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Neutronics model developments for the IFMIF-DONES test cell

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This work presents the development and evolution of the test cell (TC) neutronics geometry models for IFMIF-DONES (International Fusion Materials Irradiation Facility–Demo Oriented Neutron Source), supporting detailed Monte Carlo–based nuclear analyses for design assessment and optimization. Beginning with the IFMIF/EVEDA configuration, successive model versions have been developed to reflect major DONES design updates, including the design changes to a single accelerator and test module, revised target assembly (TA) and High Flux Test Module (HFTM) designs, relocation of the quench tank, and the introduction of removable biological shielding blocks (RBSBs). To balance modeling accuracy and computational efficiency, both high-fidelity and lightweight geometry representations were investigated. Sensitivity studies on geometry boundaries and levels of simplification demonstrate that key irradiation performance metrics, such as neutron flux and damage doses, are well preserved when essential TA and HFTM features are retained. Simplified yet representative target and HFTM models were validated for use in accelerated simulations. In parallel, an unstructured mesh-based HFTM model was successfully implemented and benchmarked against conventional CSG-based models, showing excellent agreement.

KEYWORDS
CAD, CSG, IFMIF-DONES, Monte Carlo, neutronics

1 Introduction

The IFMIF-DONES (International Fusion Materials Irradiation Facility–Demo Oriented NEutron Source) facility (Ibarra et al., 2025) is being constructed to qualify structured and functional materials for use in the design, licensing, and operation of fusion reactors such as DEMO. The facility will be based on a deuteron accelerator (125 mA, 40 MeV) that impinges on a liquid Li target, producing an intense neutron flux of up to 10^{15} n/cm^2/s. The test cell (TC) is a well-shielded, atmosphere-isolated area housing the Li target and the test modules. It is the key region where intensive nuclear analyses are performed, including DPA and gas production, nuclear heating, material activation, source term evaluation, beam-on and beam-off dose rates, and assessment of radiation impact on neighboring cells. These analyses rely heavily on the geometry model of the test cell, taking into account detailed component structures, interfaces, and areas of interest.

The neutronics models of the TC, specifically, the input geometry for Monte Carlo (MC) particle simulation codes such as MCNP (Werner, 2017), have been continuously developed yet not fully presented and documented. The DONES TC neutronics model was initially built based on the IFMIF/EVEDA (IFMIF Engineering Validation and Engineering Design Activities) design concept and was subsequently updated with major design modifications, including repositioning of the quench tank (QT), adoption of new designs for the target assembly (TA), High Flux Test Module (HFTM), removable biological shielding blocks (RBSBs), and other key components. In addition to the baseline model, simplified, detailed, and mesh-based models have also been developed. This work intends to present a summary of the evolution of the neutronics modeling of the TC since the beginning of the IFMIF-DONES project. These different versions of the TC neutronics model will be discussed in detail in the following sections.

2 Geometry modeling methods

The CAD-to-MC workflow has been well-established over the past decades to enable preparation of complex geometry models, such as in the ITER neutronics model (Juarez et al., 2021). The workflow begins with a pre-processing step, which is often time-consuming yet indispensable. This step involves CAD geometry defeaturing, volume homogenization, and integrity and interference checks. With the assistance of tools such as SpaceClaim®, this process has been significantly streamlined. The result is a neutronics-ready CAD model, often referred to as the "neutronic CAD model."

The next step involves geometry conversion using CAD-to-MC tools, such as McCad (Lu et al., 2016), SuperMC (Wu et al., 2015), and recently the GEOUNED (Catalán et al., 2024) program. These tools follow a similar workflow: first, the CAD solids are decomposed into a set of solids that enable unambiguous Constructive Solid Geometry (CSG) descriptions using surface Boolean operations. Then, the void spaces surrounding the CAD solids, which are often invisible in the original CAD model but must be explicitly represented in the MC model, are described using Boolean operations on the solid boundaries and the sub-spaces. The outputs of this process are input files for MC simulation codes, with materials assigned to each CSG solid. Alternative approaches such as using the facet geometry (Wilson et al., 2010) and the unstructured meshes in MCNP6 (Werner, 2017) reduce the restrictions on the surface types and the void space descriptions, while also bringing additional cost on faceting and meshing workflow and simulation time.

The above geometry conversion is followed by a series of geometry checks and model assembly. Geometry checking often uses a source emitting particles from a spherical surface surrounding the entire model, with empty material assignment, and particles directed inward along the sphere normals. This procedure both identifies potential geometry errors, such as overlapping cells or incorrect Boolean expressions, and computes the volume of the simulation model using the MC approach. As a standard guideline, the particle loss rate has to be less than one per million particles, assuming particles are lost in various parts of the geometry and not localized near the area of interest. The computed volumes are cross-checked against the CAD volumes of the corresponding solids and cells, sorted by volume size to identify outliers. These outliers often indicate problematic solids, except in cases of very small volumes, which usually exhibit higher relative errors in the volume calculations. The particle loss rate and the volume comparisons for the neutronics models discussed in the following section have been strictly verified according to these guidelines.

3 DONES TC model evolvements

3.1 Initial model based on IFMIF/EVEDA design

The initial version of the DONES TC neutronics model is shown in Figure 1. It has a layout similar to the current neutronics model and was inherited from the IFMIF/EVEDA model (Kondo et al., 2014), adapted to the baseline design of DONES. First main difference is that DONES uses one accelerator instead of the two used in IFMIF. The source of one accelerator is deactivated in the setup of the d-Li neutron source subroutine McDeLicious (Simakov et al., 2012), leaving one dummy beam duct in the model. Another change in the baseline is the removal of test modules in the medium flux zone (e.g., the Tritium Release Test Module and the Creep Fatigue Test Module) as well as the low-flux test modules. Only the High Flux Test Module (HFTM) is included in the DONES baseline. Note that the HFTM model is a "thin" version (Kondo et al., 2014), approximately 5 cm in thickness, arranged in 3 rows and 8 columns of capsules. The quench tank, which captures the high-speed Li from the target, is located outside the test cell to reduce tritium production from the Li-nat (n, x)H-3 reaction. Apart from these features, the magnetite heavy concrete shielding is 4 m thick at the downstream side and at the lateral walls, and 3.5 m thick at the upstream wall. The concrete shielding is manually layered in the geometry for variance-reduction purposes, allowing different cell "importance" values to be assigned to the layers to reduce statistical variance in the outer regions. This version of the model was converted using an early version of the McCad program, and is designated as version "mdl6.9" with a versioning convention inherited from the IFMIF design activities. Major version denotes a complete re-modeling of the test cell geometry, while minor version changes denote component updates and corrections.

3.2 DONES oriented TC model

Several design changes in the test cell have made the IFMIF/EVEDA-based model no longer suitable. The target assembly first adopts the so-called "bayonet back-plate" design (Micciché and Riccardi, 2005), in which the back-plate is mounted to the target assembly using a sealing gasket. In addition, the quench tank was relocated inside the TC to resolve Li-flow instabilities along the long channel (Gordeev et al., 2016) and to mitigate neutron streaming. The HFTM has also been redesigned, increasing the thickness of the 4 × 8 capsules to accommodate more material samples (Qiu et al., 2018). In the new version of the TC model shown in Figure 2, the detailed geometric features of the TA and the HFTM were constructed consistently with the engineering CAD model, allowing a renewed evaluation of DONES damage doses, gas production, heating, etc. (Qiu et al., 2018). The heavy concrete shielding with a monolithic design is still used, complemented by the neighboring rooms to assess the radiation impact of the TC on adjacent areas. The second beam duct has been blocked with a shielding plug, and the Li inlet/outlet is enclosed within an interface cell filled with shielding. This model is designated as "mdl8.3.0," representing the first DONES-based neutronics model that departs from the IFMIF/EVEDA-based configuration. A comprehensive set

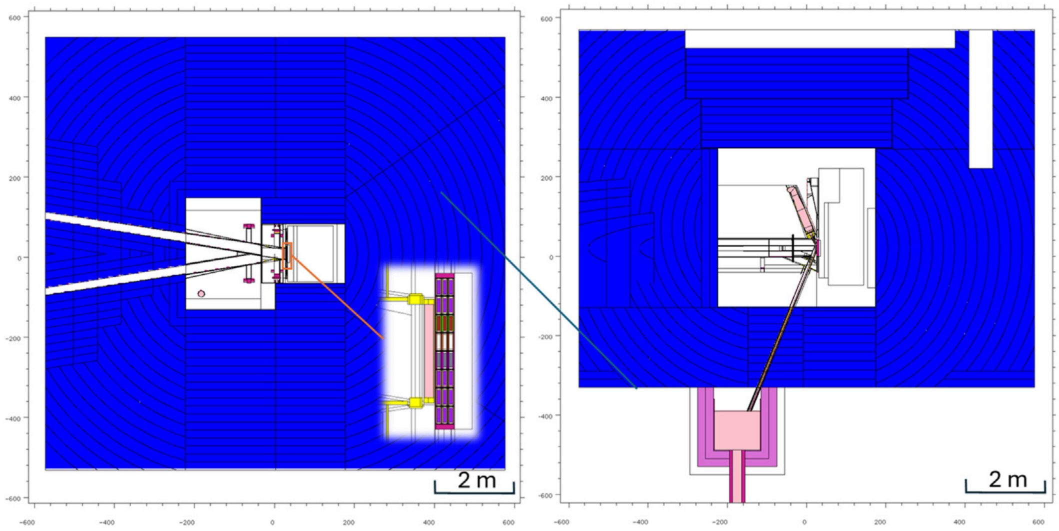

FIGURE 1
The initial version of DONES TC neutronics model based on IFMIF/EVEDA design (left: horizontal view, right: vertical view).

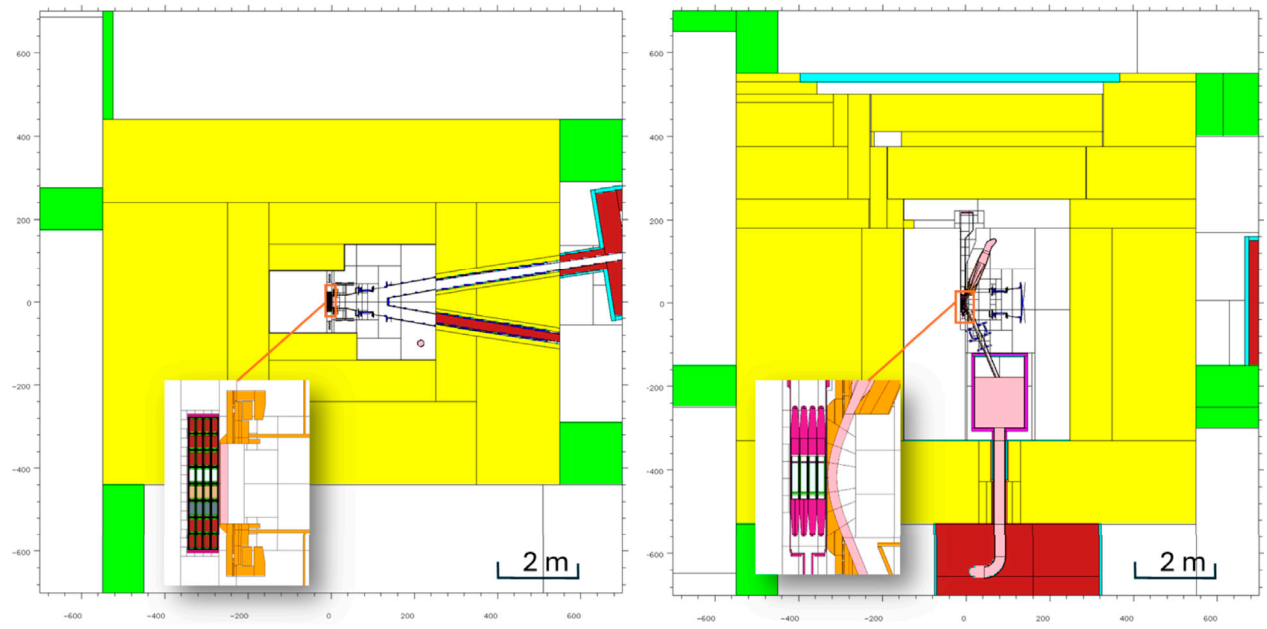

FIGURE 2
The DONES TC model with thick HFTM design and bayonet back-plate TA (left: horizontal view, right: vertical view).

of nuclear analyses has been provided in (Qiu et al., 2019) on this model.

3.3 Modular TC neutronics model

Figure 3 shows the first modular test cell model, based on a skeleton geometry concept populated with detailed components. Space-holders for the TA, HFTM, the region behind the HFTM, the shielding walls, shielding plugs, and other major structures have been implemented, except for components that are difficult to isolate geometrically, such as the steel liner surrounding the inner TC space. This model incorporates the newly introduced maintainable TC concept, in which the inner monolithic concrete shielding around the inner TC is divided into 11 removable bio-shield blocks (RBSB), designed with doglegs to mitigate neutron streaming. The bayonet back-plate TA design has been reverted to the “integrated” back-plate configuration due to the lack of suitable gasket materials capable of withstanding the intense irradiation at the target region (Nitti et al., 2025). The detailed structures of the shielding plugs—such as the lower shielding plugs—have been filled with the

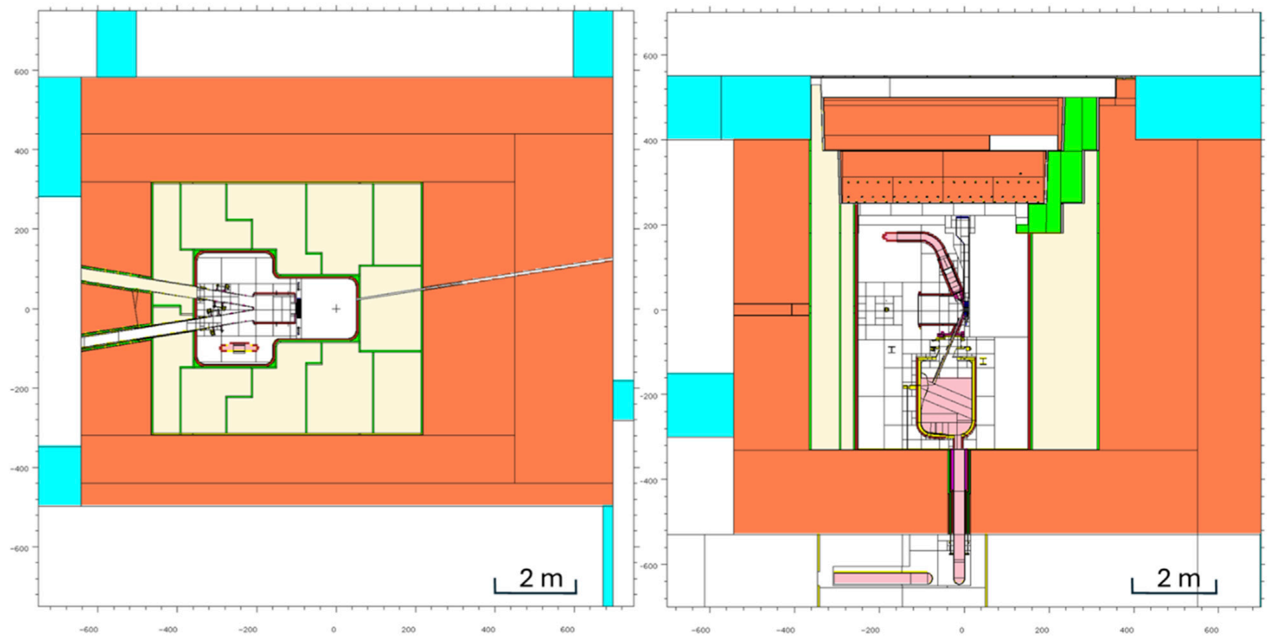

FIGURE 3
Modular TC neutronics model with RBSB design (left: horizontal view, right: vertical view).

actual piping layouts, while the piping associated with the liner and the shielding blocks remains incomplete, as the design is still under development. A neutron beam tube has also been newly introduced in this model to guide neutrons from the test cell to a neighbouring room for complementary experimental activities. The aim of this modular model is to facilitate the design updates, and reduce modelling effort in the analysis workflow. The improvements on the computational speed and memory consumption is therefore not actively monitored, yet no significant penalties are observed.

Another important update concerns the materials. The EUROFER composition from (E. F. D. Agreement, 2006) has been adopted to maintain consistency with DEMO neutronics activities. The ordinary and heavy concrete (Barabash, 2019) used in the ITER neutronics calculations has been selected as reference concrete for the TC shielding, owing to its well-characterized compositions and certified production data. The converted geometry maintains strong consistency between the neutronics CAD model and the simulation model, enabling modifications and reconversions with minimal effort. This model is designated as “mdl9.2.1,” representing a major release.

3.4 Current TC model inside the DONES global model

The latest version of the TC model is presented in Figure 4. This model addresses many of the current design requirements and incorporates several shielding optimizations. The engineering features of the RBSBs have been improved, and the thickness of the inner steel liner has been increased to enhance heat removal capability. The upper shielding plugs have been modified to accommodate HFTM piping, and the TC cover plate (TCCP) is now filled with shielding material to mitigate neutron streaming through the RBSB gaps. The floor liner thickness has also been increased to improve heat removal functions. Heavy concrete continues to be used inside the RBSBs, as it provides both effective shielding and good thermal conductivity, whereas the concrete in the surrounding bucket structure has been switched to ordinary concrete to reduce cost while shielding requirements are still met. At the beam downstream side, a beam tube and a shutter have been included to guide and control the neutron beam extracted from the inner test cell.

The entire TC geometry has been newly integrated into the main building model, which is based on the baseline IFMIF-DONES main building in 2022. This integration enables assessment of the radiation impact from the TC on neighboring areas such as the accelerator area, the access cell above the TC, and the complementary experimental room downstream. It also supports large-scale safety evaluations, including public dose assessments via sky-shine and direct radiation pathways. This model is designated as “mdl9.2.7,” and currently serves as the baseline model for TC neutronics analysis, reflecting the most relevant and up-to-date TC design.

4 Simplified and detailed model of target and test modules

4.1 Comparison of model with different geometry boundary and details

It is generally understood that the model should be as detailed as possible to obtain the best estimation of the irradiation performance of DONES. Throughout the development of the DONES TC model, the level of geometric fidelity and its impact on the simulation results

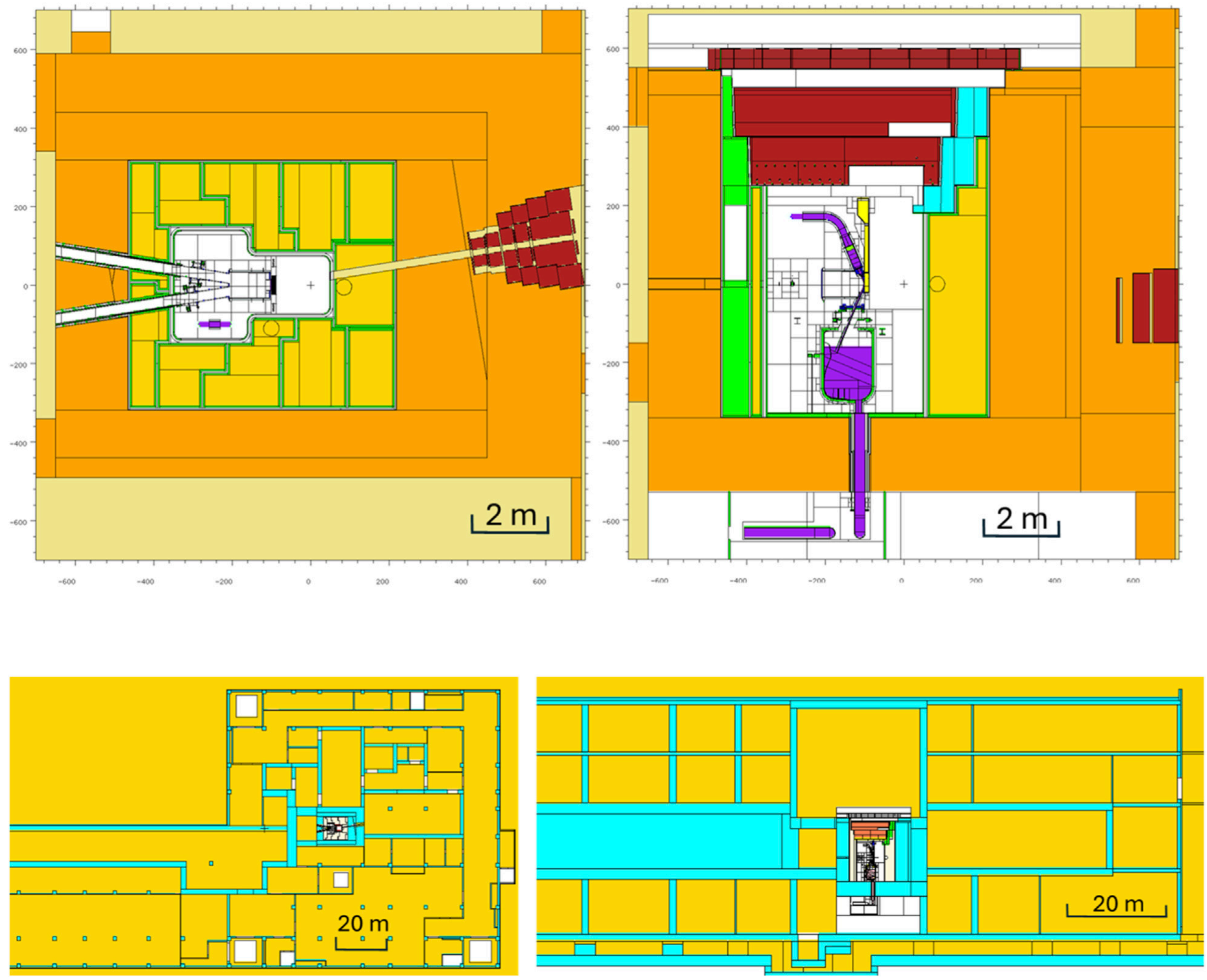

FIGURE 4
Current TC model inside the DONES global model (left: horizontal view, right: vertical view).

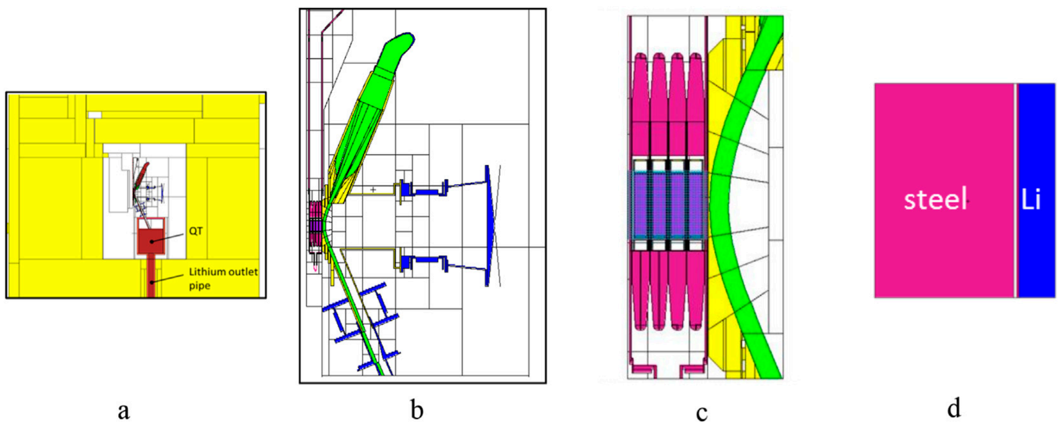

FIGURE 5
The plot of geometry model with different geometry boundaries and details **(a)**. Full DONES **(b)**. TA+HFTM **(c)**. Truncated TA+HFTM **(d)**. Simple block.

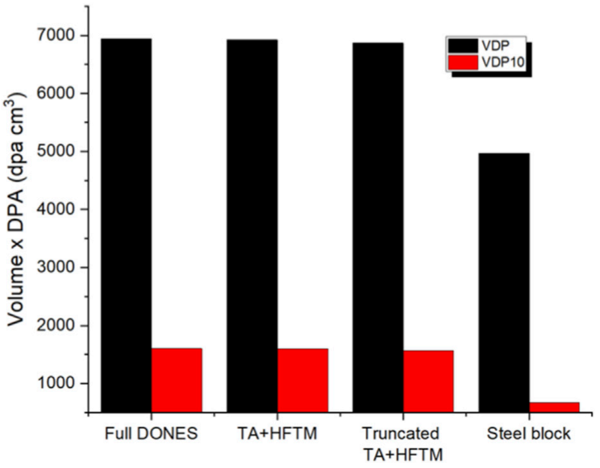

FIGURE 6
Comparison of four geometry variances on the VDP values.

have often been discussed. To address this, several model variants were created and compared so that the impact of geometry assumptions, particularly for damage dose simulations in the high-flux region, is clearly understood.

The first study focused on the geometric boundaries of the model and their influence on the calculated damage doses. The simulation model is not the latest, but the conclusions remain relevant. Compared with the full DONES model shown in Figure 5a, the first geometry variant includes most of the TA and HFTM components, as illustrated in Figure 5b. To further reduce the number of geometry cells, the second variant reduces the size of the envelope that contains the detailed TA and HFTM cells (Figure 5c). The third variant uses an extremely simplified block configuration (Figure 5d), consisting only of a Li target, a EUROFER backplate, and a uniform block made of a mixture of EUROFER, sodium, and stainless steel.

The primary concern for HFTM is the damage dose (or DPA, displacements per atom), while DPA is a distributed value that varies by orders of magnitude within the HFTM. Therefore, volume must

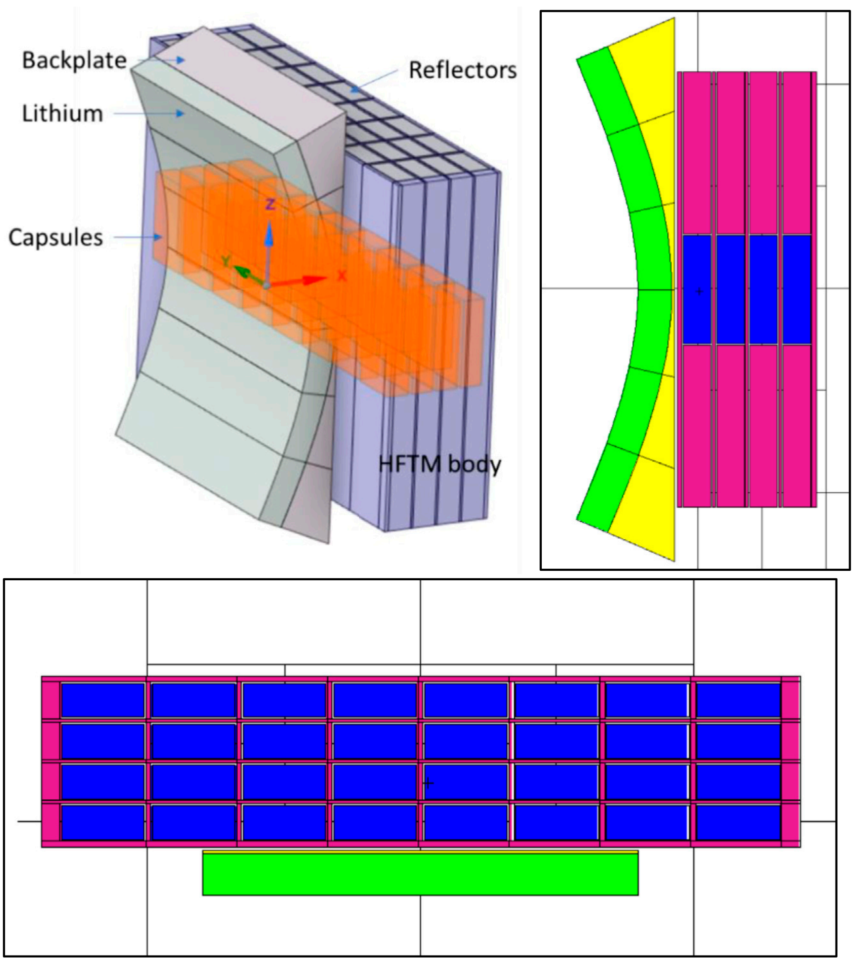

FIGURE 7
lightweight TA and HFTM model with key features and materials. The first plot (top-left) is a 3D view highlighting the capsules. The second plot (top-right) are the vertical cut view at center X-Z plane, and the third plot (bottom) is the horizontal cut-view at the center X-Y plane.

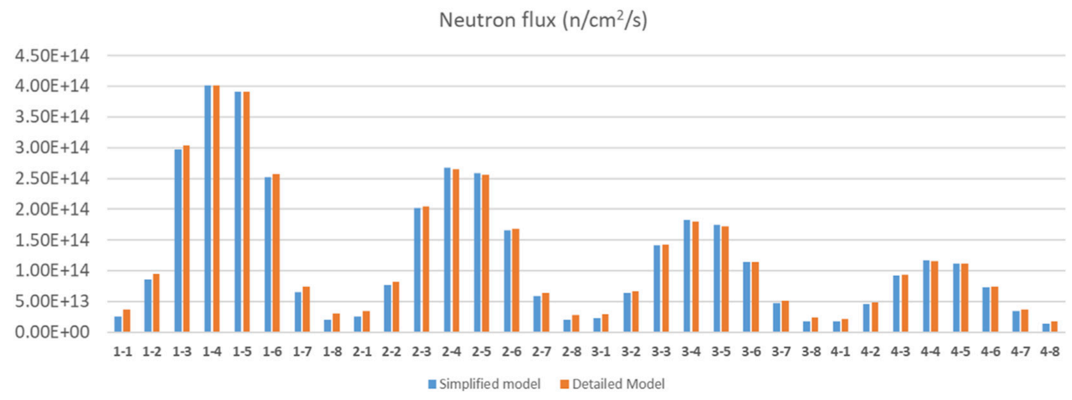

FIGURE 8
Neutron flux (n/cm^2/s) calculated for the simplified and detailed model using McDeLicious.

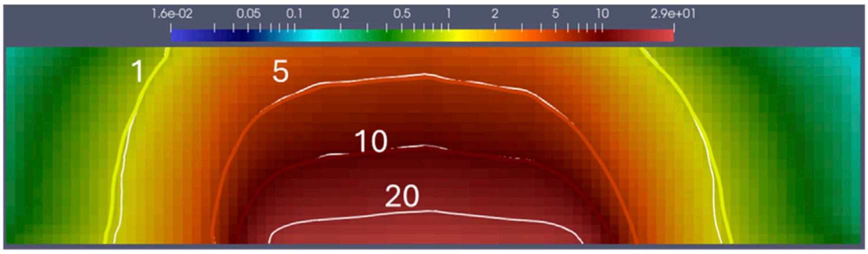

FIGURE 9
Damage dose (dpa/fpy) map plotted horizontally at the beam level. The colourful contour line is calculated using the detailed model, and the white color contour line is from the simplified model.

be integrated as a metric alongside DPA. Utilizing average DPA obscures localized high-DPA values, whereas peak DPA remains highly sensitive to the beam profile. The product of DPA and volume—named the "volume-DPA product" (VDP)—is therefore used as a metric to evaluate model discrepancies, giving higher weight to high-DPA regions. VDP10 represents the VDP over 10 dpa/fpy. Figure 6 presents the comparison of VDP values. The first two variants in Figures 5b,c, which retain detailed TA and HFTM geometry, produce similar results with <1% of deviations on VDP and <2% on VDP10, whereas the third variant shows a significantly different VDP and VDP10. This discrepancy arises because the over-simplified geometry excessively moderates the neutrons and inadequately represents the TA and HFTM structures.

4.2 Simplified version of TA and HFTM model

An over-simplified geometry is not representative of the DONES TA and HFTM. However, in many cases—particularly for accelerating simulations and optimizations—a lightweight model is necessary to reduce the number of geometry cells, thereby shortening simulation time while still preserving acceptable result quality. For this reason, a lightweight target and test-module model has been developed, as shown in Figure 7. This model preserves the key components of the TA and HFTM: the Li target, the EUROFER backplate, the HFTM body, the capsules, and the upper and lower reflectors. The TA is truncated laterally at the Li channel and vertically above and below the reflector levels. For the HFTM, the mixture of material samples follows the composition as in the full model (75% EUROFER, 25% sodium), while the capsules and HFTM body are made of SS316LN. The helium cooling channels of the HFTM are homogenized with the structural material, preserving the helium volume fraction (31%) and SS316LN fraction (69%) in the material definition.

This simplified model has been validated through comparison simulations under equivalent conditions—using the McDeLicious code with the *ad hoc* d-Li data as the neutron source and the FENDL-3.1d nuclear data library (FENDL, 2025). The comparison of total neutron flux, shown in Figure 8, demonstrates good agreement within 2% for the central four columns of capsules, with slightly higher deviations in the lateral capsules due to the absence of detailed TA structures (channels, etc). This effect is clearly visible in Figure 9, in which the DPA maps and the contours have been plotted. The DPA contour lines from the detailed model (with color lines) are plotted together with the contour lines obtained from the simplified model (white color). They are nearly overlapping in the central region but slightly diverge toward the sides. Since only the central four columns are used for irradiating material samples, and the lateral capsule volumes serve mainly as reflectors or are reserved for lower-dose

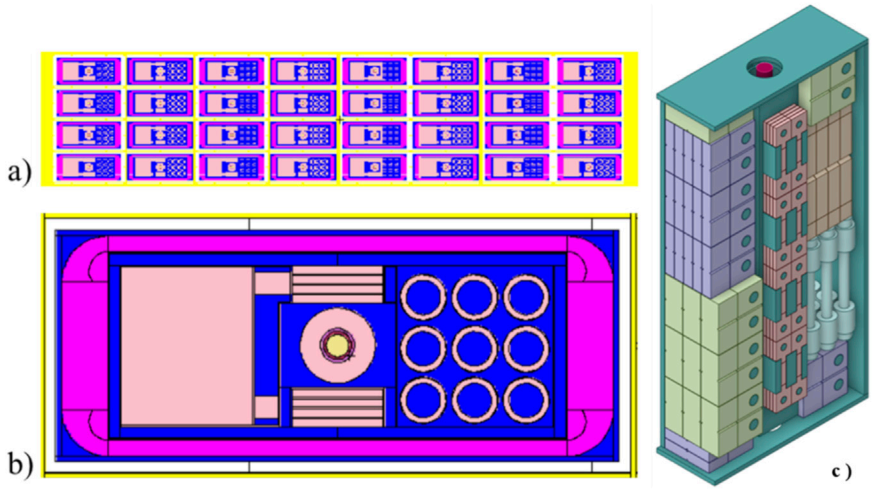

FIGURE 10
Detailed payload CLCv2.0 and the plot of neutronics model for HFTM with detailed samples (Arbeiter, 2023; Álvarez et al., 2025). The figure **(a)** is the horizontal cut view of the HFTM, **(b)** is the zooming view on one specimen capsule, and the **(c)** is the CAD model of the specimens payload.

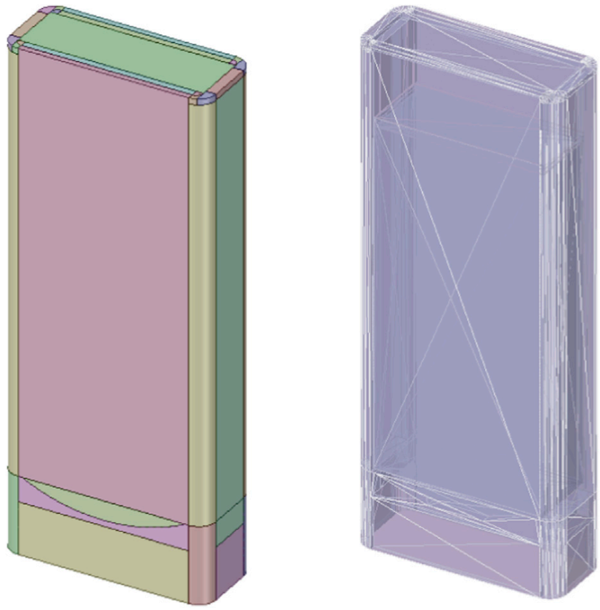

FIGURE 11
The visual comparison of the CSG model (left) and the TT mesh model (right) of a specimen capsule.

irradiation activities, deviations in the lateral regions are not critical. However, caution should be applied for any dedicated analysis involving the outer capsules.

4.3 Detailed HFTM model with geometry of material samples

Opposite of model simplifications, another direction in model development is to further increase the level of detail in the simulation geometry, for example, by explicitly modeling the HFTM specimen geometries to obtain sample-wise results. Concerns have been raised that, for a long time, the samples in the HFTM have been represented as a homogeneous mixture of EUROFER and sodium, whereas the real payload configuration has not been fully defined. The work in (Arbeiter, 2023), (Álvarez et al., 2025)provided the first attempts to model the detailed payload inside the HFTM, shown in Figure 10 with a 3D view of the CAD geometry and the cut views of the neutronics model, working with materials experts to define the number and types of specimens as well as a reference payload. Although not fully optimized, the payload version CLCv2.0 (acronym for Capsule Loading Configuration) achieves a relatively high EUROFER volume fraction of 85%, which is greater than that of the homogeneous model discussed in previous sections.

Based on the simulations reported in (Álvarez et al., 2025), the neutron flux and damage doses—both integrated values and spatial/energy-resolved distributions—are very similar between the HFTM models with detailed specimens and the one using homogeneous materials. These studies confirm that neutron irradiation performance is not very sensitive to subtle geometric features of the HFTM neutronic model, largely because neutron energies are high and the mean free path is long. Therefore, it was shown that the HFTM model with homogeneous samples is often sufficient, when the target area is not the primary focus of the analysis.

5 Mesh simulation geometry

The models above are based on the CSG modeling approach, which is the standard method for geometry representation in Monte Carlo codes such as MCNP. With the availability of the unstructured mesh capability in MCNP6, a mesh-based model of the HFTM becomes advantageous for rapid design and optimization. In this work, the fast tetrahedral meshing approach described in (Qiu et al., 2015) has been used to

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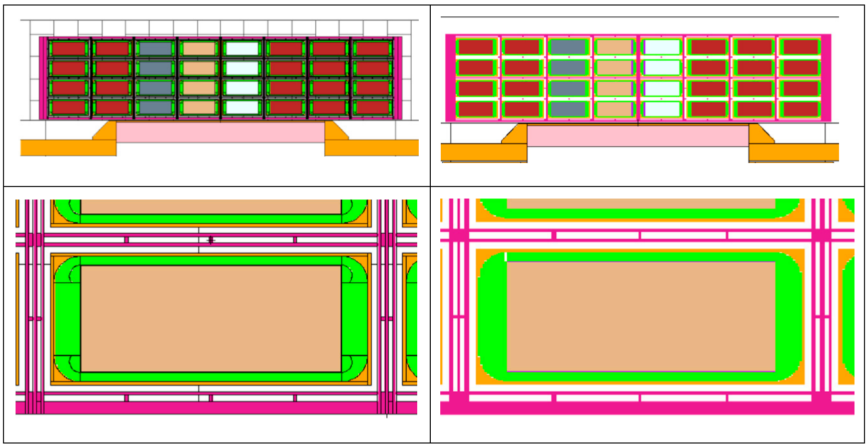

FIGURE 12
The visual comparison of the MCNP plot of the CSG model (left) and the TT mesh model (right). The mesh boundary are not possible to be visualized, only the colour is provided. Some artifacts in the right plots are due to the MCNP plot but not the geometry issue.

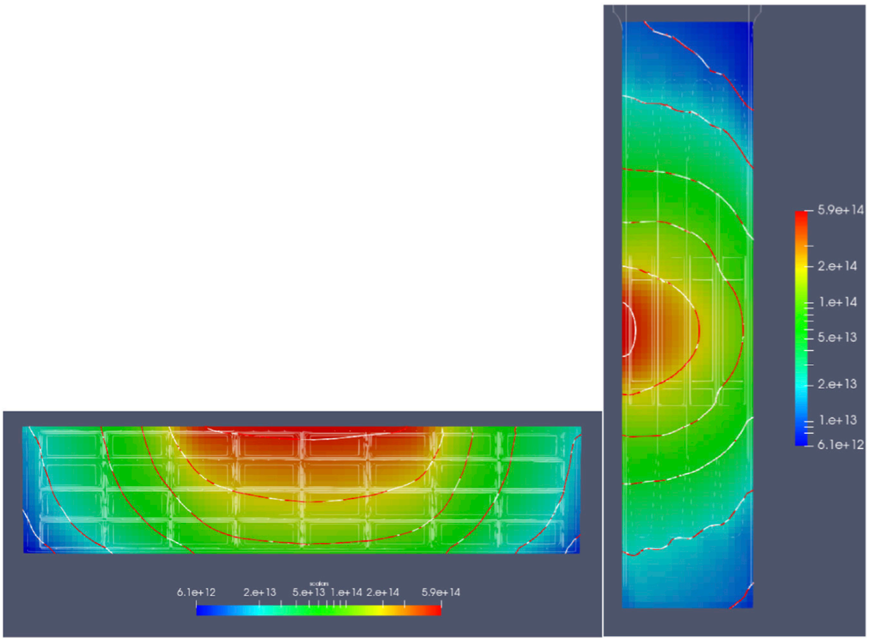

FIGURE 13
The neutron flux (n/cm^2/s) profiles calculated on the CSG and the TT mesh model. The left plot is a horizontal cut view, and right plot is the vertical cut view at target center. The red contour is produced from the CSG model, and the white contour is from the mesh model.

build the first HFTM mesh model. The neutronics CAD model shown in Figure 2 was converted into a mesh model while maintaining full consistency between the meshes and the original CSG cells. This aims to verify whether the mesh geometry can be effectively used for HFTM descriptions.

The CAD model was converted using a SpaceClaim plugin. The workflow consists of exporting the geometry to an STL file, calling the TetGen code (Si and TetGen, 2006) to generate a tetrahedral mesh, and then post-processing the resulting mesh into the Abaqus format for the MCNP6 code. Using this workflow, the mesh illustrated in Figure 11 was generated within a few minutes. The produced mesh model is plotted in MCNP6 and compared visually with the CSG model in Figure 12. The mesh model has been later integrated into the test cell model “mdl8.3.0,” replacing the previous CSG HFTM model in the envelope.

Simulations were run on the mesh model, and the neutron flux distributions computed using the CSG model and the Tessellation-Tetrahedralization (TT) mesh model are shown in Figure 13. Total mesh elements for the TT mesh model is 157 thousand. The CPU time for 10^9 histories is 950 h on the CSG model, while around 13,500 h for the TT mesh mode, which is more than 10 times than CSG model. The reason is mainly due to the fact that the CSG solids and mesh sets have been matched one-to-one, increasing particle tracking efforts. Combining mesh sets with the same material can significantly reduce the simulation time, which is to be tested in the future. The contours overlap almost perfectly, demonstrating excellent agreement between the two simulation results. A successful demonstration of the mesh-modeling approach for DONES nuclear analysis was therefore made, and further development and validation of this method are planned in order to use it for production simulations.

6 Summary and outlook

The development of the TC neutronics geometry has been presented in this work, starting from the IFMIF/EVEDA-based geometry, progressing to the first version of the DONES geometry, then to the modular design of the TC model, and finally the recent updates and integration into the global model. This evolution consists of a series of baseline changes, such as adopting a single accelerator and one test module, modifying the TA and HFTM designs, introducing the RBSB shielding, implementing detailed piping for the shielding plugs, adding the neutron beam tube and shutter, and more. These developments enable the assessment of DONES irradiation performance, facilitate design optimization of the HFTM, target, shielding, and support verification of the TC radiation safety requirements.

In addition, to provide either best estimations or accelerated simulations, the target and test module have been studied using both simplified and more detailed geometry representations. The impact of geometry fidelity on irradiation performance metrics, such as damage doses, has been evaluated. The results show good consistency (<2% of deviations) among these versions of the models on the VDP values, with the exception of the extremely simplified steel-block model. Furthermore, the HFTM unstructured mesh model has been produced and has verified the mesh-based geometry approach, demonstrating successful use of the fast TT meshing method, admitting the drawback that the CPU time is increased by more than a factor of 10.

Further improvements can be made on several fronts. One priority is enhancing the space-holder design by defining component boundaries more appropriately, taking into account the latest geometry layout. A stricter CAD-to-MC correspondence is also required, including the consistent indexing of cells according to the PBS (Product Breakdown Structure) numbers, as some manual modifications to the input currently remain. Moreover, the versioning and branching of the models need to be managed in a more structured way, ensuring that different versions can be used for specific purposes while keeping the simulation models and results traceable.

Data availability statement

The datasets presented in this article are not readily available because Available within the funding projects. Requests to access the datasets should be directed to https://euro-fusion.org.

Author contributions

YQ: Data curation, Formal Analysis, Methodology, Software, Validation, Visualization, Writing – original draft, Writing – review and editing. AS: Data curation, Formal Analysis, Software, Writing – review and editing. IA: Data curation, Formal Analysis, Methodology, Resources, Writing – review and editing. FM: Data curation, Formal Analysis, Visualization, Writing – review and editing. AČ: Data curation, Formal Analysis, Resources, Validation, Writing – review and editing. SB: Formal Analysis, Investigation, Writing – review and editing. JC: Formal Analysis, Investigation, Resources, Writing – review and editing.

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