

UKAEA-CCFE-PR(20)140

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Finite element analysis (FEA) is widely used in engineering to accurately model physical systems. FEA enables multi-physics investigations to be undertaken efficiently and increases the cohesiveness of interdisciplinary engineering assessments. Thanks to the recent implementation of the FEA Unstructured Mesh capability (UM) into MCNP6, radiation transport is now able to contribute more effectively to such multi-physics investigations. Furthermore, the use of UM in MCNP allows complicated components to be modelled more accurately since it does not have the geometrical limitations of the alternate Constructive Solid Geometry method (CSG), leading to more accurate simulations and inherent results. The ITER Electron Cyclotron-Upper Launcher (EC-UL) M3 Mirror is a complex component currently under design that had required various engineering assessments that utilise FEA such as mechanical and thermohydraulic. Therefore, this neutronics assessment took advantage of the UM capability of MCNP6.2 to be consistent with the other assessments. The peak volumetric nuclear heating for this component was found to be $3.76 \pm 22.0\%$ W/cm³ by this method. The total integral nuclear heating was found to be 6595.1 ± 0.6 W, an increase of 9.3% on the previous design but with a slightly different deposition distribution. Crucially, the total integral nuclear heating of the CuCrZr reflector was determined to be 142.92 ± 0.07 W, a decrease of 69% from the previous mirror design allowing the fulfilment of the mechanical code and standards.

Keywords:

- ITER
- MCNP
- Unstructured Mesh
- Nuclear Heating Density
- Finite Element Analysis
- ITER EC-UL M3 Mirror

1. Introduction

The unstructured mesh (UM) capability of MCNP6 is a relatively new feature of the software [1]. It allows complex geometries to be modelled more easily and accurately than with the alternate constructive solid geometry (CSG) [2,3,4] and has inherent results tallying. CSG is unable to model certain surfaces of order three and above and splines [5], necessitating simplifications for complicated models. While UM is also unable to model these surfaces, it approximates them using very fine planar or second-order surfaces. These UM approximations lead to near-full accuracy models that are much closer to the true geometry than what is achievable via CSG simplifications. To get mesh results tallying for CSG, the model must be overlaid with a structured mesh which introduces edge effect interferences [3,6], unless techniques such as the Cell Under Voxel (CUV) method are employed [7]. Whereas UM has inherent mesh tallying. Additionally, the UM feature enables more consistency between nuclear analysis and other engineering analyses that utilise finite element analysis.

The primary functions of the ITER Electron Cyclotron (EC) systems include control of magneto

hydrodynamic instabilities, plasma start-up and heating & current drive. The EC upper launcher (UL) of ITER contains mirrors to control the direction, and ultimately deposition, of EC microwave radiation beams. Like all major components in nuclear fusion reactors, the designs of these mirrors are subject to engineering assessments to ensure that they are fit for purpose and comply with requirements. The M3 mirror design contains splines and other surfaces that would require significant simplification with CSG, thus UM modelling was used to ensure greater geometrical accuracy. The water cooling channels, in figure 1, illustrate the complexity of the design.

2. Method

2.1 Preparation of the UM Model

The design of the M3 mirror consists of a reflecting CuCrZr 1 mm layer mounted upon a SS316L(N)-IG structure containing water cooling channels. The component also contains a SS316L(N)-IG support.

The finite element model (FEM) of the M3 mirror was meshed using the HyperMesh code [8] and consisted

of second order tetrahedral elements (4 pseudo-cells, 1018163 elements, 1393643 nodes). For large models such as this (> 1 million elements) it is recommended to use tetrahedral elements for better loading times and simulation rates [3]. The average element volume was $9.6e-3 \text{ cm}^3$. For consistency with other engineering disciplines involved in the wider assessment of the component, this model was unchanged from the one generated for thermo-mechanical analyses. This resulted in non-optimal voxel sizes for radiation transport purposes in terms of statistical uncertainty, since larger voxel sizes give improved sampling and statistical errors. To improve the statistics to align them with normal radiation transport uncertainties, voxels of approximately 1 cm^3 should be used. However, doing so would sacrifice the geometrical accuracy realised with smaller voxels and in this assessment, this accuracy and the consistency between engineering disciplines was prioritised over statistics.

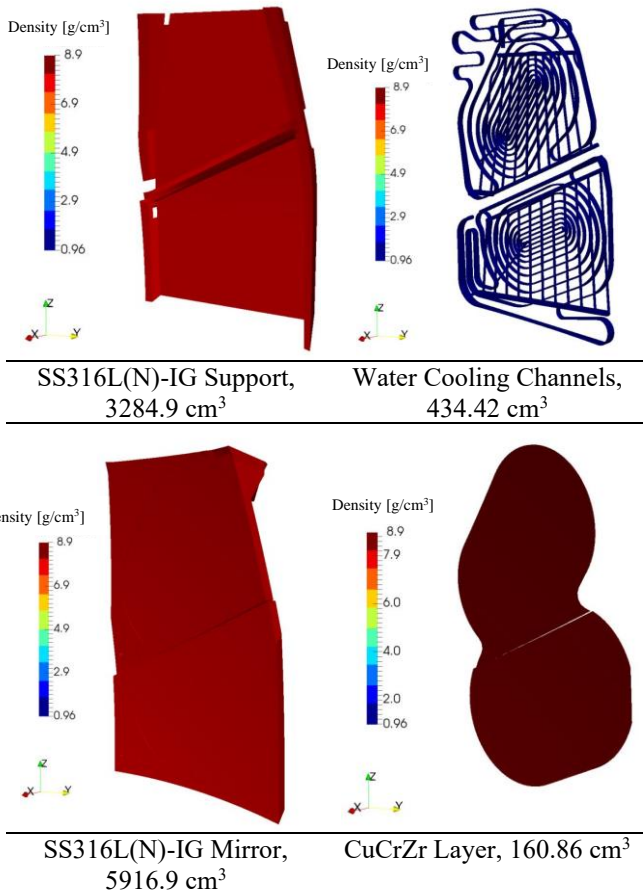


Figure 1. The pseudo-cells of the UM, their densities and volumes.

The HyperMesh model was converted to Abaqus format for MCNP integration. The Abaqus file was modified to make it fully compatible with MCNP [9], and then checked volumetrically and elementally using the MCNP pre operations utility program [1]. The volumes of the pseudo-cells were checked against the volumes in the computer-aided design file of the mirror, and the density assignments by a dedicated MCNP plot. Finally, an MCNPUM file containing additional mesh

details, such as nearest neighbour information, was created from the Abaqus file to reduce computational time for the radiation transport calculations [1]. The UM model is shown in figure 1.

2.2 MCNP Model

The UM feature of MCNP6 requires that the UM model be integrated into wider CSG geometry [1]. For this assessment, the UM M3 model was placed inside a neutronics model of the EC-UL integrated into the 40° ITER reference model, C-Model [10,11], which extends up to the bioshield. This UM-CSG integration is shown in figure 2.

Elemental edits are the UM equivalent of standard MCNP tallies; they give path length estimates of quantities as particles track from one element face to another and are inherent to the mesh elements [1]. To assess the nuclear heating of the mirror, elemental edits recording the heating due to neutrons and photons across the mesh elements were implemented.

The more traditional superimposed structured mesh FMESH tallies were also implemented as redundancies for the elemental edits. Explicit and implicit material $2x2x2 \text{ cm}$ FMESH tallies encompassing the mirror were included to assess the nuclear heating over the mirror. These were the standard FMESH tallies for this component, used for consistency with previous studies.

For variance reduction, the same methods were used as in the assessment of the previous mirror design, particularly the use of the same weight window file that was generated by global variance reduction [10].

The radiation transport simulation was run for $5e9$ NPS (number of source particle histories).

All other features of the model, such as the radiation source, were kept the same as in the original model [10].

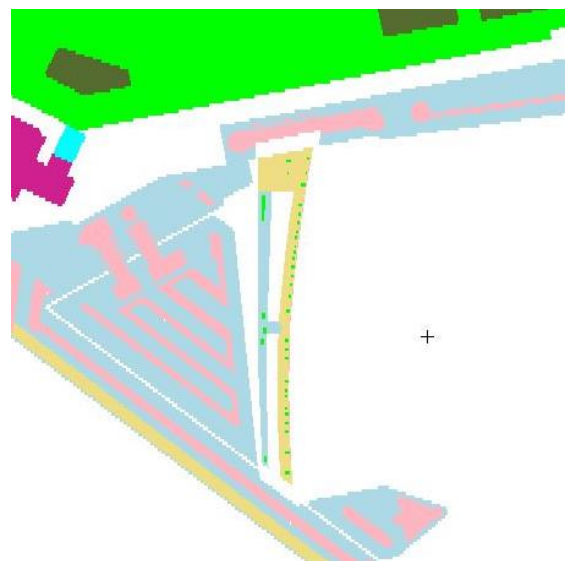


Figure 2. The UM model of the M3 mirror (centred with green markings) integrated into the CSG upper launcher MCNP model.

3. Results

3.1 Unstructured Mesh Nuclear Heating

The total integral and peak volumetric heating over the M3 model calculated by MCNP simulation are depicted in table 1 along with comparisons against the previous design of the mirror [10]. The volumetric heating over the model is shown in figure 3.

The total integral heating changes can be attributed to the volume changes of the components in the evolution of the EC UL M3 design, also shown in table 1. Specifically; the reduction of the CuCrZr layer, the increase of the SS316L(N)-IG structure and the increase of the water cooling channels.

The differences in heating peaks are due to both the evolution of the mirror design and the improved geometric modelling of the component.

Table 1. The volumetric and integral heating over the M3 model.

Pseudo-Cell		Volumetric Heating Peak [W/cm ³]		Total Integral Heating [W]	Total Integral Heating Comparison [%]	Volume Change [%]
		This UM Study	Previous CUV Study [10]			
SS316L(N)-IG	Support	2.94 ±9.82%	1.79 ±0.25%	2239.7 ±0.4	+14%	+16%
	Mirror	2.75 ±9.15%		3993.2 ±0.5		
CuCrZr		2.06 ±5.10%	2.49 ±0.82%	142.92 ±0.07	-69%	-66%
Water		3.76 ±22.0%	1.96 ±2.32%	219.20 ±0.10	+17%	+18%
Total		-	-	6595.1 ±0.6	+9.3%	+25%

The convergence criteria used for the UM elements was that the uncertainty be less than 25%. The UM elements were on average much smaller than the FMESH voxels, 9.6e-3 cm³ compared to 8.0 cm³. This necessitated the lenient UM convergence criteria to get results on an appropriate timescale. The large UM statistical errors were dominated by small elements and so only had limited effect on the Total Integral Heating, as shown by the low absolute uncertainties in column 3 of table 1. Therefore, although the UM results were more intrinsic to the component as they did not include volumes outside of the component (as is the case with FMESH, see section 3.2) and better geometrically represent the true component, for a given NPS when compared with the FMESH results, the peak values were less precise. This precision is shown by the uncertainties in column 2 of table 1 and column 3 in table 2, for an NPS of 5e9.

The comparison of volumetric heating peaks between this study that used UM and the previous assessment that used the FMESH CUV approach shown in table 1 also highlights the statistical weakness of the UM method. The CUV approach also has the same benefit as UM in that it is not subject to edge effect interferences since cells under the voxels are isolated. However, the CUV method is applied to CSG geometry and so the geometrical accuracy improvement provided by UM

over CSG is still present and especially important when the geometry is as complicated as it is with the M3 mirror. UM of course also has the benefit of improved consistency with other FEA engineering analyses, compared to the structured mesh methods, CUV or otherwise.

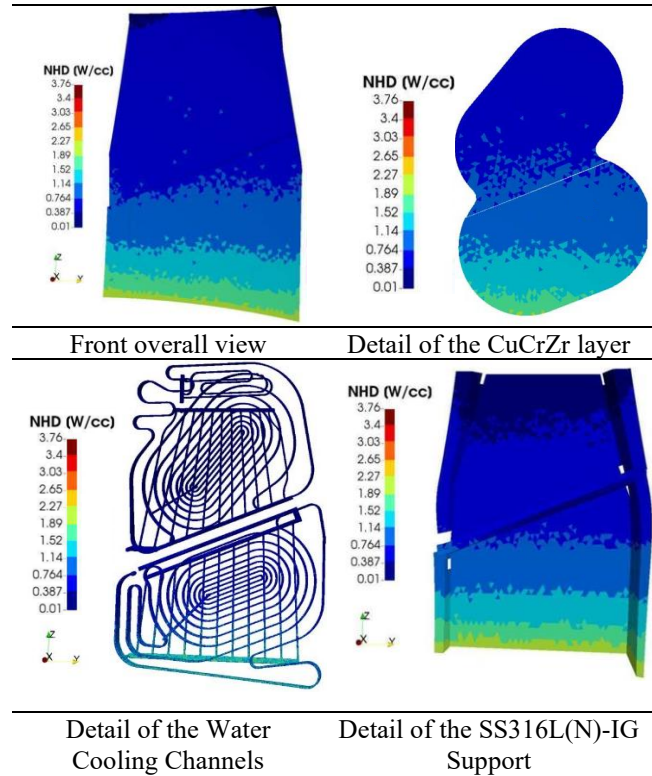


Figure 3. UM volumetric heating of the model in W/cm³, where the abbreviation ‘cc’ refers to cubic centimetre (cm³).

The plots of the mirror presented in figure 3 show that the nuclear heating it experienced was largely localised to one end. These plots were made possible due to the intrinsic results tallying of UM.



Figure 4. The 21 UM elements out of 1018163 (~0.002%) failing due to abnormal nuclear heating due to poor statistics.

Regarding the volumetric heating of the water due to neutrons; unphysically large, non-convergent results were found in a few, very small and sparsely distributed elements (21 of them, i.e. $\sim 0.002\%$ of the total), shown in figure 4. These values were treated as anomalies and discarded, however, subsequent engineering analyses that used these heating results required values for all elements in the FEA model. Therefore, with the approach used when this issue has previously been encountered [4], the structured mesh heating results (see section 3.2) were used to conservatively correct the anomalies for subsequent engineering analyses.

3.2 Structured Mesh Nuclear Heating

The maximum nuclear heating densities (NHD) for the implicit and explicit structured meshes are shown in table 2. For sequent engineering analyses the use of explicit structured meshes are recommended as they are more conservative than the implicit one. This implies the usage of three datasets, one per material, instead of the materials mixture.

Table 2. The maximum NHD for the structured meshes.

FMESH Type	Material	NHD _{max} [W/cm ³]
Implicit	All	4.72 ± 1.11%
Explicit	Water	3.58 ± 1.72%
Explicit	SS316L(N)-IG	5.12 ± 1.06%
Explicit	CuCrZr	5.76 ± 1.05%

It is worth highlighting here that the NHD maximums reported in table 2 do not correspond to the highest values of the materials, but to the highest values calculated in the structured mesh voxels. The structured mesh voxels covering the edges of the mirror also contained surrounding material since structured meshes cannot be shaped as necessary and can only be rectangular, cylindrical or spherical. Thus, the NHD maximums are highly influenced by edge effects and this inherent non-intrinsic property of structured meshes is a major weakness, which is not shared by UM. Therefore, the FMESH peaks are higher than the UM peaks, despite the FMESH voxels being much larger and thus having more averaging. This overestimation of heating at the edges of the component of interest has previously been investigated [3][6]. Structured mesh edge effects can, however, be mitigated using the CUV method which was employed in the previous assessment [10].

For subsequent engineering analyses, the maximum NHD for water was used to compute the volumetric heating where the UM volumetric heating of the water due to neutrons failed, as discussed in section 3.1.

The NHD maps of the structured meshes are shown in figure 5, overlaid on the mirror design. When compared with the plots in figures 3 and 6, the visualisation benefits associated with UM are evident.

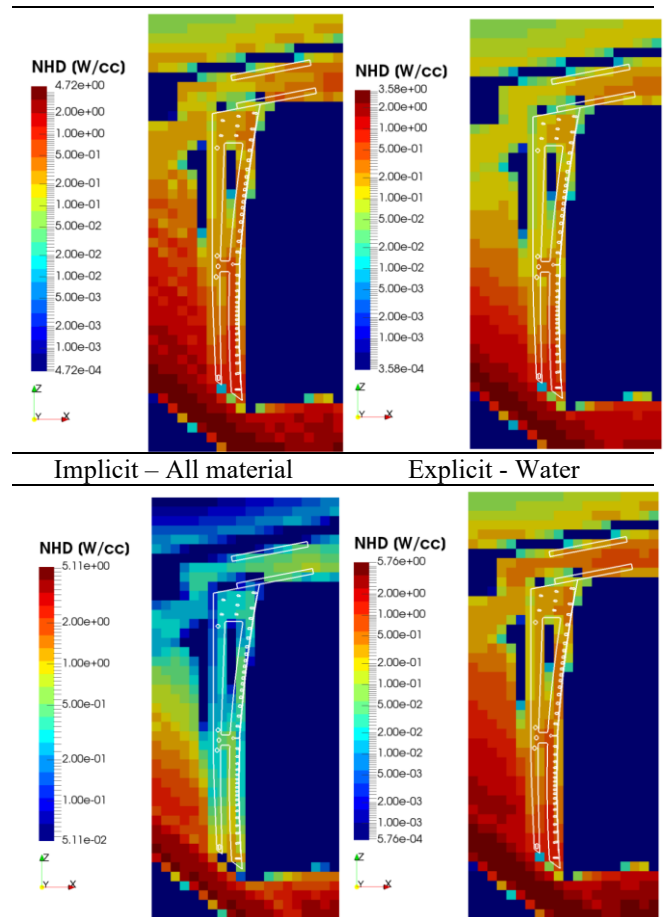


Figure 5. The NHD maps of a cross-section at $y=0$ of the structured meshes overlaid on the mirror design.

3.3 Post-Processing

The UM elemental edit output file (eeout) was converted to vtk format using mctools [9] for visualisation and preliminary nuclear analysis. For use of the data in wider, subsequent analyses, the vtk file was converted into both point cloud and IP Fluent formats using mctools [9], pandas [12,13] and a dedicated python script. A visualisation of the UM volumetric heating results in point cloud format for the mirror is shown in figure 6.

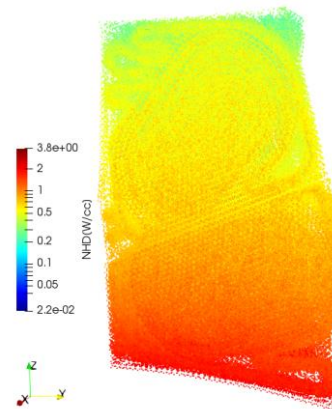


Figure 6. UM volumetric heating in point cloud format of the overall component.

3.4 Lessons Learnt

- It is recommended to order the pseudo-cells by number incrementally as well as the material number.
- It is recommended to double-check the material card/density/edit responses in the eeout file by means of dedicated isolated tests taking advantage of the vtk file generated with the tovtk feature of mctools [9]. This highlights possible mismatches in the eeout file generated.
- The FEM UM provided was of excellent quality and required no further modifications. It is understood that the preparation of the UM mesh should be assigned to an expert to optimize the UM model generation.
- The development of specific python routines enhances the data exchange between subsequent analyses.
- To account for the relatively poor statistics of small UM elements, NPS should be set as high as practicable and variance reduction should be capitalized upon, with the application of targeted weight windows for example.

4. Conclusion

The nuclear heating assessment of the EC-UL M3 mirror was computed by employing a FEM UM composed of second order tetrahedral elements and implementing it in a dedicated suited envelope within the MCNP EC-UL ITER C-Model. This was the realisation of the methodology, and the benefits of said methodology, investigated over the previous years [2,3,4,14]. Moreover, this allowed updating the M3 EC-UL mirror design with minor effort on the MCNP CSG side and having a one-to-one match with the subsequent analyses, such as thermo-mechanical analysis.

On this basis, nuclear heating (peaks and integral), were reported for the different M3 EC-UL components and compared with the previous design.

In addition, spatial structured distributions, which cover the entire EC-UL M3 and the related support, were determined for further possible applications. These proved necessary for subsequent wider engineering analyses, in order to compensate for small failures of UM elements when the UM is not optimised specifically for neutronics.

As this UM methodology is still in its infancy, it is important to take the lessons learnt from this assessment forward into subsequent applications of this methodology.

Crucially, the new design of the components passed the mechanical code assessment, of which, the nuclear analysis was executed with the use of UM.

Acknowledgments

This work was carried out using an adaption of the C-model which was developed as a collaborative effort

between AMEC Co (International), CCFE (UK), ENEA Frascati (Italy), FDS Team of INEST (PRC), ITER Organization (France), QST (Japan), KIT (Germany), UNED (Spain), University of Wisconsin-Madison (USA) and F4E (Europe). Some of the geometry modeling operations were performed using the SuperMC software kindly provided by the FDS-INEST Team.

The views and opinions here in do not necessarily reflect those of the F4E or the ITER Organization. F4E cannot be held responsible for any use which may be made of the information contained herein.

References

- [1] R. Martz. (2018). *The MCNP6 Book on Unstructured Mesh Geometry: User's Guide for MCNP 6.2.1*. LA-UR-18-27630.
- [2] H. Chohan, (2020). *Comparison between Unstructured Mesh and Simplified Constructive Solid Geometry Models of the Bioshield Airscrew*. F4E report 2JMNDB v1.0.
- [3] M. De Pietri, M. Fabbri, D. Laghi, and R. Pampin. (2019). *A preliminary assessment of MCNP unstructured mesh integration in the ITER neutronics model*. Fusion Eng. Design. 146 697-700.
- [4] D. Laghi. (2018). *Comparison UM vs FMESH on the EC Upper Launcher*. F4E memo 2EKFFF v1.2.
- [5] C. Werner (editor). (2017). *MCNP User's Manual: Code Version 6.2*.
- [6] M. Fabbri, R. Pampin. (2017). *Recommendations for the Implementation of Nuclear Heat Deposition Data in the Thermo-Hydraulic Analysis of the Vacuum Vessel Regular Sector*. F4E Memo 286648 v1.0.
- [7] P. Sauvan, J. P. Catalán, F. Ogando, R. Juárez, and J. Sanz. (2016). *Development of the R2SUNED Code System for Shutdown Dose Rate Calculations*. IEEE Transactions on Nuclear Science. 63 375-384.
- [8] Altair. (2017). *Hyperworks*.
- [9] Fusion for Energy. (2019). *Mctools*. <https://github.com/Radiation-Transport/mctools>
- [10] A. Lopez. (2019), *Upper Launcher Nuclear Heating, dpa and gas production*, MCNP Upper_Launcher_MCNP_Model_B2_used_for_D_YPP_YEL_v1_0.ABJKPGlopeza2. ITER report XKTNDB v2.0.
- [11] D. Leichtle, et al. (2018). *The ITER tokamak neutronics reference model C-Model*. Fusion Eng. Design. 136 742-746.
- [12] The pandas development team. (2020). *pandas-dev/pandas: Pandas*. Zenodo. v1.0.5
- [13] W. McKinney. (2010). *Data Structures for Statistical Computing in Python*. Proceedings of the 9th Python in Science Conference 445 56-61.
- [14] R. Pampin, et al. (2020). *Estimation of radiation conditions in the ITER electron cyclotron upper launcher with state-of-the-art simulation techniques*. Fusion Eng. Design. 157 111682.