UKAEA-CCFE-CP(23)50

Alex Valentine

Advancing methods for fusion neutronics: An overview of workflows and nuclear analysis activities at UKAEA

Advancing methods for fusion neutronics: An overview of workflows and nuclear analysis activities at UKAEA

Alex Valentine

This paper has been submitted to
The Technology of Fusion Energy, Anaheim, California, USA, 12-16 June 2022

Advancing methods for fusion neutronics: An overview of workflows and nuclear analysis activities at UKAEA

Alex Valentine ,*,[a] Thomas Berry,[a] Steven Bradnam,[a] Hari Chohan,[a] Tim Eade,[a] Callum Grove,[a] James Hagues,[a] Keir Hearn,[a] James Hodson,[a] Kimberley Lennon,[a] Jonathan Naish,[a] Joseph Neilson,[a] Chantal Nobs,[a] Lee Packer,[a] Andrew Turner,[a] Tony Turner,[a] Luke Woodall,[b] and Ross Worrall[a]

[a] *Culham Centre for Fusion Energy*
Culham Science Centre
Abingdon, OX14 3DB, Oxford, UK

[b] *University of Birmingham*
Edgbaston, B15 2TT, Birmingham, UK

*Email: Alex.Valentine@ukaea.uk

Number of pages: 30
Number of tables: 0
Number of figures: 10

Abstract

Global research programmes seeking to achieve a commercially viable model of a fusion power plant are being accelerated at an unprecedented rate. One critical element to the design and licensing is an accurate understanding of the radiation environment throughout the plant lifetime and subsequent decommissioning phase. The radiation field which results from the nuclear fusion reaction gives rise to highly complex phenomena such as flux leakage, materials activation and decay gamma fields. Demonstration of compliance with limits, the integrity of components and the permissibility of operations are all fundamental to regulatory approval and the overall safety of a nuclear device. As such, neutronics, which is used in the general sense to refer to the mapping of radiation fields in nuclear devices, is a critical design driver. The Applied Radiation Technology group at UKAEA is a world leader in this field, developing new methods and deploying state-of-the-art codes to conduct nuclear analysis. As well as applied neutronics in areas spanning fusion reactors, medical applications, spallation neutron sources and nuclear fission, there is an extensive parallel experimental program undertaking critical radiation field characterisation and conducting measurements using an array of bespoke particle detection systems. This paper highlights recent technical developments made by the group in the context of outstanding challenges in this field, as well as providing an overview of current methods and capabilities for the broader interest of the community.

Keywords — Fusion, Neutronics, Neutron Spectrometry, Radiation Detection, Radiation Transport

I. INTRODUCTION

There is a clear heightened investment both at government level and privately to expedite the pathway to commercial fusion energy as a means for generating safe, sustainable and low carbon electricity. The UK has launched its own ambitious program to develop a prototype Spherical Tokamak for Energy Production (STEP) [1] by 2040. A concerted research and development effort focused on developing a conceptual design was launched in 2019 at the UK Atomic Energy Authority with an initial £220 million government grant. STEP is a first of a kind large scale engineering project with many unique, multi-faceted challenges. To address outstanding physics and engineering gaps, innovative solutions capable of scaling to a plant level will be required. Fundamental to this is the integration across different disciplines such as plasma physics, mechanical engineering, structural engineering and neutronics such that the iterative pathway to a plant solution is performed holistically. The interface between these different areas and their unique constraints requires development of codes that can be tightly coupled and converge to a solution over the timescales that are needed as input to subsequent iterations of a design.

As fusion enters the delivery phase, accurate characterisation of the nuclear environment is a key input to the demonstration of nuclear safety. The favoured deuterium-tritium nuclear fusion reaction gives rise to 14 MeV neutrons which go on to interact with the materials in the reactor through diverse complex phenomena such as flux leakage, materials activation and decay gamma fields (see Figure 1). Systems codes including BLUEMIRA [2, 3, 4], developed in collaboration between EUROfusion and UKAEA, integrate different physics and engineering modules as a design tool for future fusion reactors. One of the core inputs is neutronics, the study of the behaviour of neutrons and more broadly the radiation environment. Integration with systems codes stipulate that the neutronics assessments must be performed on rapid timescales. With current methods and available compute infrastructure, this is feasible for scoping studies based largely on homogenised geometry representations.

Fusion neutronics is arguably one of the most demanding fields for Monte-Carlo codes, which are most commonly applied and indeed developed for the domain of fission reactor physics calculations. Beyond systems codes, the engineering level design model must determine the nuclear responses at sufficient spatial resolution, extracted from a geometry that captures the modelled system in all its complexity. The current most practiced workflow involves a multi-step process calling proprietary software, with several bottlenecks, most notably in the preparation of a CAD geometry that is suitable for radiation transport analyses. The current limitations and immediate analysis needs channels current software developments and also serves to motivate the exploration of alternative workflows. Emergent radiation transport codes such as OpenMC [5] and Serpent [6] are now at a level of maturity which permits application to most fusion modelling problems, subject to further validation.

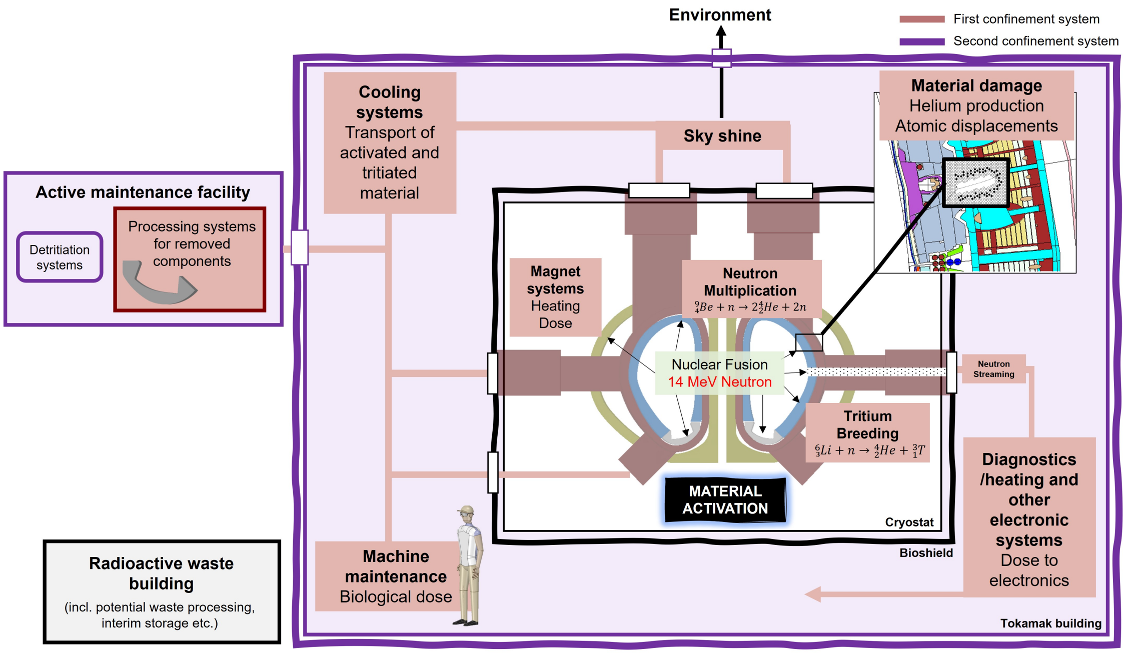

Fig. 1. A schematic illustration of the complex nuclear environment in an operating fusion tokamak. The diagram describes only some of the many complex phenomena that arise from the fusion reaction

The Applied Radiation Technology (ART) Group at UKAEA is driving the nuclear design of fusion power reactors through analysis of the radiation environment and validation through measurement. In this paper, we present specific examples from a broad portfolio of research to highlight recent advances in this field. To increase the efficiency of the workflow, a series of CAD-based tools have been developed (section II.B) built using an Application Programming Interface (API) for ANSYS SpaceClaim. For the determination of decay gamma fields, a Novel-1-Step (N1S) method (section II.C) is detailed, providing an accurate, single-step method that overcomes some of the key drawbacks of current approaches. UKAEA are also actively benchmarking different particle transport codes (section II.D) - the application of these modern workflows in the analysis of STEP and an example of their validation is presented. Efforts to advance multi-physics approaches for activated fluids in a fusion reactor are presented in section II.E. The experimental division of ART includes the on-site radiometric lab, termed the Radiological Assay and Detection Laboratory ('RADLab'), hosting a wide array of particle diagnostic systems. In the scope of immediate experimental needs in fusion, the development of a passive neutron spectrometry (PNS) system for future characterisation of neutron spectra in low dose environments is highlighted in section III.B.

II. APPLICATION AND DEVELOPMENT OF NUCLEAR MODELLING

II.A. Analysis workflow

The conventional method most widely adopted today for performing nuclear analysis of fusion reactors is outlined in Figure 2. The codes included in the figure are specific to the workflow employed at UKAEA. In the first stage, a CAD model is received at an engineering level of detail. To derive a 'neutronics' model, the CAD model is simplified such that it retains only transport relevant features i.e. those that will have a non-negligible impact on the nuclear response being studied. This typically involves the removal of interferences and small features such as rounds and bolts. Complex surface types such as splines and tori as well as other higher order surfaces must also be simplified (typically by re-drawing). Due to abundance of inherent software features that aid in the simplification process, ANSYS SpaceClaim has been the adopted CAD platform for this purpose since circa 2011. The approximations introduced at this stage are typically quantified by volumetric comparison with the original file. There is inevitably some immediate differences to the model adopted in other engineering analyses. Conversion to constructive solid geometry (CSG) format is performed using conversion software such as SuperMC [7] or McCad [8]. The CAD model preparation preceding this stage, together with the conversion process and subsequent validation of a geometrically 'clean' model, can account for over 50% of the entire workflow.

Transport calculations using the Monte-Carlo code MCNP [9] often require variance reduction techniques to reduce the stochastic uncertainty in deep shielded regions, which is generally any response external to the inner surface of the vacuum vessel in tokamaks. The ADVANTG [10] software is capable of automatically generating the variance reduction parameters for one such method, weight windows, in both the global and local scheme. UKAEA developed an alternative methodology based on iteratively populating the geometry to derive weight window bounds. This

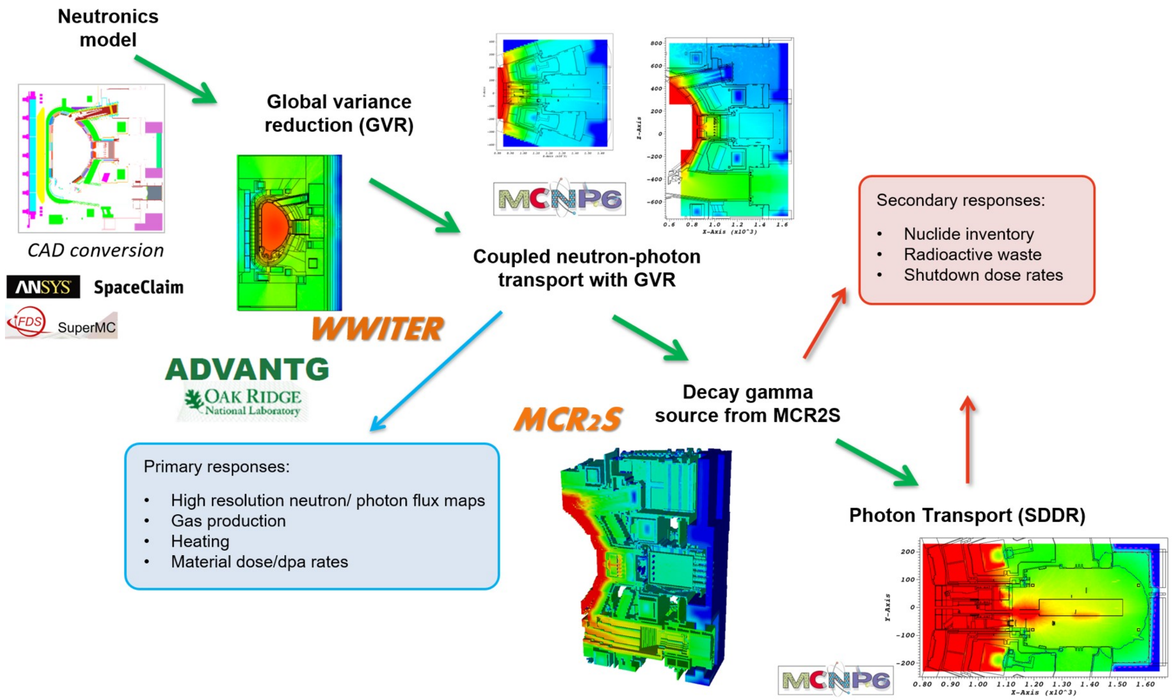

Fig. 2. Schematic overview of the conventional workflow including computational tools used for radiation transport analysis at UKAEA

method, WWITER [11], has been demonstrated for JET, ITER and DEMO applications [12, 13, 14].

To evaluate the shutdown dose rate at different decay times, UKAEA use its own mesh coupled rigorous 2 step (MCR2S) code [15]. As further detailed in section II.C, this is one of several methods for this purpose. MCR2S couples an on-load neutron transport calculation with an inventory calculation performed using an external activation solver, FISPACT-II [16], developed and maintained at UKAEA. FISPACT-II is capable of predicting of the time evolution of a material composition under irradiation. The release of FISPACT-II v5.0 in January 2022 available through RSICC and the NEA includes an API to increase its functionality and allow efficient coupling into other codes. A python based utility for parsing FISPACT output files, 'pypact' [17], is also now openly available.

II.B. Spaceclaim API tool development

To mitigate the bottlenecks in the preparation of 'conversion-ready' CAD geometry, UKAEA have developed a suite of tools which utilise the API available in SpaceClaim. Tools have been written both in C# and Python and integrated together through C# such that they are directly accessible as part of the SpaceClaim Ribbon (Figure 3).

Fig. 3. List of SpaceClaim tools developed at UKAEA using the SpaceClaim API, directly accessible in the application ribbon

The tool suite is open source [18] with accompanying user documentation detailing installation and guidance for use of each tool. The tools provide either direct automation of more arduous modelling tasks or equip the analyst with additional data to reduce the time spent identifying problematic geometry regions. One example tool is the pipe simplification tool which can be used to convert a given complex pipe network to a series of cylinders that are suitable for conversion. The internal fluid/void volume is also optionally created. An example is shown in Figure 4, along with the user interface that allows specification of pipe thickness based on a user defined input or hard coded ASME based [19] pipe standards. The option to add colour to the geometry facilitates the distinction of different materials which streamlines their assignment in the CSG model. The time to simplify a single pipe network is reduced from several minutes to a few seconds. For a geometry as vast as the ITER tokamak cooling water system (TCWS) which consists of tens of kilometers of cooling water, this tool greatly reduced the modelling effort which ultimately shifts the emphasis to the more significant analysis of nuclear responses.

Further tools have since been developed at F4E [20] which are more tailored towards specific manipulation of the geometry for MCNP once it has been simplified. There is scope to harness the API for other engineering applications which are embedded in the ANSYS suite. The simplification process means that the neutronics model can differ greatly from that used in engineering simulation. Coupling methods which may leverage the API would minimise this disparity through an intermediary model that can be adopted, for example, in high fidelity finite element analysis while being sufficiently lightweight to perform particle transport [a].

[a]The constraint on particle transport geometries is often the ability to convert them cleanly in available con-

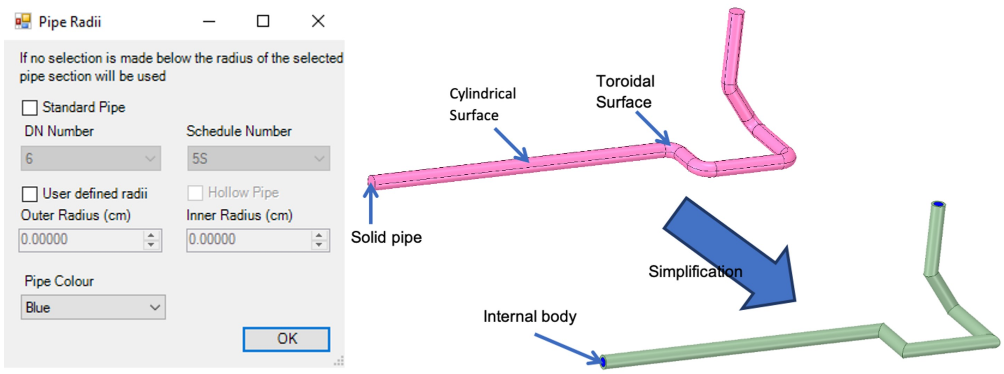

Fig. 4. User interface for the pipe simplification tool (left) together with an example of the original and simplified pipe geometry (right)

II.C. Development of a new method for shutdown dose rate calculations

The MCR2S method used by UKAEA in the evaluation of shutdown dose rates has several inherent approximations. The method is based on calculating the neutron spectra on a mesh, which at the voxel level implies a degree of flux averaging both spatially and in energy. Further, the method is in reality more like a three step process consisting of a neutron transport simulation, inventory calculation and a final photon transport calculation. The other method used widely for evaluating fusion shutdown dose rates is the Direct 1-Step method (D1S) [21, 22, 23]. Rather than discretising the problem space to derive neutron spectra, the exact position of each activation reaction is retained and the neutron and decay photon transport performed in a single Monte Carlo simulation. This is implemented through substitution of neutron induced prompt photons with decay photons using dedicated cross section libraries. This method relies on a priori knowledge of the important reactions to the dose response and the evaluation of time correction factors for each important isotope which link their activity and production rate to the irradiation schedule and decay times of interest. This information typically requires using an external activation calculation using an inventory code such as FISPACT-II.

The limitations of each method motivated the development of a Novel-1-Step (N1S) method [24] to determine the response at decay times of interest in a single transport calculation. The need for an external activation solver is removed by including the irradiation scenario as a time dependent neutron source term. Activation reactions occurring in neutron transport are evaluated

version software and the memory footprint which scales with increasing detail retained in the geometry explicitly at the location which they occur, with all the information on decay chains captured in a specially developed decay library. Full accountancy is made for self-shielding effects in materials. Each of the decay photons is assigned a weight that is essentially a probability of the decay happening at the decay times of interest specified by the analyst. The photon transport is performed in the same calculation as the neutron transport and the weights used to modify the calculated dose rates at each decay time. A flowchart of the N1S methodology is shown in Figure 5. Currently, the N1S method is implemented for MCNP and has been validated using the ITER computational port plug benchmark [25] and the FNG ITER SDDR benchmark [26] (see [24] for more detail).

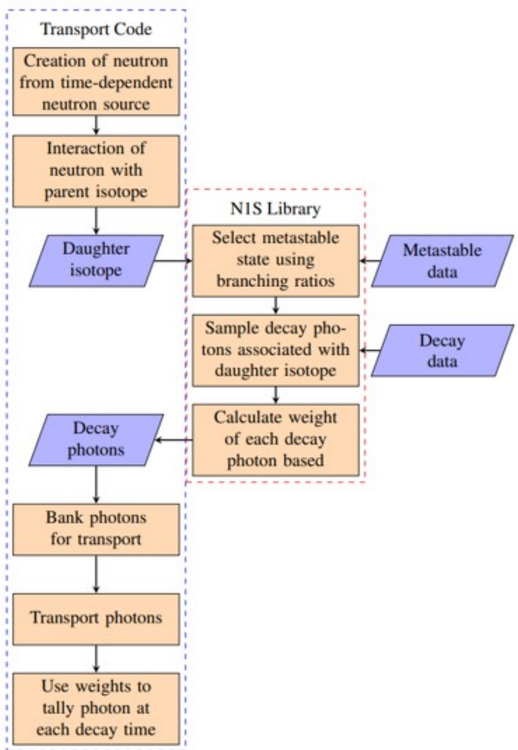

Fig. 5. Flowchart describing the workflow implemented for the Novel-1-Step (N1S) method for determining shut down dose rates

When compared to R2S method, the total time to evaluate dose rates is significantly shorter. The single transport calculation is more computationally expensive (effectively equivalent to a coupled neutron-photon calculation), however no intermediate steps are needed by the analyst. The code has been developed with the pre-requisite to be portable to different transport codes. At present, N1S has been implemented for MCNP however there is ongoing work to enable OpenMC to be used. Future effort is focused on accounting for the modification of the geometry during shutdown such as the removal of components or draining of fluids. The time dependence of the neutron source included in the neutron transport calculation gives scope to account for the time evolution of material compositions as a function of time which is not currently considered in existing methods. All of the above inherent capabilities and efficiency improvements over existing methods make N1S well suited to the parametric reactor design and/or integration with multi-physics work streams.

II.D. Benchmarking of radiation transport codes

The use of the Monte-Carlo method has long been the accepted practice for radiation transport analysis of fusion devices. MCNP, a Monte Carlo code developed at Los Alamos National Laboratory (LANL) is to date, the most widely adopted code in the fusion neutronics community. The growing capability of alternative transport codes such as Serpent 2 and OpenMC in recent years has led to the investigation of their potential for this application. Benchmarking efforts which have been conducted at UKAEA can be found in [27, 28, 29, 30, 31, 32].

Validation of the accuracy of a transport code is a fundamental where they are being deployed in fusion reactor analysis. The implications of nuclear analysis span practically all aspects of the reactor from maintenance schedules to plant economics. STEP is in a conceptual design phase with a 200+ team at UKAEA developing a viable design point for a reactor to be commissioned within the next two decades. The complex interfaces between multiple different systems and their individual requirements gives a broad design space which must be explored in an iterative manner to find the optimal solution for the plant. The workflow described in Figure 2 is not an efficient means for conducting scoping studies across multiple different design proposals. The workflow currently being used for STEP uses OpenMC with the geometry driven by parametric codes that can be automated. DAGMC [33] is a toolkit that allows for transporting particles directly on the CAD geometry based on a surface faceted representation. It can interface with several particle transport codes including OpenMC. Using the parametric workflow and harnessing direct tracking on CAD through DAG-OpenMC, several hundred design iterations can be analysed in timescales of the order of minutes. A broad design space can be quickly assessed through modifying variables and the open source nature of OpenMC alloys deployability on any HPC infrastructure without licencing restrictions. The workflow (see Figure 6) has been used to date in assessments of nuclear heating, tritium breeding ratios and neutron flux profiles. The output from the nuclear analysis is then available for other physics/engineering studies on a practical timescale, streamlining the entire design evolution process.

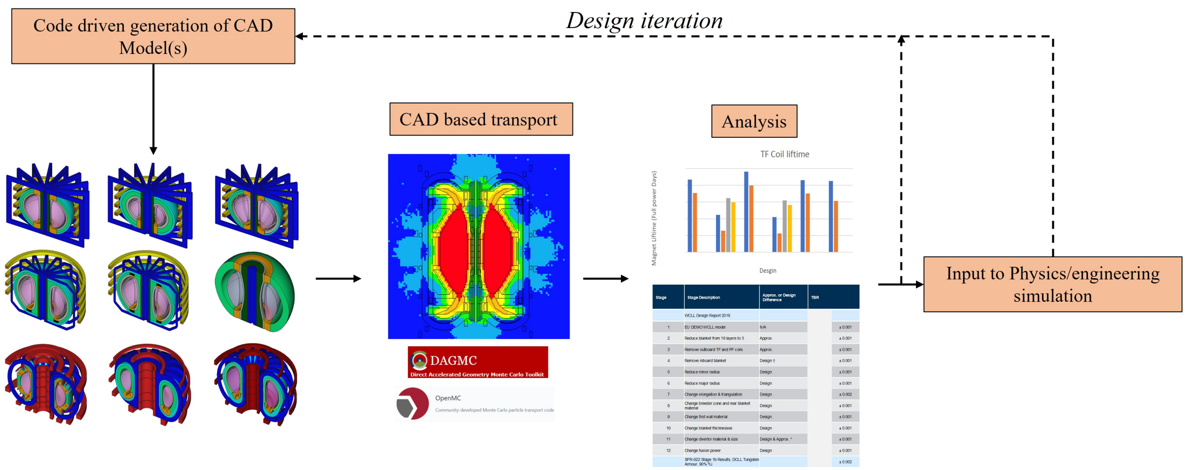

Fig. 6. Schematic overview of the workflow for nuclear analysis based on parameter driven CAD models and CAD based particle transport

The uptake of emergent radiation transport codes as alternatives to MCNP has only been possible with the conformance to a key set of code requirements for this application. These are outlined in detail in [34]. One of these is a capability to converge solutions to a sufficient level of statistical accuracy in deep shielded regions. These so called variance reduction methods are generally needed for studies external to the vacuum vessel. Current tools developed for MCNP were given in section II.A. Weight windows are one of the commonly adopted variance reduction techniques which artificially bias the simulation through increasing particle populations in the region of interest and correcting for this by accordingly adjusting a parameter assigned to each particle called its weight. Where responses are calculated, it is the sum of particle weights that is evaluated.

In 2019, Serpent developed a capability to automate the generation of the parameters controlling the bounds of the weight window [35] which has been benchmarked for several fusion relevant problems [27, 32]. In February 2022, OpenMC 0.13.0 was released with a capability to read weight window files. At present we have added two different approaches for generating weight windows. The first gives capability to convert Cartesian meshes populated in an analogue calculation to weight windows with the bounds iteratively adjusted to populate deeper shielded geometry regions. This is the MAGIC method [11] which is the basis for the WWITER tool. A second method known as PS-GVR (Pseduo-Source Global Variance Reduction) [36] also allows conversion of analog-populated meshes to weight windows, but does so in such a way that splitting is heavily reduced in mesh cells that score high enough fluxes to give acceptable statistics. The primary advantage of this method is that run times are improved versus the MAGIC method while maintaining a similar level of improvement in the stochastic uncertainties. The automated generation of weight window boundaries will remove much of the onus on the user to optimise the weight window - at the time of writing this is currently under development.

Preliminary testing of this capability has been performed using the ITER port plug benchmark. The geometry consists of an outer steel cylinder with an inner steel/water mix cylinder containing a small radius streaming channel. At the rear of the port plug mock-up is a 15 cm thick steel closure plate. The source is a 14 MeV cylindrical source with isotropic emission, 10 cm from the front face of the port plug geometry.The PS-GVR based weight window scheme was used to globally increase the particle population density in a 5×5×5 cm^3 mesh. Demonstration of this is given in Figure 7 for 10^6 source particles. It was observed that a larger proportion of voxels were populated with reduced statistical error relative to the analog simulation. There is negligbile improvement for this particular geometry beyond 2 iterations.

A comparison was made to a serpent model of the benchmark using its built in response matrix method based importance solver for generating weight windows. Both of the geometries were converted from the MCNP input file using the UKAEA developed csg2csg [37] code. The neutron spectra was determined in 175 energy groups (VITAMIN-J) in the plate at the rear of the port plug. The spectra was also determined in MCNP using a weight window generated in ADVANTG. Figure 8 shows excellent agreement between each of the codes with minor discrepancy at lower energies where the statistical error is higher. For deep shielding problems, both Serpent and OpenMC would benefit from the addition of further statistical tests such as the the 'ten statistical tests' implemented in MCNP.

The addition of this capability in OpenMC *and its validation* is fundamental to the continued adoption of the code for nuclear analysis of STEP. Nuclear responses can be studied in ex-vessel regions where, for example, the shutdown dose rate could determined using 'N1S-OpenMC' method

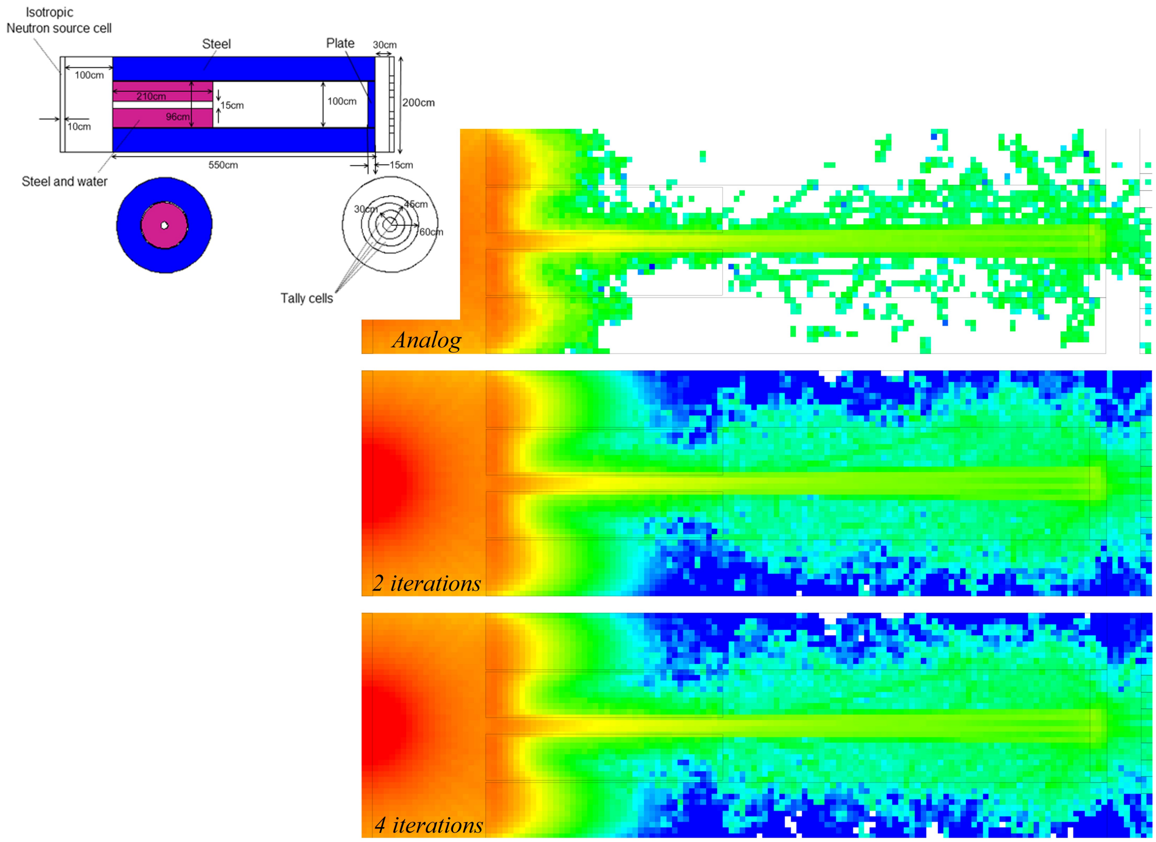

Fig. 7. Neutron flux map for the ITER port plug benchmark in OpenMC using an iterative scheme to generate global weight windows with increasing convergence across the entire mesh. The weight window boundaries are generated with the PS-GVR method.

(see section II.C). Further testing is required with more advanced geometries, an extreme case of which is the ITER reference model for nuclear analysis which has been successfully converted and demonstrated to transport particles in OpenMC [27].

II.E. Modelling of activated fluids in fusion reactors

During fusion operations a significant volume of fluid will pass through in-vessel components, including coolant and possibly liquid breeder material. The ITER Test Blanket Module (TBM) Program is investigating several different blanket concepts seeking to optimise tritium breeding with technological feasibility. Lithium-lead (LiPb) is one example of a liquid metal breeder material in several of the currently explored concepts. Flowing water is used as a coolant in certain blanket concepts, as well as more widely across ITER components to extract excess heat. In the presence

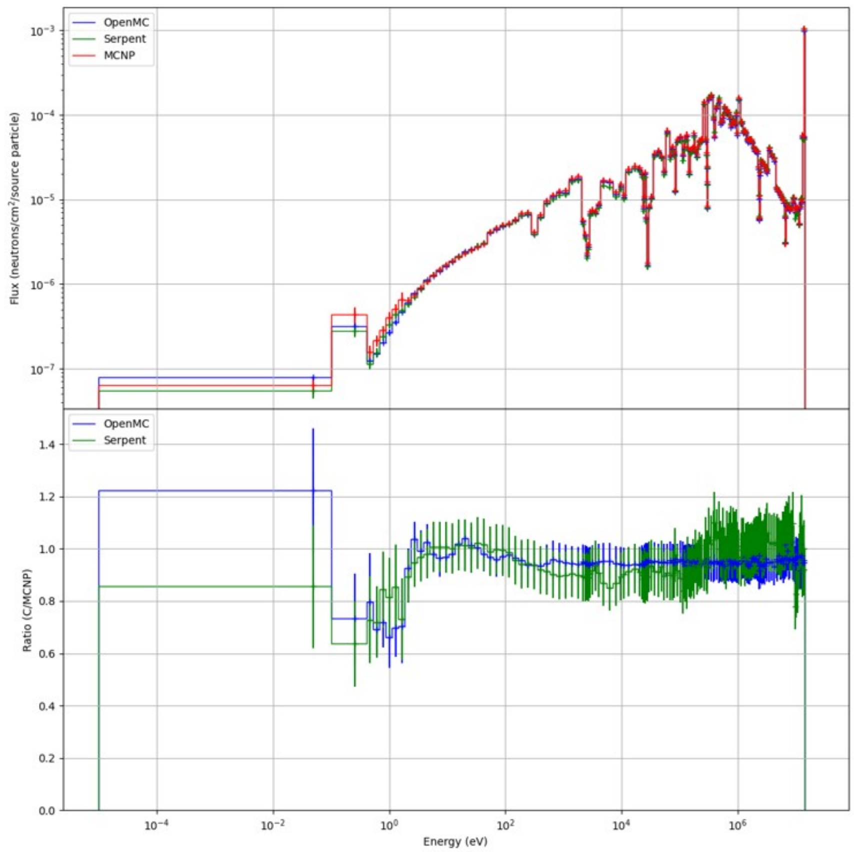

Fig. 8. Comparison of the MCNP, Serpent and OpenMC calculated neutron spectra in the closure plate of the ITER computational port plug. Each code uses an independent method of variance reduction.

of a neutron field, water is activated through (n,p) reactions with isotopes of oxygen, $^{16,17}O$. The most notable product is ^{16}N which decays through emission of 6.13 MeV (I=67%) and 7.12 MeV (I=5%) [38] photons. There is an additional gamma source term in the fluid which stems from activated corrosion products, along with secondary neutron emission from the decay of ^{17}N. Other potential coolants in future fusion devices include molten metals and salts, which would introduce different activation and corrosion profiles. The movement of activated fluids through the tokamak complex has significant implications for the demonstration of safety.

UKAEA have developed two codes for modelling the transport of activated fluids: GammaFlow [39] and ActiFlow [40]. ActiFlow calls the FISPACT-II inventory code to simulate the irradiation of a material in a path through mesh- and cell-based fluxes. GammaFlow uses a cell-based approach, relying on user-input reaction rates and decay rates to model the evolution of particular nuclides using a dedicated API. GammaFlow is well-suited to simple materials in well-defined flow paths, providing computationally inexpensive analysis scalable to the complex pipe networks anticipated in ITER and DEMO. ActiFlow is well-suited to more demanding activation analysis (such as for LiPb) without requiring detailed knowledge of fluid volumes. Both codes can account for splitting of flow paths and residence time distributions such as in fluid delay tanks (allowing for decay).

One aim of fluid activation analysis is the coupling of the neutron transport simulation with computational fluid dynamics (CFD), in order to capture the dynamics of fluid flow through a system. Originally, both codes ignored fluid dynamics effects, assuming a uniform velocity profile such that the residence time in a circuit component is proportional to the fluid volume. The assumption holds reasonably well for turbulent flow but is less accurate for laminar flow conditions. The open-source CFD software OpenFoam [41] has been used to provide input on the velocity profiles to ActiFlow and GammaFlow. This was benchmarked against the ITER first-wall (FW) mock-up water activation experiment performed with the FNG source in 2019 [42]. A clear improvement of 13% for the lowest predicted C/E has been observed when accounting for the fluid effects, with good agreement between the codes [40]. Further work is needed to more rigorously couple the codes with CFD calculations, such as implemented by F4E [43], with continuing benchmarking activities including the design of a water activation loop at the TRIGA reactor [44]. The advancement of this multi-physics approach is a key undertaking for integrated power plant design.

III. EXPERIMENTAL ACTIVITIES

III.A. Capability and expansion of radiometric activity at UKAEA

UKAEA hosts a significant portion of the Advanced Digital Radiometric Instrumentation for Applied Nuclear Activities (ADRIANA) instrument suite (see figure 9) as part of UK National Nuclear User Facility (NNUF). This includes an array of particle detection systems including a broad energy germanium (BEGe) detector with Compton suppression coincidence veto system, a high Relative Efficiency HPGe detector and a Trans-SPEC portable HPGe detector. Some examples of the broad portfolio of work conducted with this equipment includes waste assay measurements; diagnostics for JET and MAST; material characterisation for the UKAEA's Materials Research

Facility (MRF) and provision of radiometric support for private fusion companies. A brand new laboratory will be occupied in 2022 allowing significant expansion of equipment and on-site capability. The existing technologies in the ADRIANA suite at Culham will be consumed into this lab, termed the RADLab.

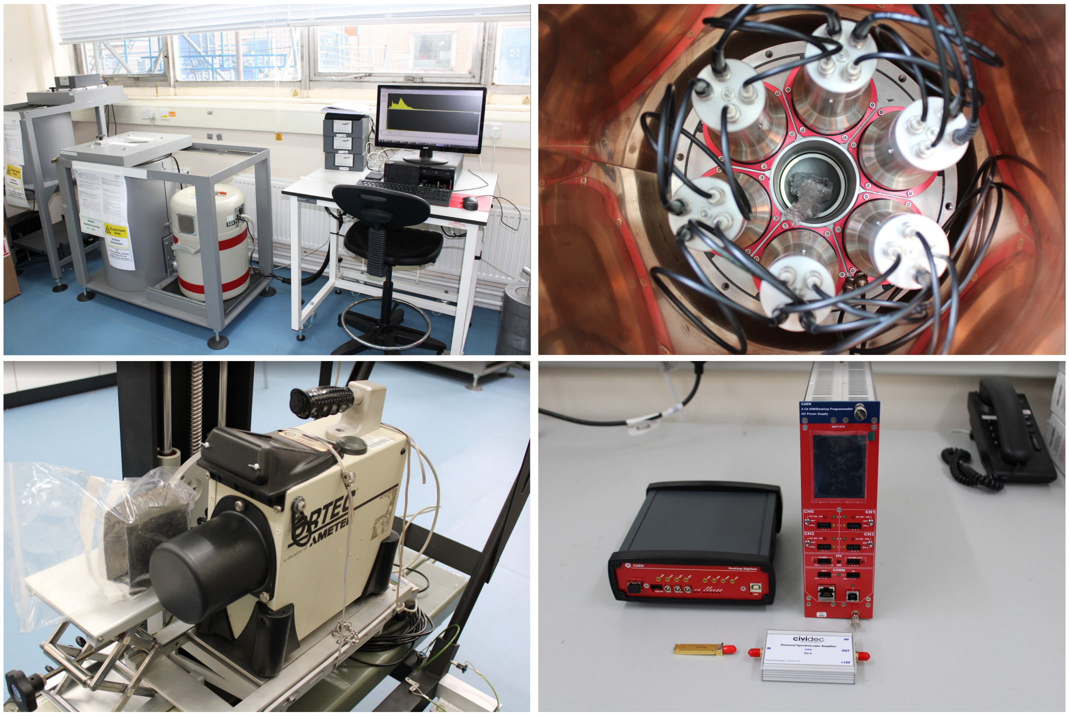

Fig. 9. The broad energy germanium (BEGe) and data acquisition setup in the current on site lab (top left), close up view of the associated Compton suppression system with several sodium iodide detectors (top right), portable Trans-SPEC HPGe (bottom left) and diamond detector with data acquisition system (bottom right)

Extensive work in supporting EU collaborative activities through gamma spectrometry, such as activation studies of ITER materials through the neutron production at JET, have been undertaken at the laboratory [45, 46, 47] with analysis also contributed through participating EU laboratories in Italy, Greece and Poland. Underpinning activation nuclear data validation activities have included use of, and data derived from, 14 MeV neutron irradiation facilities such as ASP, based in the UK, and the FNS, which was based in Japan [48, 49, 50, 51]. Support to a range of EU experimental activities at the Frascati Neutron Generator (FNG) have also been conducted, see for example [52, 53, 54]. One example of a planned future experiment is to develop an inboard shielding mock-up experiment to mitigate the risk within compact device shielding designs, where shielding space is at a premium for the protection of sensitive components such as superconducting magnets. The status of the experiment is in the design process with plans to perform the experiment at a well characterised 14 MeV neutron irradiation facility, expected in 2024. UKAEA has procured diamond detectors, activation foils and TLDs for detection of fast and thermal neutrons, and gammas in this experiment. This will validate and drive the design of shielding concepts as needed in high flux environments of future fusion devices such as STEP. It will also provide additional valuable data for validation of simulation methods, some of which were discussed in preceding sections. The diamond detectors as well as other high specification instrumentation that are part of the UKAEA radiometric lab have applications spanning fusion and fission power plants, nuclear security, decommissioning, university projects and other research areas.

III.B. Novel system for understanding operational fields

The measurement of neutron spectra provides a key understanding of the radiation environment and is an important diagnostic for fusion devices. A broad review of modern neutron detection was undertaken and published in IAEA-TECDOC-1935 in 2020, with fusion-oriented technology contributions, see for example [55, 56]. Further contributions towards resilient neutron detection instruments and neutron spectrum unfolding [57] aimed towards power plant environments and for pulsed neutron fields [58] have also been researched. Under this theme, a fusion-relevant passive neutron spectrometry (PNS) system has been designed from first principles and manufactured at UKAEA. This consists of a 30 cm diameter high density polyethylene (HDPE) sphere with as series of thermo-luminescent (TLD) badges used to measure dose. The TLDs are located along arms through the sphere in pairs comprising TLD-600 (96% ^{6}Li) and TLD-700 (96% ^{7}Li) badges. The system is highly portable and unlike active methods of characterisation, does not require any electronics or active monitoring.

The design process utilised the python package, SPECTRA-UF [59], which was developed by UKAEA to create a unified package for automating the unfolding process. To generate response matrices in the TLDs, a Python script was developed to automatically generate MCNP geometry and perform a neutron transport simulation with the dose tallied in each dosimetry disk position. To optimise the TLD locations, a synthetic data set together with the SPECTRA-UF code was utilised. A flat a-priori spectrum was used as the initial guess in this case. The spectra were compared to those determined at several low dose locations in MAST and JET which were derived using transport simulations with the respective MCNP models. The more empirical data gathered increases the population of the response matrix and therefore the fidelity of the spectrum (in energy) that can be unfolded. With increasing size of the sphere, it was found that diminishing returns are observed above 30 cm diameter. At this diameter, different arm structures as well as number of TLD badges per arm were also studied. A configuration with 14 arms (through 7 axis) with 6 TLD pairs per arm was derived as the final design as illustrated in Figure 10.

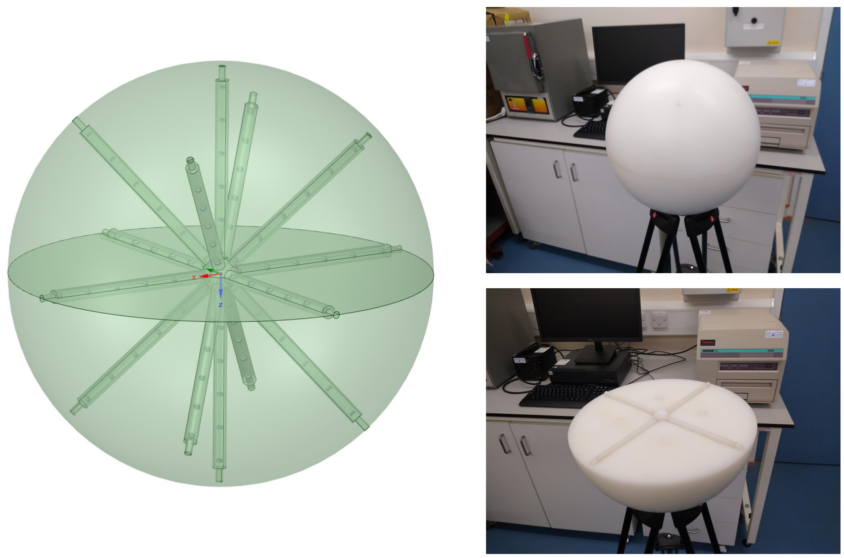

Fig. 10. CAD model (left) and manufactured model of PNS detector (right), with a 30 cm radius sphere of HDPE, 14 arms each with 6 pairs of TLD-600 and TLD-700 badges equally spaced along each arm. On the right hand side, the TLD reader can be seen in the background.

The fabrication of the PNS was completed by the manufacturing support group (MSG) at UKAEA using a specialised CNC machine. First irradiation will take place in 2022 before being deployed in either a MAST-U or JET campaign as a proof of concept and demonstration of its suitability for deployment in STEP, ITER and DEMO. As well as aiding understanding of the neutron spectra during early operations of these future devices, the data will also be valuable for the validation of simulation methods prior to full power operations.

IV. CONCLUSION

Demonstration of a commercially viable pathway to fusion energy will require novel, innovative solutions in order to address outstanding scientific and engineering gaps in present day understanding. Neutronics is the area of research concerned with the characterisation of the radiation field which impacts almost all aspects of a fusion plant. A complete understanding of the radiation environment through demonstration of the As Low As Reasonably Achievable (ALARA) principle is needed to ensure the safe and controlled operation of a fusion power plant. The codes and methods that are driving forward the design should be rigorously validated and fully capable of accurately calculating nuclear responses at a sufficient level of fidelity on the timescales required.

The ART group at UKAEA is responsible for advancing radiation analysis and validation through measurement. ART has expanded to over 18 members across the core applied analysis and parallel radiometric areas. The group has a focused research and development effort to accelerate nuclear design and address outstanding challenges where they exist in current neutronics practices. In this paper, examples of developments which increase the efficiency of the applied analysis workflow have been outlined. The set of tools integrated into SpaceClaim using the API significantly reduce the time taken to perform certain geometry simplification tasks. The development of a novel 1 step (N1S) method combines advantages of the existing R2S and D1S methods. Using a time dependent source term together with a specially prepared nuclear data library, the shutdown dose rate at different cooling times is evaluated in a single transport calculation. This method reduces the time needed for the computation of dose rates and has been developed to allow interfacing with different transport codes. One outstanding development gap is in the accurate modelling of activated fluids and their transport through a system, specifically activated corrosion products. UKAEA have developed two codes which look to couple fluid activation with the dynamics of its flow, providing a framework to develop further capabilities such as the addition of phenomena like corrosion.

The existing conventional workflow which uses MCNP for particle transport has been extensively applied across a multitude of fusion problems including JET, MAST, ITER, DEMO and others. Both OpenMC and Serpent Monte-Carlo codes are being explored as potential complimentary codes to MCNP. In the conceptual design phase of STEP, a new workflow has been devised based on the code driven generation of CAD models and particle transport on the CAD geometry using DAG-OpenMC. This allows for scoping a broad design space on timescales of the order of minutes to hours depending on model complexity. With the development of new simulation tools and methods and their deployment in shaping the design of future reactors, validation is critical underpinning that, at some stage, will fall under the scrutiny of the nuclear regulator. A benchmark case adopting the ITER port plug geometry was used as validation for a recently implemented variance reduction capability in OpenMC. This was compared to both Serpent and MCNP using independently generated weight windows, with excellent agreement observed in the neutron spectra for a cell at the rear of the port plug.

Future planned experiments will provide vital experimental data. An inboard shielding mock-up experiment is being designed in order to better understand the effectiveness of potential shielding materials in the harsh environment that plasma facing components are exposed to. As well as valuable data for code validation, this will provide crucial input for developing the most optimal shield of critical in-vessel components in devices like STEP. A fusion-relevant passive neutron spectrometry (PNS) system for the characterisation of neutron spectra in operational environments has also been detailed. This provides a highly portable and flexible system that does not require active electronics, giving many advantages over current limited methods for characterising the neutron field. The system has now been manufactured at UKAEA and will undergo irradiation in late 2022 for preliminary testing prior to deployment in MAST-U and JET.

The design, procurement of detectors and analysis of the inboard shielding mock-up and PNS system are examples of ongoing world-leading research in the sphere of fusion radiometrics. More broadly, the ART group will occupy a new facility, RADLab in Autumn 2022 that will expand the capability of existing ADRIANA instrument suite with an array of neutron and gamma diagnostic equipment. The RADlab will provide high spec and bespoke detection equipment for radiometric research. As well as providing radiometric support where it is required at UKAEA, the experimental programme works with industrial partners both in the UK and internationally, developing new techniques that address the needs of fusion technology in this area.

ORCID

Alex Valentine: orcid.org/0000-0002-6448-9701

Tom Berry: orcid.org/ 0000-0001-7087-908X

Callum Grove: orcid.org/0000-0002-3630-5637

Chantal Nobs: orcid.org/0000-0002-3630-5637

Lee Packer: orcid.org/0000-0003-3539-9587

PUBLICATIONS

A list of peer reviewed publications by the Applied Radiation Technology group dating back to 2018 can be found here.

ACKNOWLEDGMENTS

The author would like to acknowledge that this paper presents a summary of work conducted by the Applied Radiation Group at UKAEA, drawing on the wide array of ongoing nuclear analysis by each of the named co-authors.

This work has been funded by the EPSRC Energy Programme [grant numbers EP/W006839/1, EP/T012250/1 and EP/L025671/1]. To obtain further information on the data and models underlying this paper please contact PublicationsManager@ukaea.uk.

REFERENCES

[1] UKAEA, https://step.ukaea.uk/ (2022).

[2] M. Coleman and S. McIntosh, "BLUEPRINT: A novel approach to fusion reactor design," *Fusion Engineering and Design*, **139**, 26 (2019); 10.1016/j.fusengdes.2018.12.036.

[3] J. Morris, M. Coleman, S. Kahn, S. Muldrew, A. Pearce, D. Short, J. Cook, S. Desai, L. Humphrey, M. Kovari, J. Maddock, and D. Vaccaro, "Preparing systems codes for power plant conceptual design," *Nuclear Fusion*, **61**, *11*, 116020 (2021); 10.1088/1741-4326/ac18dd., URL https://doi.org/10.1088/1741-4326/ac18dd.

[4] F. Franza, L. Boccaccini, E. Fable, I. Landman, I. Maione, S. Petschanyi, R. Stieglitz, and H. Zohm, "MIRA: a multi-physics approach to designing a fusion power plant," *Nuclear Fusion*, **62**, *7*, 076042 (2022); 10.1088/1741-4326/ac6433., URL https://doi.org/10.1088/1741-4326/ac6433.

[5] P. K. Romano, N. E. Horelik, B. R. Herman, A. G. Nelson, B. Forget, and K. Smith, "OpenMC: A state-of-the-art Monte Carlo code for research and development," *Annals of Nuclear Energy*, **82**, 90 (2015); https://doi.org/10.1016/j.anucene.2014.07.048., URL https://www.sciencedirect.com/science/article/pii/S030645491400379X, joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013, SNA + MC 2013. Pluri- and Trans-disciplinarity, Towards New Modeling and Numerical Simulation Paradigms.

[6] J. Leppänen et al., "The Serpent Monte Carlo code: Status, development and applications in 2013," *Ann. Nucl. Energy* (2015).

[7] Y. Wu, J. Song, H. Zheng, G. Sun, L. Hao, P. Long, and L. Hu, "CAD-based Monte Carlo program for integrated simulation of nuclear system SuperMC," *Annals of Nuclear Energy* (2015); 10.1016/j.anucene.2014.08.058.

[8] L. Lu, Y. Qiu, and U. Fischer, "Improved solid decomposition algorithms for the CAD-to-MC conversion tool McCad," *Fusion Engineering and Design*, **124**, 1269 (2017); https://doi.org/10.1016/j.fusengdes.2017.02.040., URL https://www.sciencedirect.com/

science/article/pii/S0920379617301230, proceedings of the 29th Symposium on Fusion Technology (SOFT-29) Prague, Czech Republic, September 5-9, 2016.

[9] J. Goorley, "Initial MCNP6 Release Overview - MCNP6 version 1.0," *LA-UR-13-22934* (2013).

[10] S. W. Mosher, S. R. Johnson, A. M. Bevill, A. M. Ibrahim, C. R. Daily, T. M. Evans, J. C. Wagner, J. O. Johnson, and R. E. Grove, *ADVANTG: An Automated Variance Reduction Parameter Generator* (2015).

[11] A. Davis and A. Turner, "Comparison of global variance reduction techniques for Monte Carlo radiation transport simulations of ITER," *Fusion Engineering and Design*, **86**, *9*, 2698 (2011); https://doi.org/10.1016/j.fusengdes.2011.01.059., URL https://www.sciencedirect.com/science/article/pii/S0920379611000718, proceedings of the 26th Symposium of Fusion Technology (SOFT-26).

[12] B. Colling, T. Eade, M. J. Joyce, R. Pampin, F. Seyvet, A. Turner, and V. Udintsev, "Neutronics analysis for integration of ITER diagnostics port EP10," *Fusion Engineering and Design*, **109-111**, 1109 (2016); https://doi.org/10.1016/j.fusengdes.2016.01.013., URL https://www.sciencedirect.com/science/article/pii/S0920379616300126, proceedings of the 12th International Symposium on Fusion Nuclear Technology-12 (ISFNT-12).

[13] T. Eade, S. Lilley, Z. Ghani, and E. Delmas, "Movement of active components in the shutdown dose rate analysis of the ITER neutral beam injectors," *Fusion Engineering and Design*, **98-99**, 2130 (2015); https://doi.org/10.1016/j.fusengdes.2014.12.022., URL https://www.sciencedirect.com/science/article/pii/S0920379614006668, proceedings of the 28th Symposium On Fusion Technology (SOFT-28).

[14] A. Davis and A. Turner, "APPLICATION OF NOVEL GLOBAL VARIANCE REDUCTION METHODS TO FUSION RADIATION TRANSPORT PROBLEMS," *International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering* (2011).

[15] A. Davis and R. Pampin, "Benchmarking the MCR2S system for high-resolution activation dose analysis in ITER," *Fusion Engineering and Design*, **85**, *1*, 87 (2010);

https://doi.org/10.1016/j.fusengdes.2009.07.002., URL https://www.sciencedirect.com/science/article/pii/S0920379609002518.

[16] J.-C. Sublet, J. Eastwood, J. Morgan, M. Gilbert, M. Fleming, and W. Arter, "FISPACT-II: An Advanced Simulation System for Activation, Transmutation and Material Modelling," *Nuclear Data Sheets*, **139**, 77 (2017); https://doi.org/10.1016/j.nds.2017.01.002., URL https://www.sciencedirect.com/science/article/pii/S0090375217300029, special Issue on Nuclear Reaction Data.

[17] UKAEA, https://pypact.readthedocs.io/en/latest/index.html (2019).

[18] UKAEA, https://github.com/ukaea/SpaceClaim_API_NeutronicsTools (2019).

[19] ASME, *Stainless Steel Pipe, ASME B36.19M-2004* (2004).

[20] F4E, https://github.com/Radiation-Transport (2019).

[21] D. Valenza, H. Iida, R. Plenteda, and R. T. Santoro, "Proposal of shutdown dose estimation method by Monte Carlo code," *Fusion Engineering and Design*, **55**, *4*, 411 (2001); https://doi.org/10.1016/S0920-3796(01)00188-0., URL https://www.sciencedirect.com/science/article/pii/S0920379601001880.

[22] P. Sauvan, R. Juárez, G. Pedroche, J. Alguacil, J. Catalan, F. Ogando, and J. Sanz, "D1SUNED system for the determination of decay photon related quantities," *Fusion Engineering and Design*, **151**, 111399 (2020); https://doi.org/10.1016/j.fusengdes.2019.111399., URL https://www.sciencedirect.com/science/article/pii/S0920379619308956.

[23] R. Villari, U. Fischer, F. Moro, P. Pereslavtsev, L. Petrizzi, S. Podda, and A. Serikov, "Shutdown dose rate assessment with the Advanced D1S method: Development, applications and validation," *Fusion Engineering and Design*, **89**, *9*, 2083 (2014); https://doi.org/10.1016/j.fusengdes.2014.01.071., URL https://www.sciencedirect.com/science/article/pii/S0920379614000726, proceedings of the 11th International Symposium on Fusion Nuclear Technology-11 (ISFNT-11) Barcelona, Spain, 15-20 September, 2013.

[24] T. Eade, S. Bradnam, and P. Kanth, "A new novel-1-step shutdown dose rate method combining benefits from the rigorous-2-step and direct-1-step methods," *Fusion Engineering and Design*, **181**, 113213 (2022); https://doi.org/10.1016/j.fusengdes.2022.113213., URL https://www.sciencedirect.com/science/article/pii/S0920379622002095.

[25] M. Loughlin, "Conclusions of shutdown dose rate benchmark study," *6th ITER neutronics meeting*, 17–24 (2011).

[26] "SINBAD – Radiation shielding benchmark experiments," *Annals of Nuclear Energy*, **159**, 108254 (2021); https://doi.org/10.1016/j.anucene.2021.108254., URL https://www.sciencedirect.com/science/article/pii/S0306454921001304.

[27] A. Valentine, T. Berry, S. Bradnam, J. Hagues, and J. Hodson, "Benchmarking of emergent radiation transport codes for fusion neutronics applications," *Fusion Engineering and Design*, **180**, 113197 (2022); https://doi.org/10.1016/j.fusengdes.2022.113197., URL https://www.sciencedirect.com/science/article/pii/S0920379622001934.

[28] A. Valentine, B. Colling, R. Worrall, and J. Lepp, "Benchmarking of the Serpent 2 Monte Carlo Code for Fusion Neutronics Applications," *PHYSOR 2020 conference proceedings* (2020).

[29] A. Turner, "Investigations into alternative radiation transport codes for ITER neutronics analysis," *Transactions of the American Nuclear Society*, **116**, *17*, 251 (2017).

[30] A. Turner, A. Burns, B. Colling, and J. Leppänen, "Applications of Serpent 2 Monte Carlo Code to ITER Neutronics Analysis," *Fusion Science and Technology*, **74**, *4*, 315 (2018); 10.1080/15361055.2018.1489660., URL https://doi.org/10.1080/15361055.2018.1489660.

[31] T. Eade, B. Colling, J. Naish, L. W. Packer, and A. Valentine, "Shutdown dose rate benchmarking using modern particle transport codes," *Nuclear Fusion*, **60**, *5* (2020); 10.1088/1741-4326/ab8181.

[32] A. Valentine, R. Worrall, and J. Leppänen, "Investigation of novel weight window methods in Serpent 2 for fusion neutronics applications," *Fusion Engineering and Design*,

178, 113090 (2022); https://doi.org/10.1016/j.fusengdes.2022.113090., URL https://www.sciencedirect.com/science/article/pii/S0920379622000904.

[33] T. Tautges, P. Wilson, J. Kraftcheck, B. Smith, and D. Henderson, "Acceleration Techniques for Direct Use of CAD-Based Geometries in Monte Carlo Radiation Transport," (2009).

[34] R. Pampin, A. Davis, J. Izquierdo, D. Leichtle, M. J. Loughlin, J. Sanz, A. Turner, R. Villari, and P. P. Wilson, "Developments and needs in nuclear analysis of fusion technology," *Fusion Engineering and Design*, **88**, *6-8*, 454 (2013); 10.1016/j.fusengdes.2013.03.049., URL http://dx.doi.org/10.1016/j.fusengdes.2013.03.049.

[35] J. Leppänen, "Response Matrix Method–Based Importance Solver and Variance Reduction Scheme in the Serpent 2 Monte Carlo Code," *Nuclear Technology*, 1–17 (2019); 10.1080/00295450.2019.1603710., URL https://doi.org/10.1080/00295450.2019.1603710.

[36] Y. Hu, S. Yan, Y. Qiu, and Y. Zheng, "Implementation and benchmarking of an automatic global variance reduction method on OpenMC," *Fusion Engineering and Design*, **173**, 112829 (2021); https://doi.org/10.1016/j.fusengdes.2021.112829., URL https://www.sciencedirect.com/science/article/pii/S0920379621006050.

[37] A. Davis, S. Lilley, and J. Shimwell, "csg2csg: a Tool to Assist Validation & Verification," *European Physical Journal Web of Conferences*, vol. 247 of *European Physical Journal Web of Conferences*, 04012 (2021); 10.1051/epjconf/202124704012.

[38] D. Tilley, H. Weller, and C. Cheves, "Energy levels of light nuclei A = 16–17," *Nuclear Physics A*, **564**, *1*, 1 (1993); https://doi.org/10.1016/0375-9474(93)90073-7., URL https://www.sciencedirect.com/science/article/pii/0375947493900737.

[39] C. Nobs, J. Naish, L. Packer, R. Worrall, M. Angelone, A. Colangeli, S. Loreti, M. Pillon, and R. Villari, "Computational evaluation of N-16 measurements for a 14 MeV neutron irradiation of an ITER first wall component with water circuit," *Fusion Engineer-*

ing and Design, **159**, 111743 (2020); https://doi.org/10.1016/j.fusengdes.2020.111743., URL https://www.sciencedirect.com/science/article/pii/S092037962030291X.

[40] T. Berry, C. Nobs, A. Dubas, R. Worrall, T. Eade, J. Naish, and L. Packer, "Integration of fluid dynamics into activation calculations for fusion," *Fusion Engineering and Design*, **173**, 112894 (2021); https://doi.org/10.1016/j.fusengdes.2021.112894., URL https://www.sciencedirect.com/science/article/pii/S0920379621006700.

[41] H. Weller, G. Tabor, H. Jasak, and C. Fureby, "A tensorial approach to CFD using object oriented techniques," *Computers in Physics*, **12** (1998).

[42] Andreoli, F., Angelone, M., Colangeli, A., Besi Vetrella, U., Fiore, S., Flammini, D., Del Prete, P., Loreti, S., Mariano, G., Mazzitelli, G., Moro, F., Pagano, G., Pietropaolo, A., Pillon, M., Terranova, N., Villari, R., Naish, J., Nobs, C.R., and Packer, L.W., "Comparison between measurement and calculations for a 14 MeV neutron water activation experiment," *EPJ Web Conf.*, **239**, 21002 (2020); 10.1051/epjconf/202023921002., URL https://doi.org/10.1051/epjconf/202023921002.

[43] C. Moreno Carrero, F. Cau, and R. Pampin, "Radio-species transport model for coupled fluid dynamics-neutron activation calculations," *Fusion Engineering and Design*, **181**, 113171 (2022); https://doi.org/10.1016/j.fusengdes.2022.113171., URL https://www.sciencedirect.com/science/article/pii/S0920379622001673.

[44] A. Žohar, A. Pungerčič, K. Ambrožič, V. Radulović, I. Lengar, and L. Snoj, "Analysis of irradiation experiments with activated water radiation source at the JSI TRIGA Research Reactor," *Fusion Eng. Des.*, **161**, 111946 (2020); https://doi.org/10.1016/j.fusengdes.2020.111946., URL https://www.sciencedirect.com/science/article/pii/S0920379620304944.

[45] L. Packer, P. Batistoni, B. Colling, K. Drozdowicz, S. Jednorog, M. Gilbert, E. Laszynska, D. Leichtle, J. Mietelski, M. Pillon, I. Stamatelatos, T. Vasilopoulou, and A. Wójcik-Gargula, "Status of ITER material activation experiments at JET," *Fusion Engineering and Design*, **124** (2017); https://doi.org/10.1016/j.fusengdes.2017.01.037.

[46] L. W. Packer et al., “Activation of ITER materials in JET: nuclear characterisation experiments for the long-term irradiation station,” *Nuclear Fusion*, **58**, *9*, 096013 (2018).

[47] L. W. Packer, P. Batistoni et al., “Technological exploitation of the JET neutron environment: progress in ITER materials irradiation and nuclear analysis,” *Nuclear Fusion*, **61**, *11*, 116057 (2021).

[48] L. W. Packer, M. Gilbert et al., “UK fusion technology experimental activities at the ASP 14 MeV neutron irradiation facility,” *Fusion Engineering and Design*, **87**, *5-6*, 662 (2012).

[49] L. W. Packer, M. Gilbert et al., “Integral Cross Section Measurements Around 14 MeV for Validation of Activation Libraries,” *Nuclear Data Sheets*, **119**, 173 (2014).

[50] L. W. Packer, M. Angelone et al., “A comparison of oxide decay heat simulations and nuclear data libraries with fusion irradiation experiments,” *EPJ Web of Conferences*, vol. 247, 09011, EDP Sciences (2021).

[51] T. Stainer, M. R. Gilbert, L. W. Packer et al., “14 MeV NEUTRON IRRADIATION EXPERIMENTS-GAMMA SPECTROSCOPY ANALYSIS AND VALIDATION AUTOMATION,” *EPJ Web of Conferences*, vol. 247, 09010, EDP Sciences (2021).

[52] M. Angelone, M. Pillon et al., “Measurement of delayed neutron emission from water activated by 14 MeV neutrons in a FW mock-up of ITER,” *Fusion Engineering and Design*, **160**, 111998 (2020).

[53] M. Angelone, U. Fischer et al., “Neutronics experiments, radiation detectors and nuclear techniques development in the EU in support of the TBM design for ITER,” *Fusion Engineering and Design*, **96**, 2 (2015).

[54] M. Savva, T. Vasilopoulou et al., “VERDI detector benchmark experiment at the ENEA 14 MeV Frascati Neutron Generator,” *Fusion Engineering and Design*, **146**, 1877 (2019).

[55] L. W. Packer, Z. Ghani et al., “Neutron Detection Technologies and Measurement Challenges at JET and ITER,” *IAEA TECDOC SERIES*, 313 (2020).

[56] I. E. Stamatelatos, M. I. Savva et al., “Novel Neutron Activation Detector for Fusion,” *IAEA TECDOC SERIES*, 301 (2020).

[57] C. R. Nobs, L. W. Packer et al., "Neutron spectrum unfolding for the development of a novel neutron detector for fusion," *Fusion Engineering and Design*, **146**, 2658 (2019).

[58] L. W. Packer, S. Allan et al., "Backwards extrapolation activation diagnostics and their dynamic range for pulsed neutron source measurements," *Fusion Engineering and Design*, **160**, 111923 (2020).

[59] R. Worrall, B. Colling, M. Gilbert, E. Litherland-Smith, C. Nobs, L. Packer, C. Wilson, and A. Zohar, "The development, testing and comparison of unfolding methods in SPECTRA-UF for neutron spectrometry," *Fusion Engineering and Design*, **161**, 112038 (2020); https://doi.org/10.1016/j.fusengdes.2020.112038., URL https://www.sciencedirect.com/science/article/pii/S092037962030586X.