedule is given as a normalised source strength with 1 reflecting the full source strength of 2.0×10^{19} n/s.

Source Strength	Duration	Repetitions
5.36×10^{-3}	2 years	1
4.13×10^{-2}	10 years	1
0.00	0.667 years	1
8.30×10^{-2}	2 years	1
0.00	3920 sec	17
1.00	400 sec	
0.00	3920 sec	4
1.40	400 sec	

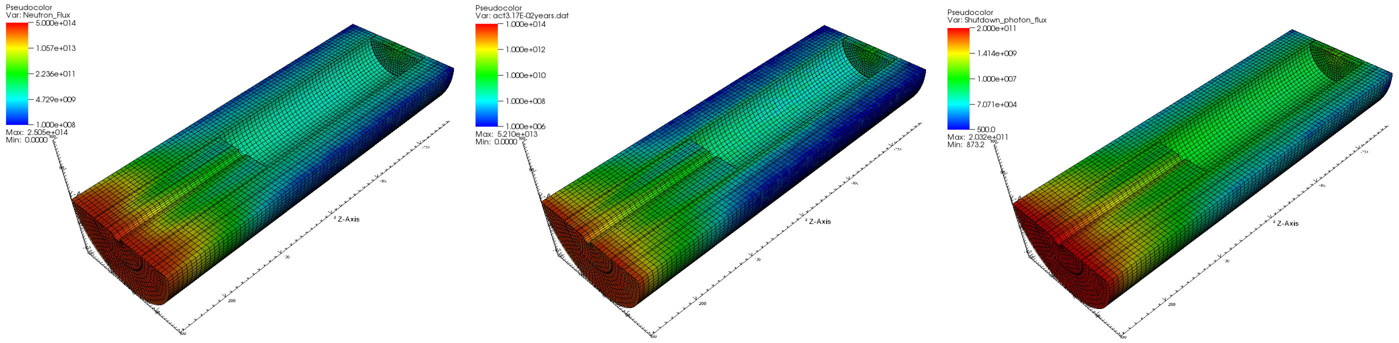
Table 2: ITER computational benchmark irradiation scenario

The specific activity of the ITER computational benchmark at a time of 10^6 s after the end of the irradiation can be seen in Figure 8b. Using the shutdown photon source calculated by MCR2S a photon transport calculation was carried out. The shutdown photon flux within the unstructured mesh can be seen in Figure 8c and results for the shutdown dose rate in the cell tallies at the end of the port plug can be seen in Figure 9. These are plotted alongside results from existing R2S codes using superimposed structured mesh tallies and a MCR2S CSG structured mesh calculation using the latest version of MCR2S. The R2S codes used for comparison are R2Smesh developed by KIT and the R2S tool developed by FDS [12].

The shutdown dose rate results from the tally cells for both the unstructured mesh and structured mesh MCR2S calculations appear to be higher than the results for the other R2S codes. The difference between the results for the MCR2S unstructured mesh calculation and the MCR2S structured mesh calculation range between 5% and 30% with the unstructured mesh predicting lower shutdown dose rates for all tallies.

The unstructured mesh shutdown dose rates are approximately 15% higher than the results from the KIT R2Smesh for all of the tally cells and approximately 24% higher than the FDS results.

As with a superimposed structured mesh R2S approach the resolution of the voxels/elements will affect the predicted shut-



(a) Neutron Flux (n/s/cm^2) (b) Activation (Bq/kg) (c) Shutdown Photon Flux (p/s/cm^2)

Figure 8: ITER computational benchmark results clipped through the centre line of the port plug

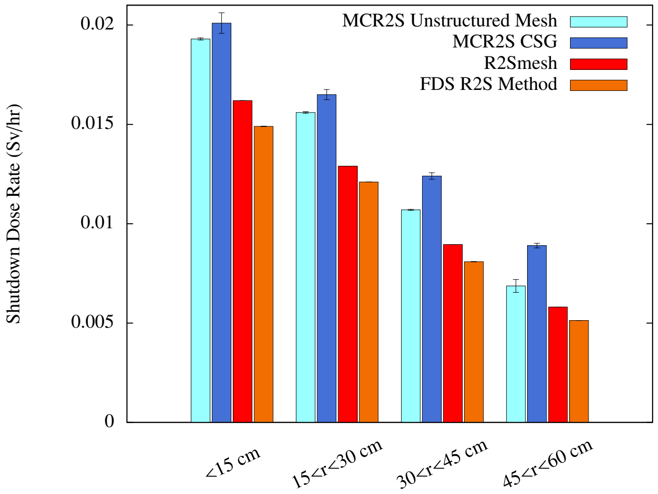


Figure 9: ITER Computational Benchmark Cell Tally Results Comparison

down dose rate result. For unstructured meshes larger elements result in greater flux averaging in areas with a high flux gradient. The averaging of fluxes in this way can result in over- or under-prediction of the shutdown dose rate levels; depending on the location relative to the flux gradient. As the size of the unstructured mesh elements are reduced the flux averaging is reduced and therefore its impact on the shutdown photon flux is also reduced.

In order to study the effect of unstructured mesh resolution on the shutdown dose rate for the ITER computational benchmark several models of the port plug were created with varying numbers of mesh elements. The models have been meshed using an adaptive algorithm to try to model the geometry more faithfully. Adaptive meshing allows for refinement of the mesh in certain regions such as curved surfaces. This allows for a better representation of the geometry for a given number of elements. All models were meshed using hexahedral elements. The number of elements used for each model can be seen in Table 3. All other aspects of the models were kept the same.

Model Number	Number of Mesh Elements
1	4959
2	7230
3	23396
4	56757

Table 3: ITER Computational Benchmark Mesh Resolution

Each model was run through the MCR2S process to ascertain the shutdown dose rate in the tally cells at the rear of the port plug. The results for each model can be seen in Figure 10.

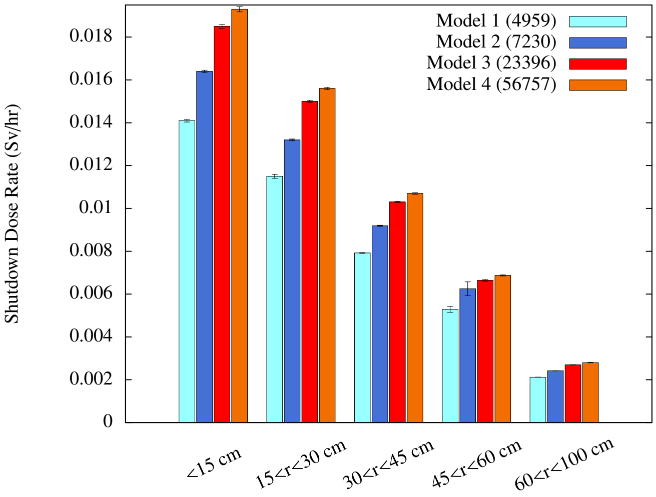


Figure 10: ITER Computational Benchmark Cell Tally Results Resolution Study

The results show the dose rate at the rear of the port plug increases as the number of elements increase. It can also be seen that the shutdown dose rate results seem to be converging as the number of elements is increased. Increasing the number of elements above 56,757 is expected to lead to a converged shutdown dose rate as the flux averaging in the elements tends to zero.

3.3. DEMO Computational Benchmark

A more complex shutdown dose rate computational benchmark, based on a 11.25°sector of the concept design for the DEMOnstration (DEMO) fusion reactor, was also been carried out using unstructured mesh geometry. A similar benchmark exercise has previously been carried out using superimposed structured meshes [13] on a MCNP CSG model to calculate the shutdown dose rate at four locations within the reactor vessel at decay times of 1 hour and 10 days after shutdown.

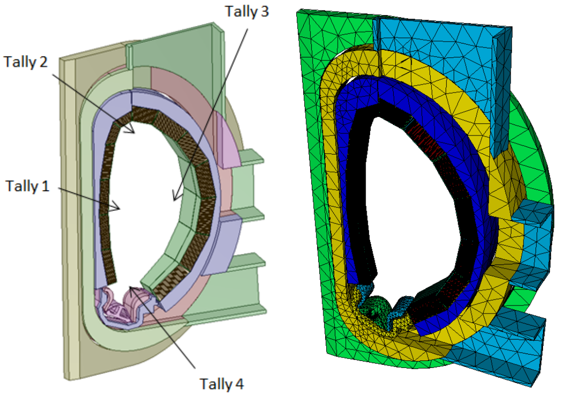
While previous benchmark results are available using the DEMO MCNP model, differences between the available CAD and MCNP models, such as the addition of first wall armour and torodial field coil casing, meant that a direct comparison was not appropriate. In addition only a sub-set of DEMO components had been activated, a feature which is not yet available in the MCR2S unstructured mesh implementation. Instead two calculations using MCR2S have been carried out; one using CSG and a superimposed structured mesh, and the other using an unstructured mesh. The MCNP CSG model used in the previous studies was modified to match the CAD model by removal of the first wall armour and the toroidal field coil casing. A superimposed structured mesh was placed over the entire geometry at a resolution of 10 cm. The same material definitions, irradiation schedule and decay schedule were used for both the unstructured mesh and CSG structured mesh calculations.

The DEMO model is made up of a number of parts containing several materials. The materials used in the study are listed in Table 4. The unstructured mesh was created by meshing the parts of the demo model individually. This allowed flexibility in the number of elements required for each part. Parts such as the blankets, first wall and divertor, which will have the largest influence on the shutdown dose rate in the reactor vessel, have been meshed relatively finely (between a resolution of 2cm and 20cm). In order to reduce the number of elements in the model and aid in speeding up the calculation, parts which are positioned away from the plasma, and therefore less likely to have a significant impact on the shutdown dose rate in the reactor vessel, have been meshed coarsely with resolutions in the order of metres. The unstructured mesh geometry for the 11.25°sector of DEMO can be seen in Figure 11, along with the original CAD and the in vessel shutdown dose rate tally locations.

The DEMO unstructured mesh contains 733,813 elements, with a mixture of first order tetrahedra, pentahedra and hexahedra. The majority of these elements have been used in the meshing of the blanket and first wall modules which will have the greatest effect on the shutdown dose rates in the reactor vessel.

Material	Reactor Component
Eurofer Steel	Blanket Encasing, divertor and ports
Lithium Lead	Breeder Blanket Material
Niobium-Tin	Magnetic Coils
Water, Stainless Steel, Eurofer and boron mixture	Vacuum Vessel
Lithium Lead, Eurofer and helium mixture	Manifold blankets

Table 4: DEMO Model Materials



(a) DEMO CAD Model (b) DEMO Unstructured Mesh

Figure 11: a) The DEMO CAD model showing the shutdown dose rate tally locations within the vessel and b) the corresponding unstructured mesh.

A 14 MeV parametric plasma neutron source has been used for both the unstructured mesh and CSG models. For both the unstructured mesh and superimposed structured mesh the neutron flux was recorded over the entire geometry. MCR2S was used to calculate the activity and shutdown photon source for each element/voxel in each mesh. Unlike the previous DEMO benchmark comparison [13], where only the blanket and divertor were irradiated, due to current limitations in the unstructured mesh MCR2S routines full model activation had to be carried out. This also means that all components have to be irradiated with the same schedule which does not allow for replacement of components to occur at different times. It was therefore decided to base the irradiation schedule for the models on the irradiation seen by a blanket module; assumed to be replaced every 8 years in the final phase of DEMO. The irradiation schedule used by MCR2S for all components is given in Table 5.

Source Strength	Duration	Repetitions
0.5	7.9 years	1
1.0	0.5 days	60
0.0	0.5 days	

Table 5: DEMO Computational Benchmark Irradiation Schedule

The activity and shutdown photon sources were acquired 1 hour and 10 days after shutdown. Both shutdown photon sources were then used in photon transport calculations, allowing the shutdown dose rate to be acquired at the four locations within the reactor vessel at both decay times. The shutdown photon flux within the components of the DEMO reactor can be seen in Figure 12 for 1 hour and 10 days after shutdown. Due to a programming error in MCNP6.1 at the time of the calculation it was not possible to obtain a shutdown photon flux on a mesh tally within the void for the unstructured mesh model. It should be noted that this programming error has recently been fixed in the beta release of MCNP6.1.1.

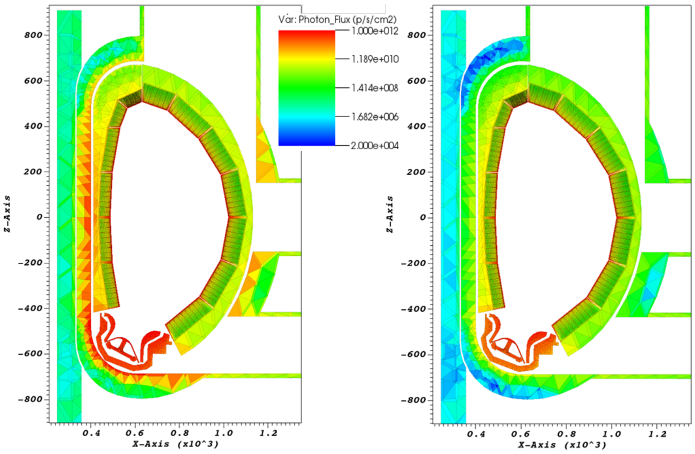


Figure 12: DEMO Benchmark Shutdown photon flux (p/s/cm^2), Left: 1 hour after shutdown, Right: 10 days after shutdown

The shutdown dose rate results at the four locations, see Figure 11, for both the unstructured mesh and CSG structured mesh models can be seen in Figure 13. The shutdown dose rate results are presented for 1 hour and 10 days after shutdown.

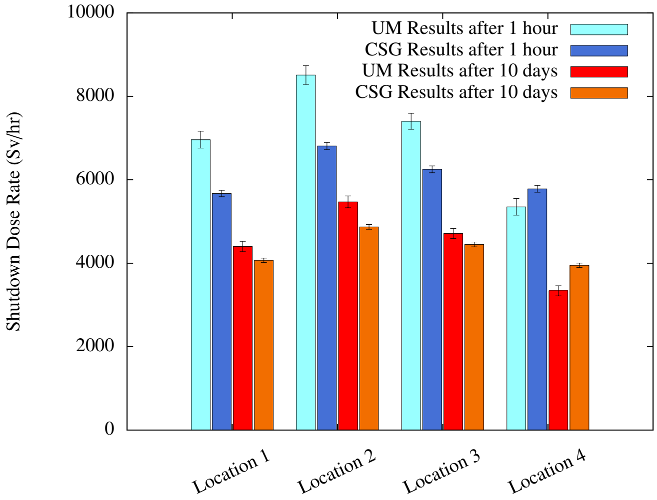


Figure 13: DEMO Computational Benchmark Cell Tally Results at the four tally locations

For tallies 1-3 the predicted shutdown dose rate for the unstructured mesh is generally around 20% higher than the predicted shutdown dose rate for the CSG model an hour after shutdown and 10% higher 10 days after shutdown. This trend is reversed in the region around the divertor (Tally 4, see 11) where the predicted shutdown dose rate for the unstructured mesh is approximately 8% lower than the predicted shutdown dose rate for the CSG model an hour after shutdown and 15% lower 10 days after shutdown.

Some differences in results could be partly due to the different mesh resolutions. The CSG structured mesh has a 10 cm resolution everywhere, however the resolution of the unstructured mesh changes dependant on the model part. The blanket areas, which are expected to have the greatest effect on the shutdown dose rate at tallies 1-3, have been meshed with hexahedral mesh elements at resolutions in the range of a few centimetres. This means there is less flux averaging in the blankets of the unstructured mesh which would lead to higher shutdown dose rates at tallies 1-3.

The divertor, which is likely to have a significant effect on the shutdown dose rate results at tally 4, due to its shape has been meshed using tetrahedral element at a resolution of approximately 20 cm. This lower resolution results in higher flux averaging for the divertor in the unstructured mesh compared to the CSG model. This might be one of the contributing factors to the lower predicted shutdown dose rate for the unstructured mesh around the divertor region. However, further detailed investigations on the impact of the mesh resolution on the shutdown dose rate would be required to understand all contributing factors.

4. Discussion

4.1. Results

The shutdown dose rate results for the sphere model compare very well for the unstructured mesh and CSG structured mesh with 80% of the results lying within two standard deviations of each other. The majority of the points lying outside two standard deviations occured were observed at a few data points close to the edge of the sphere. The differences can be explained by a the poorly fitting structured mesh which resulted in the averaging of neutron fluxes from void into the material and an artificially high material activation.

The shutdown dose rate results for the unstructured mesh ITER benchmark model have been compared to other R2S codes. The MCR2S unstructured mesh calculation predicted higher shutdown dose rates in all of the tally cells compared to the R2Smesh and FDS codes. However, the MCR2S unstructured mesh calculation predicts lower shutdown dose rates for all tally cells compared with the MCR2S CSG structured mesh calculations. It is therefore likely that the higher prediction by the unstructured mesh calculation compared to R2Smesh and the FDS code is due to a difference in the MCR2S method and not the unstructured mesh. In order to confirm the cause of this difference a further investigation would be required.

The resolution study performed on the ITER benchmark model showed that while using unstructured meshes, mesh resolution effects can still significantly affect shutdown dose rate results. The difference in shutdown dose rate results between the model with 4959 elements and the model with 56757 element is as much as 20%, and even the results with 56757 elements do not appear to be fully converged.

The DEMO benchmark model shows reasonable agreement between the shutdown dose rate predicted by the unstructured mesh and the CSG structured mesh models. Up to a maximum of 20% differences were noticed in the shutdown dose rate at the four tallies. However these are likely to be due to mesh resolution effects where the divertor was mesh more coursely. Mesh resolution effects are not just an issue with the unstructured mesh models but also an important issue for CSG structured meshes. In the DEMO study only a single unstructured mesh resolution has been used. Ideally, in order to show a converged solution it would be necessary to use several different mesh resolutions, some with very high numbers of elements. However, to run the DEMO benchmark with very high numbers of elements is not practical at present with Culham Centre for Fusion Energy's computational resources due to memory limitations and time considerations.

Throughout the calculations for all three models presented in this report, unstructured mesh and structured mesh resolution effects have been an important consideration. Significant differences in the shutdown dose rate results occur when different mesh resolutions are used. However, mesh resolutions have different effects on results dependant on the location of interest. If the location of interest is behind shielding the shutdown dose rate reduces with increasing mesh resolution (i.e. decreasing element size), if the location of interest for the shutdown dose rate calculation is the same side as the neutron source then the shutdown dose rate increases with increasing resolution.

With unstructured meshes it is possible to mesh different parts of the model at different resolutions. Therefore consideration should be given at the time of model creation to the areas of interest and which parts of the model are most likely to affect results and which parts have high flux gradients across them. These parts of the model should ideally be meshed with a relatively high resolution in order to best predict the shutdown dose rates in the areas of interest.

5. Conclusions and Recommendations

Based on the work and assumptions documented in this paper the following conclusions have been made:

1. MCR2S has been successfully modified to enable shutdown dose rate calculations on tetrahedral, pentrahedral and hexahedral geometrical meshes. Although currently it is computationally more expensive to track particles on an unstructured mesh compared to CSG for a typical fusion DEMO problem there are clearly some significant advantages of using unstructured meshes with MCR2S calculations. It prevents the need for materials and void mixing in voxels at the edge of components. It also prevents artificially high neutron fluxes in materials occurring around streaming paths with a voxel that completely covers the streaming path and surrounding material. It also increases the ability in neutronics calcuations to model more complex geometry and results in a significant speed up in the time taken to create neutronics models. It should therefore be investigated further
2. The unstructured mesh implementation of MCR2S has been successfully run with several unstructured mesh geometries. The results compared well to those from MCR2S CSG structured mesh calculations. The sphere model demonstrated the unstructured mesh MCR2S capability on a simple model. The ITER Port Plug Benchmark was performed with a hexahedral unstructured mesh. The calculated shutdown dose rate results compared resonably well to other R2S shutdown dose rate codes. The DEMO benchmark model shows a good comparison between the shutdown dose rate predicted using an unstructured and a CSG structured mesh, for a relatively complex model with >700000 elements.
3. As with CSG structured mesh calculations, mesh resolution was found to be an important factor in determining the shutdown dose rate using unstructured mesh. Care is needed in both CSG structured mesh and unstructured mesh calculations to ensure the mesh resolution is sufficiently high in areas of the model which contribute to the shutdown dose rate in the area of interest. Unlike CSG, unstructured mesh geometry allows parts of the model to be meshed individually, thus allowing the components which make a significant contribution to the shutdown dose rate to be meshed with a higher resolutions.

6. Acknowledgements

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