

## Methodological approach for DEMO neutronics in the European PPPT programme: Tools, data and analyses



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### HIGHLIGHTS

- Development of computational tools for neutronics simulations.
- Development of nuclear data for fusion applications.
- Generation of neutronics DEMO models.
- Nuclear analyses for breeder blankets, shield systems and toroidal field coil.
- Activation, decay heat and shut-down dose rate analyses.

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### ABSTRACT

The methodological approach employed for the neutronics in the PPPT (Power Plant Physics and Technology) programme of EUROfusion is presented. It encompasses development works on advanced computational tools and activities related to the nuclear design and performance evaluation of the DEMO power plant including safety, maintenance, and waste management issues. Development work is conducted on Monte Carlo codes, on the CAD geometry conversion for Monte Carlo simulations, and on coupled radiation transport and activation computation systems. The role of nuclear data for reliable DEMO neutronics design analyses and uncertainty assessments is also addressed. Specific examples of nuclear analyses are presented including breeder blanket and shielding analyses for the different DEMO blanket concepts as well as related activation, decay heat and shut-down dose rate analyses.

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## 1. Introduction

The European Power Plant Physics and Technology (PPPT) programme, organised as activity of the EUROfusion Consortium, aims at developing a conceptual design of a fusion power demonstration

plant (DEMO) as a central element of the European roadmap to the realisation of fusion energy [1].

Various integrated PPPT projects are being conducted to meet this ambitious goal including Breeder Blanket (BB), Safety and Environment (SAE), Magnets (MAG), Materials (MAT), Diagnostic and Control (DC), Divertor (DIV), and Remote Maintenance (RM). Neutronics plays an important role for all of the related activities since it has to provide essential data for the nuclear design of DEMO, assess and verify its performance. This requires, on one hand, the

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availability of suitable computational tools and data to ensure reliable neutronics simulations of DEMO, and, on the other hand, a consistent approach for the variety of nuclear analyses to be performed within the different PPPT projects.

Accordingly, the PPPT programme builds on a co-ordinated approach for the DEMO neutronics including both development works on advanced computational tools as required for nuclear, activation and shielding analyses, and a variety of activities related to the nuclear design and performance of the DEMO power plant and specific reactor components and issues.

In the following, the methodological approach for the PPPT neutronics is presented including the development works on advanced simulation tools and their application to DEMO. The focus is on the approach for DEMO nuclear analyses including blanket design, shielding, activation and radiation dose issues with the discussion of specific examples. In addition, the role of nuclear data for reliable DEMO neutronics design analyses and uncertainty assessments is addressed.

## 2. Computational tools and data for neutronics simulations

Neutronics simulations form the basis for providing the nuclear responses which are needed for the engineering design and the performance evaluation of DEMO. The related issues include the Tritium breeding capability, shielding performance, nuclear power generation, activation and radiation damage of irradiated materials/components as well as the resultant radiation dose loads to sensitive components, and related biological dose rate distributions.

Suitable computational approaches, tools and data need to be available to provide the required response data with sufficient accuracy. This includes a suitable method for the simulation of neutron transport in complex 3D geometries, high quality nuclear cross-section data to describe the nuclear interaction processes, and simulation models which replicate the real geometry without severe restrictions. Such requirements are satisfied with the Monte Carlo (MC) particle transport technique which can handle any complex geometry and employ the nuclear cross-section data without any severe approximations. Furthermore, suitable computing schemes for coupled radiation transport and activation calculations are required for safety, maintenance and waste related analyses including the assessment of the activity inventories produced in DEMO over the anticipated lifetime, the decay heat power generation, and the calculation of shut-down dose radiation maps.

Key issues for faithful neutronics simulations of DEMO are thus related to (i) the reliability of the employed MC particle transport code and its coupling to nuclide inventory calculations (to be validated with fusion relevant benchmark experiments), (ii) the capability to describe in the simulation the real reactor geometry with high fidelity and sufficient detail, and (iii) the quality of the nuclear cross-section data available for fusion applications (to be checked against integral experiments). The first two key issues are addressed in specific activities of the PPPT programme within the BB and SAE projects while the latter is conducted so far in a dedicated programme on Nuclear Data Development and Analysis supported by F4E, Barcelona.

### 2.1. Monte Carlo codes and related development work within PPPT

The Monte Carlo code MCNP with the current versions 5 and 6 [2,3], developed by the Los Alamos National Laboratory (LANL), USA, is the standard code for ITER nuclear analyses. MCNP is very powerful in its capabilities, well validated and benchmarked, and most suitable for fusion applications. MCNP is also used for most of

the analyses conducted within the PPPT programme. MCNP, however, is subject to US export control regulations and thus not freely available, in particular with regard to the source code which is required for adaptation to many DEMO applications. Several alternative MC codes have been considered in a previous exercise on their suitability for fusion neutronics applications and, in particular, DEMO nuclear analyses [4]. The TRIPOLI-4 code [5], developed by CEA Saclay, France, was selected as most promising candidate and was accepted as analysis code for PPPT neutronics. TRIPOLI-4 is a mature code, well advanced in its functionalities, successfully validated for fusion neutronics and benchmarked against MCNP for the application to DEMO [6,7].

The further development of TRIPOLI-4 as alternative European MC code for DEMO nuclear analyses is supported within the BB project of PPPT [8]. The open source codes SERPENT [9] and GEANT [10], both freely available, are considered as long-term alternatives which still require substantial development and qualification effort for fusion neutronics applications including the adaptation to DEMO analysis needs. Related development work on these codes is not conducted within the PPPT programme.

### 2.2. CAD to MC geometry conversion tool

The requirement to represent the real reactor geometry within the neutronics simulation with high fidelity and sufficient detail can be satisfied by using a modelling approach which ensures a true one-to-one translation of the CAD geometry model, as produced for the engineering design of the reactor, into the MC geometry representation. Such an approach is enabled with software tools like MCAM, developed by the FDS Team, Hefei/China [11], or McCad, developed by KIT as open source project [12]. The development work on McCad is conducted within the BB project of PPPT with the objective to provide a mature European software tool for the conversion of CAD geometry models into the semi-algebraic geometry representation utilized in MC particle transport simulations with MCNP or TRIPOLI. Such capabilities are essential for the generation of the DEMO models used for the breeder blanket analyses. The McCad interface for TRIPOLI-4 has been developed only recently on the basis of the already existing conversion functionalities developed for MCNP. The interface has been successfully tested and applied for the generation of a TRIPOLI model of the HCLL DEMO used for the design analyses within the BB project [13].

The latest enhancements to McCad include improved algorithms for the decomposition of solids with the addition of splitting surfaces, a collision detecting technique based on mesh triangles, and an algorithm for the sorting of the splitting surfaces. These improvements were verified with several test models derived from a PPPT DEMO model and were shown to result in a more efficient conversion process with a better, less complex, geometry representation.

The McCad software, originally developed under the Linux operation system, has been ported to the Windows platform. This has been achieved through its implementation on the SALOME simulation platform [14]. A new Graphical User Interface (GUI) was developed to this end on SALOME under Windows. It provides the users with a higher flexibility and extended interactive features. The McCad code package, including the source code and pre-compiled binaries, is available on the GitHub software development platform [15].

### 2.3. Coupled radiation transport and activation calculation schemes

The calculation of the radiation fields after shut-down (“post irradiation”) requires a suitable coupling scheme of codes, data and interfaces capable of simulating both the neutron induced material

activation during operation and the decay photon transport in the real 3D geometry of DEMO. Two different computational schemes have been developed, pre-dominantly aimed for shut-down dose rate analyses of the ITER tokamak: the Rigorous 2-Step (“R2S”) [16], and the Direct 1-Step (“D1S”) method [17,18]. Both of them rely on the MC technique for the transport simulation and are under further development within the SAE project of PPPT for application to DEMO.

The D1S approximation method is based on the assumption that a radioactive nuclide generated during irradiation spontaneously emits the associated decay photons. Neutron and decay photon transport can be treated in one single MC calculation run using a modified version of the MCNP code together with special purpose activation data libraries. The Advanced D1S method (“AD1S”) [19] includes the capability to provide shut-down dose rate (SDR) distributions on spatial meshes superimposed to the real geometry by utilizing MCNP5’s mesh tally feature. The further development of the AD1S method aims at its adaptation for SDR calculations of DEMO. This requires the extension of the data libraries for nuclides and reactions important to DEMO and taking into account sequential two step activation reactions which are neglected so far.

The R2S approach reproduces, in a rigorous sense and sequential order, all computational steps which are required for the estimation of SDR distributions. It includes particle transport calculations in two steps, the first one on the neutron transport to provide the neutron flux spectra distribution, the second one on the decay photon transport to obtain the radiation doses at the specified locations of interest. Nuclide inventory calculations, succeeding the neutron transport simulation, provide the decay gamma source distribution. The transport calculations, both for neutrons and decay gammas, are performed with MC codes such as MCNP or TRIPOLI. The activation calculations are performed with an inventory code like FISPACT [20] or ACAB [21]. MC and inventory codes are linked through interfaces for the automated routing of the neutron flux spectra and the decay gamma source distribution.

The R2S methodology has been also extended for calculations of high resolution shut-down dose rate distributions on spatial meshes. Thus proper account is taken of the spatial variations of the flux and the decay gamma source distribution without the need to modify the MC geometry model. This functionality also enables exporting of the decay gamma source distribution from the irradiation site in the reactor to any external location for the determination of shutdown dose rate distributions around an activated component. Independent implementations of the mesh-based R2S approach were developed by CCFE [22], KIT [23] and UNED [24] with the MCR2S, R2Smesh and R2S-UNED codes, respectively.

Within the PPPT programme, a unified European R2S code system, called cR2S (“common R2S”), is under development by CCFE, KIT and UNED. A suitable architecture has been elaborated for the coupling scheme including programme structure, interfaces, and data management. A common decay gamma source (CDGS) representation, with data format specification and coding in a MCNP source routine, has been developed and tested. The CDGS is already established as standard and used in ITER applications to enable the exchange of decay gamma source distributions calculated for activated components.

The cR2S code system is developed from scratch and will be first based on the MCNP6 MC code which provides advanced unique features such as unstructured meshes. Special functionalities as already available in the various mesh based R2S approaches will be integrated as useful and needed. A dedicated methodology is elaborated to include in the cR2S scheme the propagation of errors over the whole calculation sequence, from neutron transport over the activation calculations to the decay photon transport. The practical implementation of the cR2S approach is conducted on the GitHub software development platform to enable the joint development

by the participating institutions using a versioning control system.

Validation of the computational approaches is an essential precondition for the application to SDR analyses of a fusion power plant such as DEMO. A series of related benchmark analyses has been previously conducted on the SDR experiments conducted on the JET tokamak and the 14 MeV neutron generator at ENEA Frascati (FNG) [25]. Within the EUROfusion programme, dedicated validation activities on shut-down dose rate predictions are conducted in the JET3 project (“Technological Exploitation of DT operation”), sub-project NEXP (“Neutronics Experiments”) with measurements and analyses of SDR inside and outside the JET vessel. Available SDR measurements from previous experiments on JET mostly agree within about  $\pm 30\%$  with the AD1S and R2S calculations [26].

#### 2.4. Nuclear data for fusion applications

Neutronics simulations need to describe the interactions of neutrons and atomic nuclei including the formation of (stable or radio-active) product nuclei and the emission of secondary particles such as neutrons, photons and charged particles. The interactions are governed by quantum mechanical probabilities described by means of neutron cross-section data (“nuclear data”) which depend on the nucleus species, the reaction types and on the neutron energy. The availability of high quality nuclear data is thus a pre-requisite for reliable design calculations to ensure sufficient prediction accuracy for the nuclear responses to be provided. The data quality thus affects significantly the nuclear design and performance of DEMO including safety, licensing, waste management and decommissioning issues.

Work on the development and qualification of nuclear data for fusion so far has been conducted by the European “Consortium on Nuclear Data Development and Analysis” within a framework partnership agreement with F4E, Barcelona [27]. The related programme, conducted through specific grants, addresses the nuclear data needs of ITER, the IFMIF neutron source and DEMO. The activities include the evaluation and validation of relevant nuclear cross-section data, the development/extension of codes and software tools required for nuclear model calculations and sensitivity/uncertainty assessments. After passing a thorough benchmarking and validation process, the cross-section data evaluations are fed into the Joint Evaluated Fusion File (JEFF), maintained and disseminated by the NEA Data Bank of the OECD, Paris, France [28]. Special data libraries were developed for activation/transmutation, gas production and displacement damage calculations. Dedicated evaluations, based on advance modelling approaches, were performed for the displacement damage cross-sections of the Eurofer steel [29]. These data, available via the IAEA, Vienna, are used as reference data for the calculation of displacement damages to Eurofer components in the PPPT programme.

### 3. DEMO nuclear analyses

#### 3.1. General methodological approach

A multitude of nuclear analyses is being constantly performed in the various PPPT projects, pre-dominantly PMI, BB, SAE and the Early Neutron Source (ENS) project (not covered in this work), involving nuclear analysts from several European research institutions including e.g. CCFE (UK), CEA (France), CIEMAT (Spain), ENEA (Italy), KIT (Germany), IPPLM/NBJ (Poland), LEI (Lithuania), and UNED (Spain). This requires a co-ordinated approach to ensure all the analyses for DEMO are performed in a consistent manner and the results are comparable. Accordingly, a dedicated “transversal” activity was implemented in the PPPT programme to co-ordinate

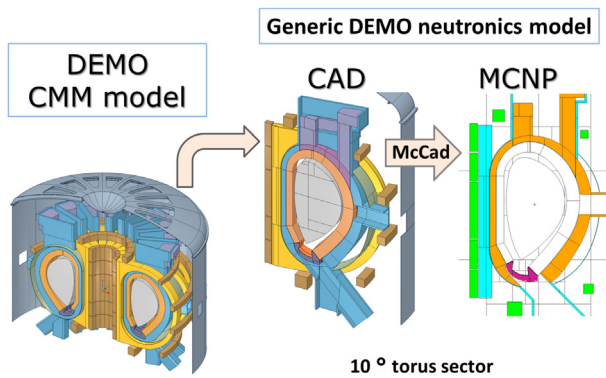


Fig. 1. Generation of generic DEMO neutronics model.

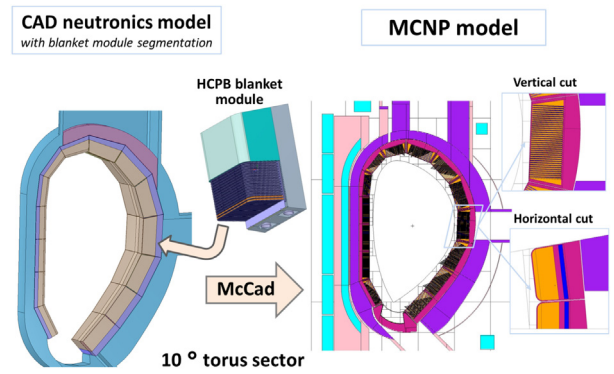


Fig. 2. Generation of HCPB DEMO neutronics model.

the neutronics activities across the projects. The consistency of the analyses, e.g., is ensured by a methodological approach specified in the guidelines for DEMO nuclear analyses. These include recommendations on the computational tools and data, specifications of the geometry models and the neutron source, general recommendations on calculation techniques, assumptions to be made (such as the irradiation scenario for activation calculations), targeted accuracies, as well as specific recommendations for the provision of nuclear responses. The guidelines are constantly updated and adapted to the progress of the various PPPT projects.

An essential feature of this approach is the mandatory use of a generic neutronics model which is consistent with the underlying DEMO design and then is individually adapted as required and useful for the investigation of different tasks and problems.

In the following a few examples are presented of specific PPPT nuclear analyses performed for DEMO including the neutronics model generation.

### 3.2. Generation of neutronics DEMO models

The general approach is to generate first a generic CAD neutronics model from the CAD Configuration Management Model (CMM) of DEMO as provided by PPPT's PMU. This model includes the Toroidal Field Coil (TFC), vacuum vessel (VV), divertor, blanket segment box, vessel ports, and plasma chamber, represented in a single torus sector with envelopes. All components are thus described by their bounding surfaces ("envelopes") without any internal structure specified, as shown in Fig. 1 for the latest DEMO baseline model called "EU DEMO1 2015". This model is converted to analysis models for the MCNP and TRIPOLI MC codes using the McCad conversion software and serves as basis for the adaptation to specific tasks as demonstrated in the following section.

### 3.3. Breeder blanket design and shielding analyses

The development of a technically mature breeder blanket design for DEMO is a major aim of the PPPT programme. Four different design options of a breeder blanket are under investigation, the Helium Cooled Pebble Bed (HCPB) blanket with Beryllium as neutron multiplier and Helium gas as coolant, the Helium Cooled Lithium Lead (HCLL) with PbLi as breeder and Helium gas as coolant, the Water Cooled Lithium Lead (WCLL) with PbLi as breeder and water as coolant, and the Dual Coolant Lithium Lead (DCLL) with both the liquid PbLi breeder and Helium as coolant.

The nuclear design analyses are performed with specific models derived from the generic DEMO model by integrating blanket modules of the different breeder blanket concepts. The engineering CAD model of a single blanket module is processed and converted into an MC analysis model. It is then repeatedly filled into the

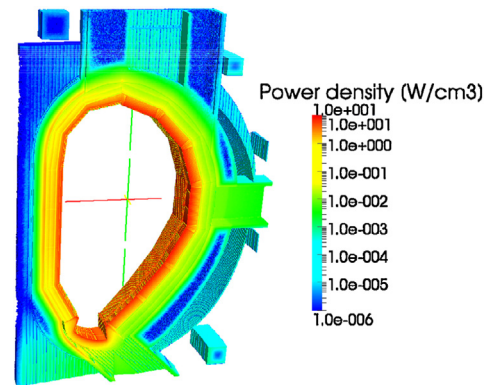


Fig. 3. Spatial distribution of the heating in a HCPB DEMO torus sector.

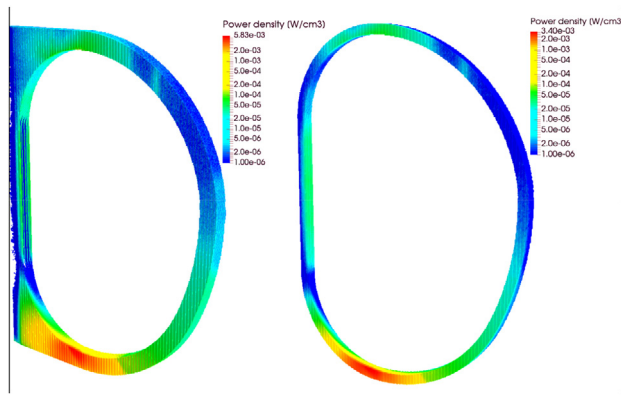
empty blanket segment envelope of the generic DEMO model. Thus specific HCPB, HCLL, DCLL and WCLL DEMO models are generated which are consistent with the DEMO baseline configuration and the specific engineering blanket design with the internal structures of the blanket modules. Fig. 2 illustrates this process on the example of the HCPB DEMO.

The model development and the calculations for the considered DEMO variants are performed by the KIT (HCPB), CEA (HCLL), CIEMAT (DCLL) and ENEA (WCLL) expert teams using MCNP or TRIPOLI-4 and nuclear cross-sections from the JEFF data library [28].

The calculations of the Tritium Breeding Ratio (TBR) showed that the design target of  $TBR \geq 1.1$  [30] can be safely achieved for all blanket variants. For the DEMO 2015 baseline there is actually a large safety margin due to the assumed compact and small divertor. Significant progress has been also achieved in improving the engineering blanket design for an enhanced Tritium breeding as compared to the DEMO 2014 design [31].

The nuclear power generated in the blanket and the other reactor components exceeds the primary fusion neutron power due to the release of binding energy in the various nuclear reactions. The related energy multiplication factor is at 1.20 for the PbLi based blankets and 1.35 for the HCPB blanket with Be neutron multiplier. The nuclear power densities in the steel structure are in the range from  $10 \text{ W/cm}^3$  at the first wall down to ca.  $0.1\text{--}0.5 \text{ W/cm}^3$  at the back, see Fig. 3 for the HCPB DEMO.

The shielding analyses performed so far allow drawing the general conclusion that the super-conducting TFC can be sufficiently protected against the radiation penetrating the blanket/shield system (BSS). This applies even for the highest loaded locations behind the BSS at the inboard torus mid-plane with a design limit of  $50 \text{ W/m}^3$  for the TFC heating. The shielding efficiency of the blanket modules (with back support structure and manifold) was also shown to be sufficient to keep the displacement damage to the VV



**Fig. 4.** Power density distribution in the TFC casing (left) and the super-conductor (right) of DEMO.

below 2.75 dpa over the anticipated DEMO lifetime of 6 full power years so as to prevent the radiation induced degradation of the steel strength.

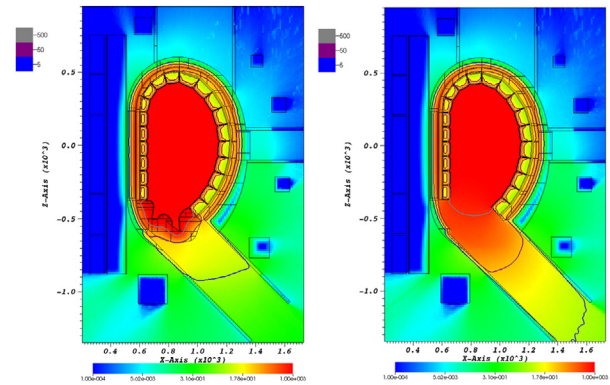
### 3.4. Nuclear heating of the TFC

Dedicated analyses were performed on the TFC system with the objective to estimate the total heating power and identify locations with insufficient shielding due to the presence of open ports or gaps. To this end the HCPB DEMO model was adapted with a suitable description of the TFC with casing and interior structure, as provided by the magnet designers, and a steel plug in the equatorial vacuum vessel port. Fig. 4 reveals that the TFC is insufficiently shielded in the (open) divertor port area where heating rates in the order of  $1 \text{ kW/m}^3$  can be reached thus exceeding the assumed design limit by a factor 20. The heating in one TFC is 620 W and 1.62 kW in the casing. For DEMO1 2015 with a fusion power of 2037 MW and 18 TFC this sums up to a total heating of 11 kW for the entire TFC and 29 kW for the casing.

### 3.5. Activation, decay heat and SDR analyses (many)

Safety, maintenance and waste related analyses require the knowledge of the activity inventories accumulated during DEMO operation in the irradiated components, the related decay heat generation and the resultant radiation dose fields as function of time. Such issues are addressed in several PPPT activities making use of the coupled code systems described in section 3.3 and specific “ad-hoc” DEMO models. The general approach for this kind of calculations is to use a common DEMO model with empty blanket boxes in which homogenized material mixtures according to the layout of different blanket concepts are filled in. Such analyses have been performed for the DEMO 2014 with a fusion power 1572 MW to evaluate and compare the decay heat of the considered four blanket concepts [32] and assess their impact on the activation of the VV and the divertor with the ultimate objective to enable the classification of the accumulated radio-active waste [33].

The decay heat generated in the blanket modules amounts to 21.4, 17.5, 22.7, and 22.7 MW for the HCPB, HCLL; DCLL and WCLL, respectively, at 1 s after shut-down. It decreases to the order of 1 MW or less after one week. Most of the decay heat is due to the activation of the Eurofer steel used as structural material. The VV, designed as lifetime component made of SS-316, is less activated with HCPB and WCLL blanket modules than with DCLL and HCLL. This is due to the softer neutron spectra in the HCPB and WCLL resulting in a better shielding capability. At 1 s after shut-down, the VV decay heat power is at 1–2 MW for the HCLL and DCLL blankets and around 0.4 MW for the HCPB and WCLL. The analyses revealed



**Fig. 5.** Map of the biological dose rate [Sv/h] in DEMO, 8 weeks after shut-down with divertor in place (left) and removed (right).

that most of the VV must be categorised as intermediate level waste until about 200–300 years when some of it can be handled as low level waste [32]. Typical radiation dose rate distributions are shown in Fig. 5 for the case with HCLL blankets and divertor in place, and the divertor removed.

## 4. Conclusions

The methodological approach employed for the neutronics in the PPPT programme has been presented. It encompasses development works on advanced computational tools and activities related to the nuclear design and performance evaluation of the DEMO power plant including safety, maintenance, and waste management issues. Specific examples of nuclear analyses were shown including breeder blanket and shielding analyses for the different DEMO blanket concepts as well as related activation, decay heat and dose rate analyses.

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