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# **Development of neutronics analysis techniques for radioactive waste assessment**

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# Cover page

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Title: Development of neutronics analysis techniques for radioactive waste assessment

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## **Abstract**

Computational models created for neutronics assessment through solid geometry conversion are often specific to the analysis being performed. The use of unstructured mesh geometry has the potential to reduce the build time of MCNP models, reduce inaccuracies introduced through flux averaging over different components and material mixing, and make use of CAD models that can also be suitable for other types of analysis. In this paper three neutronics methods were investigated for suitability in performing a radioactive waste assessment of a fusion demonstration reactor. The methods included the conventional cell-based approach, a superimposed structured mesh and the use of a recently developed capability with unstructured mesh geometry. As a result of this research it was concluded that an unstructured mesh approach has the potential to not only be an important tool for assessing radioactive waste to inform reactor design and waste management planning, but also significantly reduce neutronics model build efforts.

**Keywords:** DEMO, neutronics, radioactive waste, unstructured mesh, MCNP

## 1 Introduction

A fusion reactor device will become radioactive during operation as a result of irradiation by neutrons generated in the D-T fusion reaction. A fusion power plant will typically receive approximately  $1 \times 10^{21}$  neutrons per second during full power pulses. Consequently radioactive waste will be produced through neutron activation of materials [1]. Significantly, however, only a small proportion of long-lived radioactive waste is generated. It is foreseen that fusion power reactors will not produce radioactive waste requiring significant active cooling for substantial periods of time, such as that arising from fission plants [2]–[4].

Radioactive waste needs to be disposed of using methods that ensure safe isolation from biological systems. There is also a need to reduce the amount of permanent radioactive waste; an important issue with regards to public acceptance of fusion power. Several paths are identifiable depending on how the waste is classified, national regulations and existing facilities. Examples include direct disposal into deep geological disposal facilities, near surface disposal, recycling and clearance of material that is not active waste. Due to the limited availability of waste burial facilities in the EU and the associated social perceptions regarding radioactive waste, an optimum waste management plan for fusion power plants needs to be developed [4].

In this paper the neutronics methods used for the assessment of radioactive waste are investigated for a conceptual model of a demonstration fusion power plant (DEMO). Recent advances in the use of unstructured mesh are also considered and a method for use in radioactive waste assessment developed.

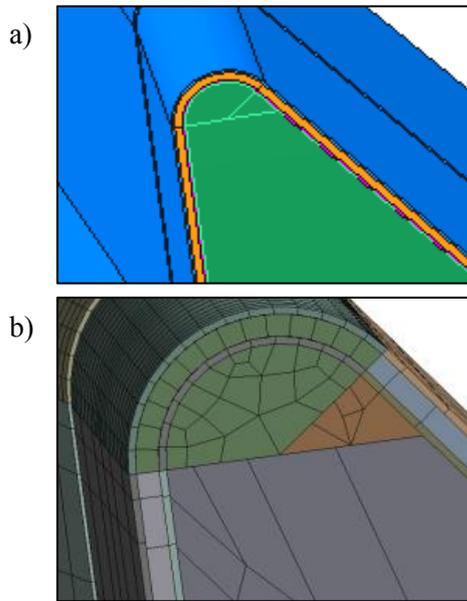
## **2 Neutronics analysis for radioactive waste assessment**

To compute the radioactive waste inventory for a given geometry, the spatial distribution of the neutron flux is determined through a transport calculation (such as with the Monte Carlo N-Particle transport code 'MCNP') and subsequently used for irradiation in an activation calculation (for example with the inventory code FISPACT-II [5]). MCNP transport calculations require a 3 dimensional (3D) neutronics model. Until recently this has been provided in constructive solid geometry (CSG) form, either through manual writing of the CSG model definition or through CAD [computer-aided design] to CSG conversion tools. CAD to CSG conversion is often a lengthy and troublesome process. Difficulties with poorly defined geometries and lost particles within the simulation are a common problem. Some codes are available to automate some of the conversion process, however these still require 'good', 'clean' and defeatured CAD. The latest version of MCNP (version 6 [6]) now includes the capability to read the geometry of a model represented using an unstructured mesh in Abaqus<sup>®</sup> [7] form.

The neutron flux can be estimated through the use of MCNP using a number of different particle history tally approaches; in this work cell tallies and 3D superimposed structured mesh tallies. If the new unstructured mesh geometry feature of MCNP is used it is also possible to tally directly on the mesh elements that make up the geometry. The calculated neutron flux from either the cell, 3D structured mesh or 3D unstructured mesh tally can then be used to perform an activation calculation. The activation calculations are performed for the materials within each cell, structured mesh voxel or unstructured mesh element that comprise the neutronics model. Using FISPACT-II this activation calculation provides the material inventory at various cooling periods which in turn can be used to deduce the waste classification for the material in that cell, structured mesh voxel or unstructured mesh element.

There are a number of key disadvantages regarding the use of the cell-based and structured mesh-based tallies for waste classification through neutronics analysis. Firstly, the neutron flux spectrum used in the irradiation phase of the activation calculation is averaged over the whole cell tally. If the cell is particularly large or comprises a thick shielding material this assumption that the neutron flux is uniform throughout the entire cell provides a poor representation of the actual flux in some parts of the cell; this can be minimised through splitting large cells into a number of smaller ones, but this is a time-consuming activity. In turn the material within the large cell will all be classed as the same waste type; examples of this are evident in the results of this research. Secondly, the use of the structured mesh tally which is superimposed over the CSG geometry creates a material mixing problem. Where the mesh voxel covers two or more different materials, and or void region, the activation calculation in the current implementation of this method assumes a homogeneous mix of the materials.

An unstructured mesh approach allows the neutron flux to be tallied directly on the elements comprising the geometry mesh and therefore the tally is not confined to a structured shape, either rectangular or cylindrical, and instead conforms to the geometry shape. The mesh elements consequently contain only one material which removes the effects of material mixing of different components and void mixing (see Figure 1). Mesh refinement can be used to readily create elements much smaller than the original CAD solid body volume, thereby reducing flux averaging problems. The mesh elements can take the form of tetrahedral, pentahedral or hexahedral shapes. In this work a combination of all three types were used.



**Figure 1. Example of unstructured mesh conformity to the CAD geometry: (a) rounded feature on the divertor CAD, (b) unstructured mesh elements used to provide the model geometry and tally volumes.**

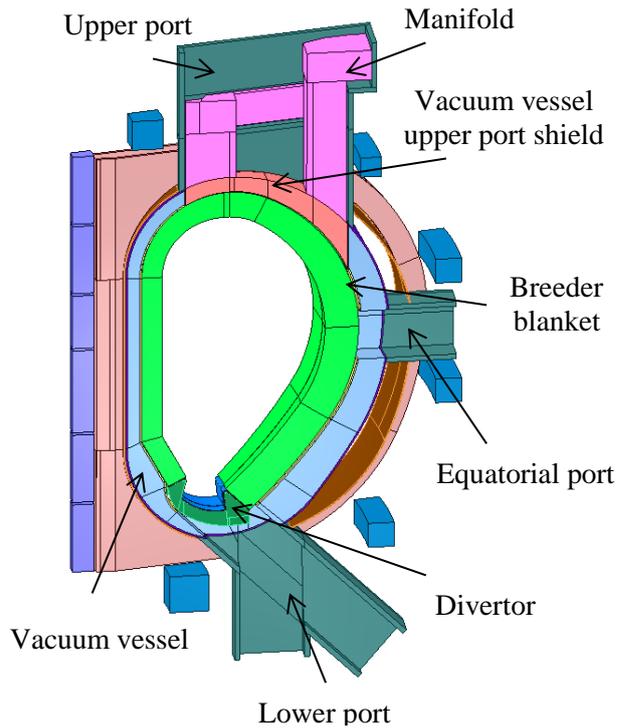
The quantities of radioactive waste calculated using these methods are sensitive to the size of the volume being considered, i.e. the size of the cell, mesh voxel or element. Absolute quantities of waste will depend on the individual waste packages, packaging type and disposal route. In turn the waste packages will be affected by the type of material, size of component and dismantling opportunities. As the design of a DEMO reactor is in the pre-conceptual phase there is insufficient information to determine absolute values of radioactive waste as packaged. Assessment can be made on approximate quantities of waste based on the current neutronics model, not taking into account the packaging of wastes. The cell-based approach assumes the materials to be separated by cell, the structured mesh approach assumes the materials to be separated by mesh voxel and the unstructured mesh by mesh element. It would be impractical to separate the components to the size of the structured mesh voxels or unstructured mesh elements used in this work. Calculating absolute quantities of radioactive waste, however, is not the focus of this analysis. Instead the aim is to investigate methods for assessing the

radioactive waste of varying DEMO reactor designs to inform on future component design and a suitable radioactive waste management strategy.

### **3 Neutronics modelling and calculations**

#### **3.1 Model description**

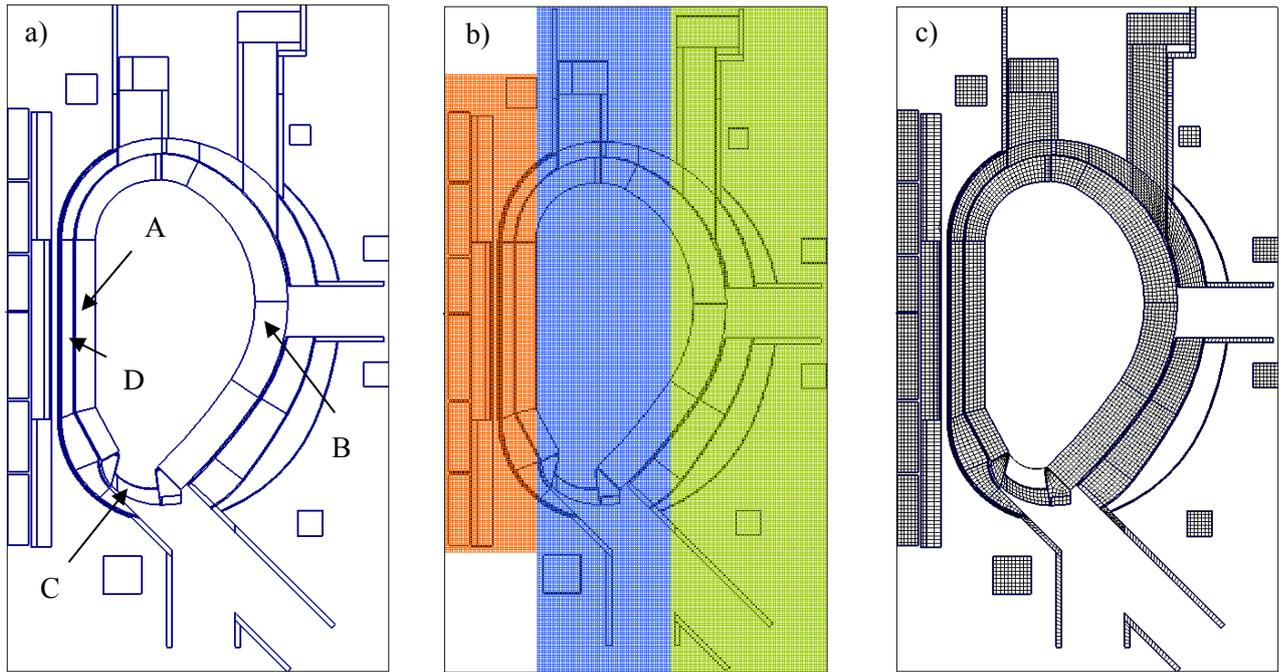
A neutronics model based on a preliminary EU generic DEMO 2015 baseline model (shown in Figure 2), with a helium-cooled pebble bed blanket concept, was used to compare the neutronics response and radioactive waste inventory calculated using an unstructured mesh method against the conventional CSG definition with cell-based and superimposed mesh tallies. The MCNP input file was provided which had been created via the conversion of the CAD model to MCNP with McCad [8]. Using this MCNP input file both the cell-based and structured rectangular mesh-based (9 cm voxel size) tallies were used to record the neutron flux.



**Figure 2. EU generic DEMO 2015 baseline model.**

The unstructured mesh file for MCNP was created in Abaqus<sup>®</sup> form using the ANSYS<sup>®</sup> [9] workbench package and recently developed tools at CCFE. The CAD model was prepared for meshing in the SpaceClaim module [10] of ANSYS<sup>®</sup> and then imported into the mechanical modeller of ANSYS<sup>®</sup> to create the mesh. A curvature and size refinement of 5 degrees and 15 cm respectively was used creating a mesh with 112305 elements. Each component within the tree structure of the CAD model in ANSYS<sup>®</sup> creates a pseudo-cell definition in the MCNP input deck - similar to the standard CSG-type cell definition.

A visual representation of the three tally methods is provided in Figure 3.



**Figure 3. Three tally methods: (a) cell based, (b) superimposed rectangular structured mesh based and (c) unstructured mesh based. (Labels on (a) show the point locations in 2D for the neutron flux values in Table 1.)**

### **3.2 Neutronics calculations and waste classes**

Neutron transport calculations were carried out using MCNP6v1 with FENDL2.1 [11] neutron cross-section data and where this was unavailable, ENDF-B-VII [12]. This neutron flux spectrum, tallied in the 175 VITAMIN-J energy group structure [13], was then used to irradiate the materials comprising the various components of the EU DEMO 2015 model using FISPACT-II (release 2.20 and release 3.00) [14] with the EAF-2010 activation data [15] and the 2-phase operation scenario planned for a European DEMO [16]. The simulation codes, nuclear data and irradiation/decay scenario were common in all methods.

The IAEA safety standards [17] were used to formulate a set of ‘general classes’ for fusion generated radioactive wastes as the allowable limits of a specific disposal facility are not

defined in this work. Radionuclide specific activation concentration levels in becquerels per gram (Bq/g) presented in the UK Government guidance on the scope of and exemptions from the radioactive substances legislation [18], which originate from RP-122 [19], were used to assess cleared or 'not active waste' (NAW).

Within the IAEA guidelines, any material that does not meet the clearance level requirements is classed as either low-level waste (LLW) or intermediate-level waste (ILW). The classification of higher activity waste is not considered here as it is currently considered that there will be no high-heat generating wastes requiring significant active cooling.

LLW is radioactive material that is above the clearance levels but with limited amounts of long-lived radionuclides. For this EU DEMO study this waste class is defined by the beta+gamma activity concentration which must be less than 12 GBq/tonne (there is also a limit on the alpha activity though this was assumed to be a small contribution and not included for this comparison). All other radioactive material is classed as ILW; although this type of waste requires a greater degree of containment and isolation than that provided by the near surface disposal routes available to LLW, it requires no or little provision for long-term heat removal.

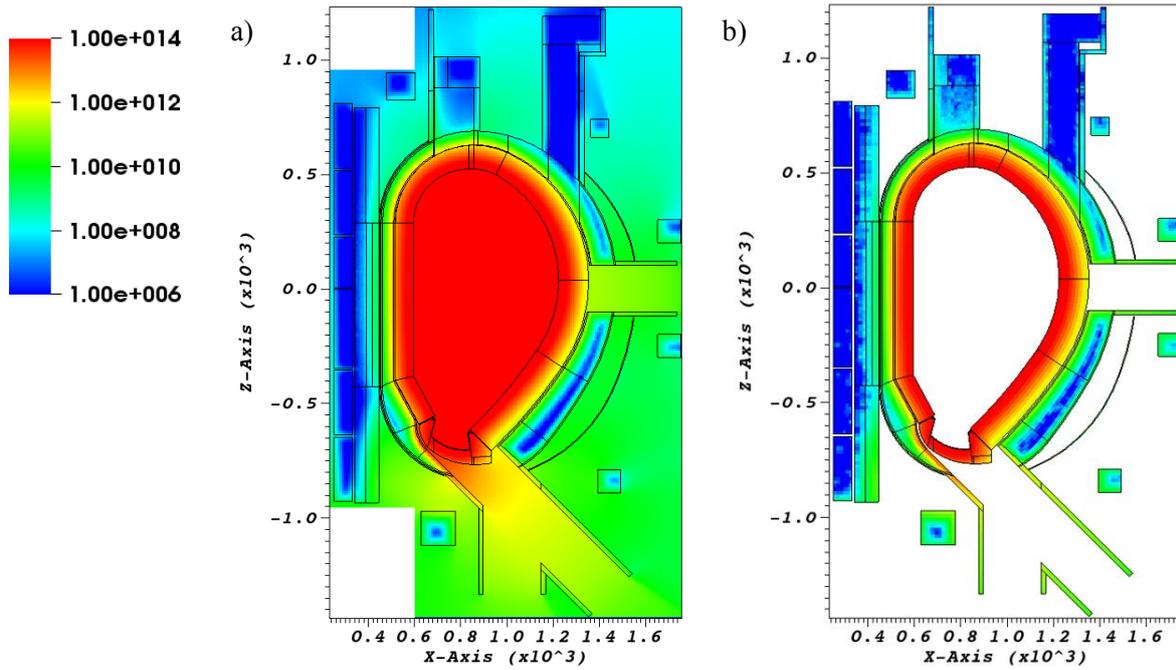
Material recycling after a fusion reactor is dismantled and the reuse of components is preferred due to the more economic use of materials and reduced quantities of radioactive waste for disposal. The criteria for recycling vary by country [20] and in some studies arbitrary recycling limits are used; realistic criteria for recycling need to be established based on viable processes. In this study recyclable materials (RM) were identified separately to the activated waste class. Both materials classed as LLW and ILW were assessed for potential recycling based on a contact dose rate limit of 2 mSv/hr [21], below which shielded hands-on handling could be possible and therefore potential for a relatively simple recycling process.

To determine the quantities of waste and classification for the materials comprising the EU generic DEMO 2015 model a material activation calculation was performed for each cell, structured mesh voxel or unstructured mesh element. A scripted approach was used to perform the activation calculation for each of the cell tallies. A modification to the CCFE developed MCR2S code [22], [23] was used for the assessment of the waste classification using the 3D structured mesh with a further modification to the code for assessment of the unstructured mesh tally.

## **4 Results and discussion**

### **4.1 Neutron flux and radioactive waste results**

As described previously in this paper a potential issue encountered in neutronics analysis is neutron flux averaging effects. The neutron flux maps from the structured and unstructured mesh tally results are shown in Figure 4. The reduction in flux through the blanket and vacuum vessel is evident.



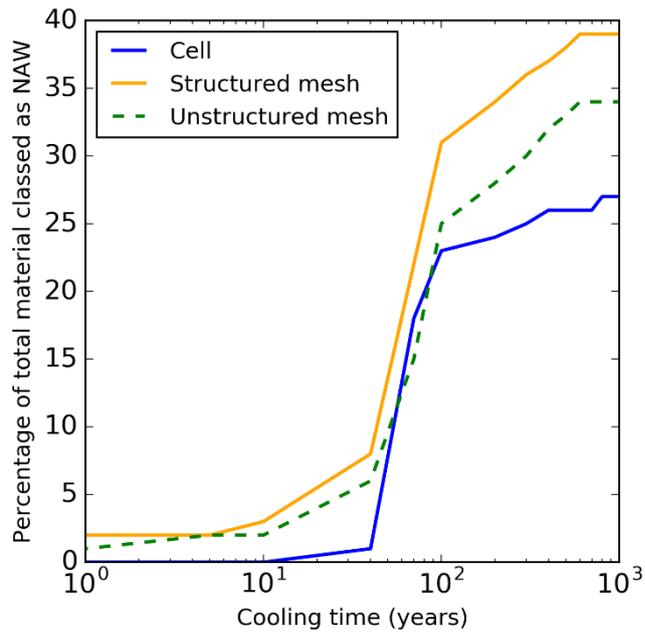
**Figure 4. Neutron flux map (neutron flux neutrons/s/cm<sup>2</sup>) using a) superimposed structured mesh tally and b) unstructured mesh.**

**Table 1. Neutron flux method (neutron flux neutrons/s/cm<sup>2</sup>) values at four points within the model (see Figure 3 for a visual reference to location). \*Statistical error values for the unstructured mesh method are from a superimposed structured mesh included in the calculation and not directly on the unstructured mesh element. The size of the voxel in the structured mesh will have some differences to that of the unstructured mesh element. Further information on the uncertainties is provided in section 4.3.**

		Cell-based		Structured mesh		Unstructured mesh	
		Flux	Statistical error	Flux	Statistical error	Flux	Statistical error*
A	Inboard blanket	1.10E+14	0.01%	9.12E+13	0.14%	8.45E+13	0.03%
B	Outboard blanket	7.18E+13	0.01%	2.42E+13	0.10%	2.33E+13	0.06%
C	Divertor	1.04E+14	0.02%	1.55E+14	0.04%	1.37E+14	0.02%
D	Inboard vacuum vessel	8.14E+11	0.06%	1.43E+11	3.17%	2.15E+10	0.65%

The neutron flux in some point locations is presented in Table 1 calculated using the three different neutronics methods considered in this study: cell-based, structured mesh and unstructured mesh based. Predominantly the cell-based method over estimates the flux compared to the structured and unstructured mesh results. This is because the flux is assumed to be uniform over the entire cell volume which in the case of the blanket, for example, is a thick shielding material with a large gradient in flux from front to back. These variations in the calculated neutron flux impact on the subsequent activation and material inventory calculations which are in turn used to assess the waste classification.

Although a fusion power plant will not produce what was previously described in this paper as higher activity wastes, the tokamak could create substantial quantities of ILW and LLW due to the activation of materials that comprise the reactor. The quantity of activated material and the nuclide inventory is used to determine the waste classification. The percentage of the total material comprising the DEMO neutronics model that can be cleared, i.e. considered as NAW, is shown in Figure 5 for the cooling period of 1 - 1000 years after shutdown. Results from each of the three methods are shown together. By 100 years cooling approximately 25 - 30 % of the reactor material could be cleared from regulatory control. Using a cell-based calculation there is no material that can be considered as NAW until after 10 years.



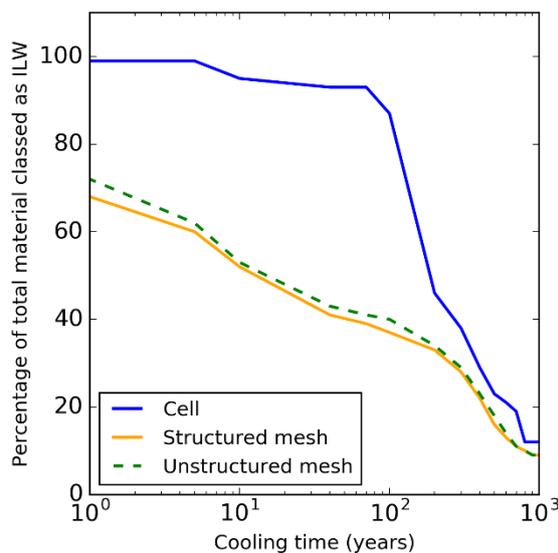
**Figure 5. Variation of the percentage of NAW comprising the total model over the time period 1 - 1000 years after shutdown. Results shown for each of the 3 methods: cell-based, superimposed structured mesh and unstructured mesh.**

As discussed earlier in the paper, the conventional cell-based approach relies on flux averaging over cells comprising the geometry, although this can be reduced through time consuming cell-splitting. The mesh-based approach allows the potential dismantling and separation of waste to be investigated by providing neutron flux, and therefore activation and inventory data, in voxels or elements. We can therefore consider the waste classification of components and parts on a more refined scale, as opposed to each cell. Although it would be impractical to separate the components into the size of mesh voxels and elements used in this work, analysis on this scale is very important for informing on the design of components and where provision should be made to allow for dismantling and segregation during decommissioning and waste packing.

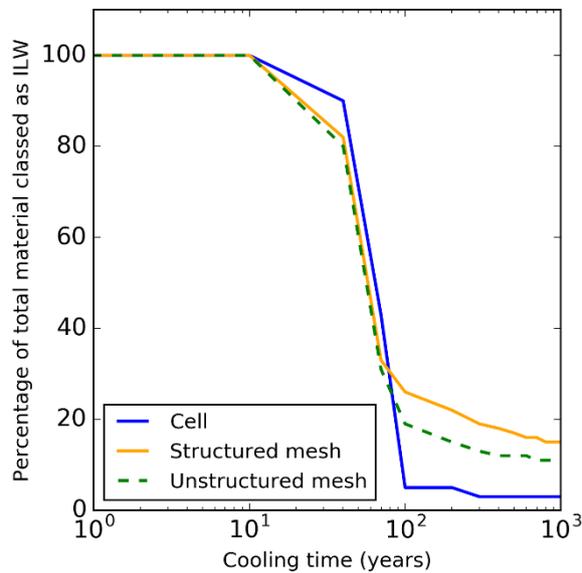
Both the structured and unstructured mesh approaches allow the potential of dismantling to be considered. For example, by considering the sections of the outboard vacuum vessel by

voxel/element the quantity of ILW from the vacuum vessel at 100 years can be reduced to nearly 50% (Figure 6). It is therefore evident that some utilisation of component dismantling within the vacuum vessel could be used to reduce the quantities of ILW. Less difference is observed between the percentage of NAW from the three methods for the divertor (Figure 7) due to the smaller cells.

In this work the cell-based technique tends to provide an overestimation of the radioactive waste quantities, though this is not always the case as shown in the divertor results (Figure 7). The quantity of ILW above 100 years calculated using the cell-based approach is lower than that from the mesh-based results. The effect of averaging the neutron flux over cells that have regions very close to the plasma is observed; in the mesh-based methods the few voxels or elements in this region would be classed as ILW. A cell-based approach is therefore likely to provide conservative values for quantities of radioactive waste which could be considered advantageous. However, as discussed earlier in the paper, the level of information for a DEMO reactor model is currently insufficient for realistic absolute radioactive waste quantification.



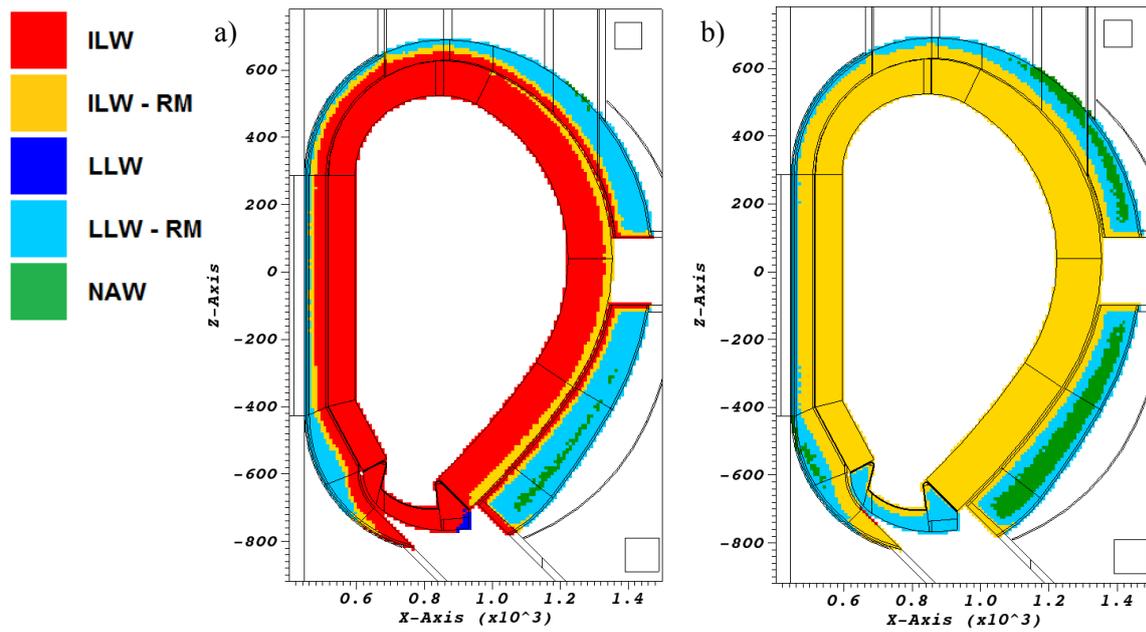
**Figure 6. Variation of the percentage of ILW comprising the vacuum vessel over the time period 1 - 1000 years after shutdown. Results shown for each of the 3 methods: cell-based, superimposed structured mesh and unstructured mesh.**



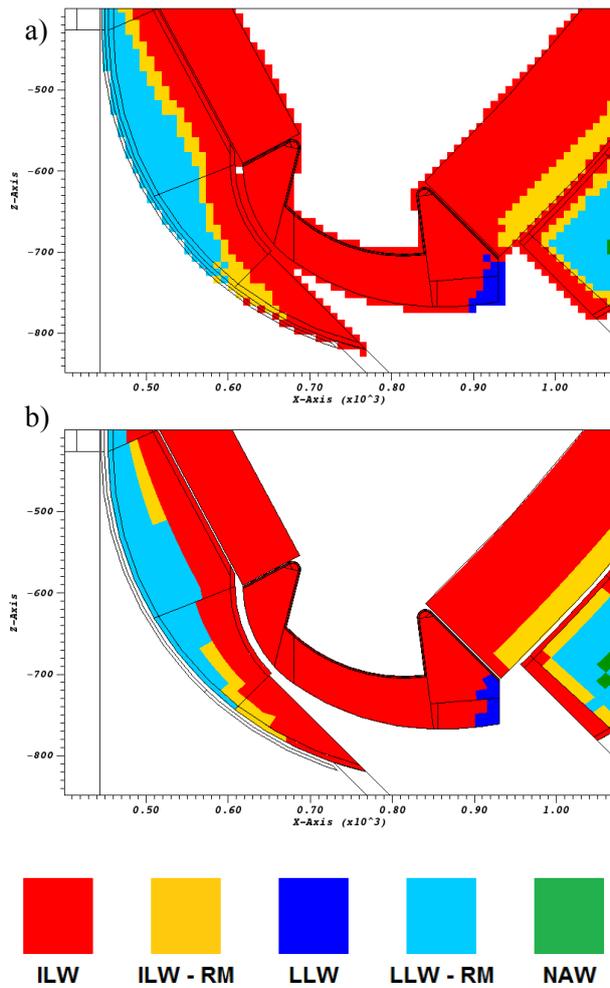
**Figure 7. Variation of the percentage of ILW comprising the divertor over the time period 1 - 1000 years after shutdown. Results shown for each of the 3 methods: cell-based, superimposed structured mesh and unstructured mesh.**

An important output from the mesh-based developed approaches is the ability to visualise the mesh voxel/elements by waste classification on a 3D map. This enables quick evaluation of components that show potential for reducing quantities of radioactive waste through dismantling. For example, it was shown that dismantling the vacuum vessel has the potential to significantly reduce the quantities of radioactive waste after 100 years cooling. In Figure 8 a 2D section of the waste map is shown for the structured mesh results at 40 and 100 years. The significant portion of the vacuum vessel that can be considered as NAW is observed in this image. This type of analysis is important for identifying where the design of specific components needs to consider future dismantling.

Some of the advantages from using the unstructured mesh-based approach can be seen in Figure 9 by comparing the waste map between the structured and unstructured mesh approach. There are no results shown for areas of void when using the unstructured mesh approach, i.e. no material and void mixing, and there are no mesh elements that comprise more than one component.



**Figure 8. Radioactive waste map using structured mesh tally after a) 40 years b) 100 years shutdown.**



**Figure 9. Comparison of radioactive waste map from a) structured and b) unstructured mesh approach.**

#### 4.2. Use of the unstructured mesh capability

Radioactive waste assessments for fusion power plants using neutron flux data from MCNP have in the past been carried out using a cell-based approach. In this work, recent developments regarding the coupled use of MCNP and FISPACT-II with mesh-based neutron spectrum results, has been considered, along with the state-of-the-art unstructured mesh capabilities within the latest release of MCNP.

In theory the unstructured mesh approach is the most appropriate radioactive waste analysis method for informing design; there are no introduced errors through material mixing of

different components and materials, and reduced flux averaging by effective use of mesh elements. The method of using unstructured mesh in calculations is also advantageous as the mesh only covers the solid bodies of the model, increasing the efficiency of the mesh and removing unnecessary elements that take up valuable computing resource but are not needed. For example, in the 10° fusion tokamak sector model used in this work the structured rectangular mesh approach required breaking down into three individual mesh tallies to reduce the number of unused mesh voxels. Coupled 3D neutronics and activation analysis is ‘expensive’ both in terms of computational requirements and human time. The majority of human time is often spent creating neutronics compatible models for CAD to CSG conversion. The use of unstructured mesh modelling could better facilitate the use of ‘shared’ models between analysis teams, and shared time in creating suitable models. Currently the geometry requirements for a model to be converted into CSG result in neutronics specific and even analysis specific models being created. This is a large amount of human time which could be reduced with the development of unstructured mesh neutronics methods.

When creating the mesh geometry, the use of varying mesh refinements for different components, based on required detail and the complexity of the component, should be used carefully in order to make efficient use of computational memory resources.

### **4.3. Uncertainties**

Uncertainties regarding the results presented in this paper arise from a number of areas including, but not limited to: statistical methods, cross-section and decay data, resolution of result tallying and error propagation in the two-step method. Further uncertainties arise from the model itself: material definitions, location and design of components etc. The propagation of uncertainties using a two-step approach with FISPACT-II to perform radioactive waste calculations is an ongoing area of research. It is assumed that provided the statistical

uncertainty on the neutron flux is low, these propagation errors will be much smaller than those associated with activation cross-section uncertainties.

To produce neutron flux results with sufficient statistical uncertainty, and within an acceptable time frame, global variance reduction using a weight window generated from the Automated Variance Reduction Parameter Generator (ADVANTG) software was performed with the DEMO 2015 baseline neutronics model. This variance reduction was used with the cell-based and structured mesh simulations. The statistical uncertainty in the total neutron flux is below 5 % in the majority of mesh voxels for the structured mesh method used, with some higher errors in regions that present a 'deep shielding problem'. Statistical uncertainties within the cell tallies, as used for the cell-based method, were in general significantly lower, as the result is a neutron flux averaged over a large volume, which will be based on more histories than the result in a relatively small mesh voxel volume.

Global variance reduction using weight windows was not achievable with the unstructured mesh method therefore a long calculation time was required to increase the number of particle histories. The uncertainty information was not computed for each of the mesh elements comprising the unstructured mesh due to memory limitations and difficulties in interpreting and visualising the data. A structured mesh, computing total neutron flux and associated error, was superimposed and included in the unstructured mesh calculation. This showed that in-vessel components had reasonably good statistical uncertainty, below 5 - 10 % in the majority of mesh elements apart from some within the vacuum vessel. In some surrounding components outside the vacuum vessel there were poor statistics and in the case of the centre coils there were no results at all. A variance reduction technique is required with this model to achieve reasonable statistics in the ex-vessel areas.

## 5 Summary and conclusions

Three neutronics methods have been compared for use in radioactive waste assessments of fusion relevant computational models. The following conclusions and recommendations are made regarding the neutronics methods:

- The unstructured mesh approach has the potential to be a very useful tool to inform on component design, materials and dismantling to reduce quantities of radioactive waste.
- The conventional cell-based approach to radioactive waste analysis relies on flux averaging over cells comprising the geometry. This method is better suited to a well-established reactor design including detailed component geometry, where cells comprising the model are defined based on dismantling and separation plans.
- A mesh-based approach allows the dismantling and separation strategy of waste to be investigated. A significant increase in the level of detail acquired from simulation outputs can be obtained using a mesh-based method in comparison to cell-based, from what is essentially the same calculation. There is an increase in computational time as a FISPACT irradiation calculation is performed on every voxel instead of every cell, however these calculations are relatively quick compared to the neutron transport - which must be performed for either approach.
- In the case of a structured mesh, a material mixing step is introduced which is not ideal.
- The use of unstructured mesh geometry alleviates the materials mixing problem. The neutron flux is tallied directly on the mesh elements comprising the geometry with a FISPACT calculation performed on each of the elements.

Calculation of realistically representative absolute values for the quantity of waste produced from a demonstration power plant is not yet practical due to a number of factors. This would require definite waste classification limits for specific identified disposal routes, knowledge of the exact components, materials and dismantling opportunities (including bolts and fixings), and how the waste can be packaged. However, scoping calculations to inform the design of components for eventual decommissioning and disposal are very important and the unstructured mesh-based approach has the potential to be an advantageous method. Calculations with the current design information can also provide useful approximations regarding quantities of waste for development of a waste management plan.

The radioactive waste assessment using the EU generic 2015 DEMO model demonstrates some of the important aspects for a fusion relevant waste management plan. The results suggest that the use of dismantling techniques will be imperative in reducing the amount of ILW and LLW.

## **6 Future work**

The effect of different waste classes will be considered in further work, for example a system that does not allow for the clearance of any waste material created on a nuclear site.

Further testing of unstructured mesh geometry with global variance reduction techniques is a particularly important development requirement for producing a robust neutronics analysis method.

## **Acknowledgments**

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To obtain further information on the data and models underlying this paper, please contact [PublicationsManager@ccfe.ac.uk](mailto:PublicationsManager@ccfe.ac.uk).

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