# Safety Reports Series No.95

Methodologies for Assessing the Induced Activation Source Term for Use in Decommissioning Applications



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SAFETY REPORTS SERIES No. 95

# METHODOLOGIES FOR ASSESSING THE INDUCED ACTIVATION SOURCE TERM FOR USE IN DECOMMISSIONING APPLICATIONS

INTERNATIONAL ATOMIC ENERGY AGENCY VIENNA, 2019

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# FOREWORD

A number of nuclear facilities in IAEA Member States are approaching the decommissioning phase of their lifetimes. Planning is key to ensuring that decommissioning is carried out safely and effectively, and various types of information are required to prepare a suitable and complete decommissioning plan. For proper planning and safe decommissioning, a good estimate of the radioactive inventory (i.e. the source term) of the facility is needed. The largest fraction of the radioactive inventory within a reactor or an accelerator facility is that created by the activation process (i.e. the creation of radioactive activation products induced by neutrons or other particles).

This Safety Report provides information on the methodologies, approaches and practices currently available and in use in Member States to assess activation source terms for decommissioning applications. It presents an overview of the process used for the activation calculations, including: (i) the requirements for input data; (ii) details about the modelling and calculation process; (iii) a summary of the most commonly used computer codes with their capabilities and limitations; and (iv) details about the use of the results of the activation calculations. This information is intended to help users in selecting an appropriate methodology for activation calculations that can provide reliable results for material characterization, the decommissioning planning process and the selection of appropriate waste disposal options.

The IAEA would like to express its appreciation to all the experts who contributed to the development and review of this Safety Report. The IAEA officer responsible was V. Ljubenov of the Division of Radiation, Transport and Waste Safety.

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# **1. INTRODUCTION**

#### 1.1. BACKGROUND

A number of nuclear facilities in IAEA Member States are approaching the decommissioning phase of their lifetimes. Planning is one of the most important preparatory tasks for ensuring that a decommissioning project can be implemented safely and effectively [1]. To prepare a proper and complete decommissioning plan, which will help ensure the objective of safe and effective decommissioning is achieved, various types of information need to be developed and secured [2].

For the proper planning and safe implementation of decommissioning, a well developed estimate of the radioactive inventory of a facility (i.e. the source term) is needed. For the purposes of this report, the source term is defined as the quantity of radionuclides (and their spatial distribution in the host material of structures, systems and components (SSCs)) that needs to be processed, treated or removed in order to meet the regulatory requirements for releasing the facility from regulatory control. The amount of radioactivity is normally expressed in units of activity (e.g. becquerels or curies). The largest fraction of the source term inventory for reactor and accelerator facilities is created by neutron activation or activation by other energetic particles (e.g. in the case of accelerator facilities). For other types of facilities, such as manufacturing or processing plants, radioactive contamination often represents the predominant factor in the source term. Experience in Member States with material activation calculations is limited to a small number of countries, and there is a strong interest in specific information about source term determination as it relates to activation processes.

### 1.2. OBJECTIVE

The purpose of this report is to provide Member States with information concerning the assessment of particle induced activation source terms for reactors and accelerators by focusing on: (i) a review of approaches and practices currently available for use in performing activation calculations; and (ii) providing guidance in the selection of an appropriate activation calculation methodology that can provide information required for the material characterization, decommissioning planning, and the selection of the appropriate waste management options.

# 1.3. SCOPE

The source term for facilities that use or generate radioactive material generally consists of: (i) activated materials; (ii) SSCs with loose or fixed radioactive contamination; and (iii) spent fuel elements, operational waste and other radioactive sources.

This report primarily focuses on the induced activation source term, as this source provides a major contribution to dose commitment, the quantity of waste generated during decommissioning activities, and the radiological content of the waste. The determination of source term contributions from other sources (i.e. contamination, fission products) is only briefly discussed in this report because these source term components have been discussed in other IAEA decommissioning publications [3].

The results of activation calculations are particularly applicable to nuclear facilities where neutron or other particle interactions either occur (e.g. in a reactor) or are generated (e.g. in an accelerator) during operations and thereby cause material to become activated. In the case of nuclear power plants and research reactors, the main mechanism is neutron activation. In the case of accelerators, two factors contribute to the induced activation; the first is related to the interaction of the accelerated beam with equipment, especially targets, beam dumps or high beam loss areas, and the second arises from the interactions of secondary particles produced by the beam (mainly neutrons and photons) with the accelerator components and structures.

The information available from activation calculations can also be used to determine the activation characteristics of components that have been removed from a facility and are undergoing testing or analysis at a research or testing laboratory, or are being analysed for waste characterization purposes.

After the source term is determined, shielding and dose calculations can be performed in support of initiatives to assess and control radiation exposures during the implementation of decommissioning activities. Similarly, the information can be used for safety assessments, including those being undertaken in support of, for example, a radioactive waste disposal facility. However, information about the identification and implementation of a dose assessment methodology, dose optimization, and performance assessment methodologies are not explicitly addressed in this report.

# 1.4. STRUCTURE

Section 2 presents: (i) information on the basic processes used in the calculation of particle induced activities; (ii) an overview of proven methods and

codes that can be used to perform activation calculations; and (iii) a discussion centred on the importance of establishing a good understanding of the principles underlying the activation calculations in terms of processes, assumptions and limitations so that the results can be used effectively and with adequate technical confidence. Section 2 also presents a discussion of parameters or factors that may warrant consideration in evaluating and selecting methodologies for calculating the activation source term. Section 3 discusses the means by which to verify and validate the software and data. Section 4 briefly discusses other possible contributors to the total source term for a facility. Section 5 describes how the results of the activation calculations can be applied to the decommissioning planning process. In addition to the information contained in the body of this report, there are five annexes. Annexes I and II provide examples of output data from two of the computer codes discussed in the report. Annex III describes lessons learned during the application of activation calculation techniques. Annex IV provides an example of a validation process for use with numerical simulations of neutron activation in a 300 MW(e) pressurized water reactor plant. Annex V provides an example of an assessment of the induced activities in the graphite components of a 1500 MW(e) high-power channel-type reactor plant.

# 2. PARTICLE INDUCED ACTIVATION SOURCE TERM CALCULATIONS

# 2.1. GENERAL

In general, the decommissioning source term has its origins in both activated components and contaminated SSCs.

The calculation of induced activities is a process that helps to determine the radionuclide content of SSCs exposed to a particle flux (in particular charged hadrons, neutrons and photons) as a function of time. In some nuclear facilities, the activated components can represent a substantial source term requiring carefully developed particle transport and activation model results, as well as careful planning when using the results of the activation calculations. The care required in calculating these activities results from the fact that even a small deviation between the actual and calculated activity levels could have significant effects in terms of safety and radioactive waste management.

Activation calculations can be performed using various computer codes, and Section 2.9 summarizes the models and computational tools which can be used to perform the calculations. However, a precautionary note is warranted: the application of these codes without a detailed understanding of the mathematical and physical principles that underlie the code, or without a considerable amount of experience in the use of the code, could lead to erroneous conclusions. Section 6.2 of Ref. [3] presents a general approach for the calculation of neutron induced activity in reactor facilities.

Two different types of code are needed to perform activation calculations (i.e. a particle transport code and an activation code). Figure 1 provides an overview of the activation calculation process. For nuclear reactors, there are typically two distinct steps; first, a particle transport code is used to calculate particle fluxes at various points in the structure undergoing study, and then an activation code helps determine what activation products result from the reactions between the flux and the materials in the structure. For accelerators, these two steps are not as distinct and can generally be performed simultaneously.

Activation calculations involve four sequential steps:

- (1) Assembling code inputs: Physical, operational and measurement data are assembled and studied to: (i) determine parameter values for use as code inputs; and (ii) provide data required for geometric and spatial modelling.
- (2) Performing particle transport calculations: Using the code inputs identified in the previous step, particle flux levels are determined at locations of



FIG. 1. General approach to activation calculations.

interest. Codes based on Monte Carlo or discrete ordinate  $(S_n)$  methods are used to develop the particle flux levels and energy spectra. Basic assumptions used in these calculations are identified and documented as part of the calculation process.

- (3) Performing activity calculations: Using the code inputs (e.g. facility operating history, material compositions including impurities) and the particle flux levels calculated in the previous step, radionuclide distributions are determined using radionuclide generation and depletion codes. Again, basic assumptions are identified and documented as part of the calculation process.
- (4) Developing results: Using the results of the activity calculations, in terms of both total and specific activities, the radionuclide distributions in specific components, subcomponents and regions can be developed. Upon completion of steps to validate the calculated results, those results can be used for further applications.

Following the completion of the above four steps, the results of the particle induced activation calculations can be applied to decommissioning planning. Areas of planning that specifically benefit from the availability of activation calculations include waste disposition planning, decommissioning scenario selection, cost estimating and dose optimization.

There are two different fundamental approaches that can be used for particle transport calculations (i.e. deterministic and probabilistic). The deterministic approach applies transport codes that solve the Boltzmann transport equation with certain approximations. Deterministic codes based on the  $S_n$  method are adequately suited to this task. However, deterministic codes using the diffusion approximation (which are more often used for reactor core calculations) may not be well suited for the types of activation calculation applications required by decommissioning. At issue is the fact that in decommissioning applications, the range of interest in terms of activation reactions extends into spatial regions which lie at comparatively large distances (i.e. a few metres) from the particle sources. For the components or regions that are in close proximity to the particle sources, diffusion codes may be used, but these are of significantly less value at greater distances from the particle source.

The probabilistic approach is based on the Monte Carlo method. According to the Monte Carlo particle transport theory, if the random walk of a large number of particles is simulated with the aid of statistical estimations, values for physical quantities such as particle flux can be derived. The proper modelling of the random walk and particle trajectories requires values for the differential cross-sections for all possible nuclear interactions in the material region being investigated. Monte Carlo based codes normally assume that the space of the modelled system is divided into segments or cells composed of homogeneous material.

# 2.2. DATA QUALITY

Before proceeding with discussions about the methodologies for the assessment of the induced activation source term for use in decommissioning applications, the topic of data quality merits introduction. A substantial portion of the discussions in this report will focus on the topic of data and information, particularly as it relates to:

- The input and output data used by and resulting from the source term calculations;
- The use of a graded approach;
- The process of ensuring that input and output data are suitable for the intended uses.

At issue is how best to characterize data and information in a manner that accommodates the different possible uses of the data. For example, characterizing data as needing to be "more accurate" or "more precise" may not adequately capture the changes required if those data are to move from being used in scoping calculations to being used in detailed calculations with safety implications.

This issue has been recognized by the United States Environmental Protection Agency, and addressed through a parameter referred to as data quality.

Definitions relative to data quality are as follows [4]:

- Data quality: A measure of the degree of acceptability or utility of data for a particular purpose.
- Data quality indicators: The quantitative statistics and qualitative descriptors used to interpret the degree of acceptability or utility of data to the user. The principal data quality indicators are bias, precision, accuracy (bias is preferred), comparability, completeness, representativeness and sensitivity.

In the context of data quality, references to an increase or improvement in data quality could refer to improvements in any or all of the data quality indicators. Use of the terms data quality or quality of data in this report will be in reference to these definitions.

# 2.3. EVALUATION OF METHODOLOGIES FOR ACTIVATION SOURCE TERM ASSESSMENTS

Two of the principal objectives of this report are: (i) to provide Member States with insight into methodologies available for assessing an induced activation source term and (ii) to help users in selecting an appropriate methodology for activation calculations that can provide reliable results for application to material characterization, decommissioning planning and the selection of appropriate waste disposal options.

In preparation for the evaluation and selection process, it can be useful to systematically identify those parameters that may be important in choosing a methodology. Having identified the parameters, it is then possible to determine if there are any for which critical criteria must be met in order for the selected methodology to be useful. Table 1 provides examples of possible parameters that can be considered when evaluating activation methodologies, as well as some general discussions concerning these parameters.

# 2.4. ACTIVATION PHYSICS

Activation by neutrons is the result of nuclear reactions. A neutron can interact with an atomic nucleus in several ways, and in most cases, these reactions lead to the production of a radioactive nucleus. If a neutron has high energy (in the MeV range), the reactions that most often occur are the types that result in the emission of charged particles. Examples include (n,p), (n, $\alpha$ ), (n,d) and (n,t) reactions. In most cases, the result of these reactions is an altered nucleus, with atomic and mass numbers different from those of the target nucleus. In most cases, the resultant nucleus is found in an excited state. The neutron absorption cross-sections associated with these reactions strongly depend on the energy of the incident neutron, and in most cases that are relevant to activation, the nuclear cross-sections are in the millibarn range.

After being slowed down by the scattering processes (e.g. thermalization), the energy of a neutron becomes very low (in the eV range or below). In this energy range, the most important nuclear reaction is radiative capture  $(n,\gamma)$ . The cross-sections involved with these types of reaction are usually orders of magnitude higher than those for reactions involving higher energy neutrons. Given that a nuclear reactor is generally designed to effectively thermalize neutrons, it is reasonable to assume that in the vicinity of a high intensity neutron source, such as a nuclear reactor core, the products of radiative capture reactions will dominate the generation of radionuclides.

# TABLE 1. EXAMPLES OF POTENTIAL SELECTION ANDEVALUATION PARAMETERS

Potential selection and evaluation parameters	Discussion An assessment of the accuracy of input, as in the case of precision, will dictate the confidence that can be placed in calculated results. The validation measurements may provide insight into the accuracy of input data such as material compositions, but precautions need to be taken to ensure that sources of error are well understood before using output results to adjust input values. As in the case of precision, the availability of records, drawings, etc. can also be used in evaluating the accuracy of the input.			
Accuracy of input data				
Accuracy of results	To help ensure consistency in the use of the term <i>accuracy</i> , it is best defined on a statistical basis (i.e. the closeness of a measurement to a true value). The assessment of the accuracy of calculated results will rely in large measure on the results of code validation studies. Validation studies may need to be specifically designed to ensure that key parameters of particular concern to a user are effectively validated.			
Application of results	<ul> <li>It is of paramount importance to identify how the calculated results will be used. Typical uses could include:</li> <li>Radiation protection;</li> <li>Safety assessments;</li> <li>Environmental assessments;</li> <li>Transportation requirements and compliance;</li> <li>Performance assessments for waste disposal safety cases;</li> <li>Development of decommissioning operational procedures;</li> <li>Selection of decommissioning options;</li> <li>Cost estimation;</li> <li>Risk management.</li> </ul>			
Code limitations	Each code has specific limitations, and part of the evaluation process will be to consider the nature of those limitations, and whether they will adversely affect the planned applications.			

# TABLE 1. EXAMPLES OF POTENTIAL SELECTION ANDEVALUATION PARAMETERS (cont.)

Potential selection and evaluation parameters	Discussion The availability of expertise and support for using the various codes may warrant consideration. For example, it could be beneficial if internal staff have expertise and experience with a particular assessment methodology.		
Code support			
Computational requirements	The availability of required computational resources, including both support staff and equipment, may be important in examining the various assessment options.		
Conservative scenarios	Where input data are unknown, uncertain or highly variable, it may be possible to invoke conservative scenarios that will help ensure that important parameters are not underestimated. However, a structured approach to developing the conservative scenario would be advisable to ensure that the scenario does not unrealistically overestimate other parameters.		
Data quality	A measure of the degree of acceptability or utility of data for a particular purpose [4].		
Data quality indicators	The quantitative statistics and qualitative descriptors used to interpret the degree of acceptability or utility of data to the user. The principal data quality indicators are bias, precision, accuracy (bias is preferred), comparability, completeness, representativeness and sensitivity [4].		
Decommissioning option	This report has been developed for use in decommissioning activities. The results of source term assessments may be pivotal in making key decisions about a preferred decommissioning option (e.g. entombment versus complete removal). Alternatively, key decisions may have already been made concerning a decommissioning strategy, in which case the source term calculations will then play a role in operational considerations such as radiation protection and waste management. The specific role of the source term assessment calculations (i.e. decommissioning planning or execution) may be important in code selection.		

# TABLE 1. EXAMPLES OF POTENTIAL SELECTION ANDEVALUATION PARAMETERS (cont.)

Potential selection and evaluation parameters	Discussion		
Graded approach	One of the topics discussed in this report is the concept of using a graded approach in the assessment of an induced activation source term. The extent to which the various methodologies and codes permit the use of a graded approach may constitute a useful evaluation criterion.		
Key radionuclides	Further to discussions concerning the anticipated uses of the calculated source term, explicitly listing those radionuclides of primary concern to decommissioning activities will help ensure that any issues surrounding those radionuclides are identified and considered during methodology selection.		
Precision of input data	A value describing the variability in the input data will be necessary if, for example, sensitivity analyses are performed. Values for precision can be based on a statistical analysis of measurements, or on material specifications for components of interest. In other cases, it may be necessary to make assumptions and estimate variability. One example is the variability in aggregate density in a concrete structure; another is variability in beam strength and neutron flux.		
Precision of results	To help ensure consistency in the use of the term <i>precision</i> , it is best defined on a statistical basis (i.e. closeness of agreement among a set of results). A user may wish to specify requirements with respect to key parameters such as precision in terms of the codes being considered. For example, a radionuclide of particular importance to a disposal safety case may require a defined level of precision.		
Result portability	The extent and ease to which the calculated results can be used as input to other codes may warrant consideration.		
Risk management	In considering the applications of the source term calculations, it may be useful to ascertain if any risk mitigation measures could benefit from specific capabilities of the codes and methodologies under consideration.		

# TABLE 1. EXAMPLES OF POTENTIAL SELECTION ANDEVALUATION PARAMETERS (cont.)

Potential selection and evaluation parameters	Discussion		
Sensitivity	Sensitivity refers to the effect of variability in input data on the variability of output data. The topic of sensitivity analysis is raised in a number of sections in this report, and plays an important role in assessing the usefulness of calculated results in terms of planned applications. If results are found to be very sensitive to input parameters, and the variability in the input parameters is largely unknown or high, then the results may be of limited use.		
Spatial and energy resolution	The resolution of the results in terms of both spatial and energetic parameters may be a key consideration. If, for example, a reactor is to be disassembled into individual components, the granularity of the calculated results will be more important than if the reactor is removed as a single component.		
Trueness of results	Trueness is defined on a statistical basis (i.e. closeness of the mean of a set of measurement results to the actual (true) value). As in the case of accuracy, the trueness of calculated results is primarily assessed through validation studies.		
Type and nature of facility	<ul> <li>As will be discussed in Section 2.9, the nature of the facility requiring modelling by the assessment codes is an important consideration in code selection. Specific aspects include:</li> <li>Whether the facility is an accelerator or reactor;</li> <li>For reactors, whether it is a power, research, material testing, or isotope production reactor;</li> <li>Unique characteristics of the facility (e.g. non-symmetrical configurations, complex, multiple void spaces, unusual materials of construction);</li> <li>Availability and quality of facility information.</li> </ul>		

Particle accelerators of intermediate energies (from about 50 MeV up to a few GeV per nucleon), and high energies (above a few GeV per nucleon) generate secondary radiation fields which are usually referred to as 'complex radiation fields', since they comprise different types of hadronic and electromagnetic particles extending over a wide energy range. For a primary beam of charged hadrons, the secondary radiation is mainly neutrons. Apart from the high energy particles, other contributions come from photons, protons, electrons, pions (above the threshold energy for their generation) and muons (from pion decay). For a primary beam of electrons, bremsstrahlung X rays are the main component of the secondary field generated in a target (plus synchrotron X rays produced in circular accelerators). Hadrons from photonuclear reactions (mainly neutrons) provide a further contribution. Neutron production occurs via three mechanisms: the giant dipole resonance (the dominant process in energies up to 35 MeV), the quasi-deuteron effect (dominant in the energy range 30–300 MeV) and the photopion reaction (occurring in energies of about 150 MeV and higher) [5–7].

If the production rate of the nuclides induced by the activation process is considered time dependent (i.e. dependant on the facility operational history), the following differential equation has to be solved for each nuclide:

$$\frac{\mathrm{d}N_m(t)}{\mathrm{d}t} = -N_m(t)\beta_m + \overline{Y_m(t)} + \sum_{k \neq m} N_k(t)\gamma_{k \to m} \tag{1}$$

where

- $\beta_m$  is the total transformation probability of isotope *m*;
- $\gamma_{k \to m}$  is the probability of the transformation from isotope k into isotope m, assuming that the nuclear transformation only involves single capture and  $\beta$  decay;
- $Y_m(t)$  is the production rate of isotope *m*;

 $N_k(t)$  is the time dependent atomic density of the isotope k;

and  $N_m(t)$  is the time dependent atomic density of the isotope m.

By applying a numerical integration method to solve the above equation, the total or specific activity values for various radionuclides can be determined.

# 2.5. GRADED APPROACH

In principle, the application of a graded approach represents a process whereby the level of effort applied to an activity corresponds exactly to that needed to achieve the required results. Therefore, the effective use of a graded approach requires a clear understanding of: (i) what constitutes the required results; (ii) what parameters can be adjusted to change the 'grade' of the approach; and (iii) the impact of the adjustments on the results.

From the perspective of a graded approach as applied to activation calculations, the requirements for the results could be varied, for example, in terms of:

- Spatial details and resolution;
- Quality of output data (e.g. precision and accuracy);
- Extent and comprehensiveness of the output (e.g. the suite of radionuclides calculated).

The types of parameters that might be adjusted to change the grade could include:

- Model complexity;
- Quality of input data (e.g. precision and accuracy).

As an example of a graded approach to activation calculations, the quantities and types of radionuclide produced by the activation process can be roughly estimated with the aid of relatively simple codes, and these rough estimates may be sufficient for preliminary estimates to be made of waste volumes and their total and specific activities. Alternatively, more sophisticated computational codes (e.g. codes based on probabilistic methods) can be used if the activated material needs to be characterized in greater detail. The requirements in terms of the results are principally determined by the operator of the nuclear facility, requirements of the regulatory authority, the method of planned decommissioning, and in particular, the nature of the inputs required for safety, environmental and performance assessments. Significant differences in results can be found with different types of activation calculations; consequently, the method of calculation needs to be carefully chosen, taking into consideration the use to which the results will be put.

During the early stages of decommissioning planning, it may be sufficient to have a general radionuclide inventory of the activated components. In order to assess the total activity and specific activity of the components closest to the particle source, calculations using simplified models may be sufficient. In the case of nuclear reactors, the highest levels of activation are usually concentrated in the metal components closest to the reactor core. Similarly, in the case of particle accelerators, the most activated regions are close to targets or beam loss areas. Therefore, if the objective of the calculations is to determine those regions where the majority of activation products reside, sophisticated computational models may not be required.

Depending on the type of calculation, computational cost can be reduced by: (i) simplifying the particle transport calculation; (ii) reducing the number of spatial mesh intervals or energy groups ( $S_n$  method) applied; or (iii) reducing the number of material regions into which the model geometry is sectioned (with a Monte Carlo method). However, if the calculation methodology or the system model is overly simplified, the reliability and usefulness of the results may be significantly reduced. Similarly, if, as part of the graded approach, different levels of data quality are being considered in terms of input data (e.g. in terms of details about the intensity of the activation source), it is important to note that the quality of the input data will affect the quality of the results.

In line with the precepts of a graded approach, it is often best to let the level of detail (granularity) in the spatial model be largely based on the dismantling methods that will actually be applied during the decommissioning operations. For example, if some or all of the metal components are to be removed and disposed of as one piece (e.g. in cases where a reactor vessel is removed intact), a high level of spatial resolution for the activation results may not be required. On the other hand, if components are to be segmented into several smaller pieces based on dimensional, storage, transport or handling limitations, then the geometric model may need to be divided into regions with dimensions in line with the segmenting plans.

The nature or quality of the required results in a graded approach may also need, for example, to consider the expected or planned disposition routes for the decommissioning waste. In general, disposal cases for radioactive waste are supported by performance assessment cases which consider potential doses to critical individuals based on: (i) source term; (ii) transport mechanisms for radionuclides through the environment; and (iii) radiation exposures to certain individuals as a function of time. Essentially all disposal cases, ranging from high level waste to free release, are based on performance assessments of various levels of sophistication. As a result, waste acceptance criteria (including clearance criteria) are principally those levels of radioactivity below which dose levels to human and non-human biota will be acceptable. Therefore, it is critical that the activation calculations include all of the radionuclides of importance to the proposed disposal option.

# 2.6. CODE INPUT

Physical, operational and measurement data are required in order to develop the models that will ultimately provide the activation calculations. The

level of detail and quality of the inputs will determine the level of detail and quality of the results. Assumptions are necessary for model development, and these assumptions need to be explicitly identified and documented to allow their potential effects on the results of activation calculations to be assessed. In order to ensure that the calculated activities are not underestimated, these assumptions will need to be appropriately conservative. It may also be beneficial to assess the level of uncertainty in the assumptions, and to determine the impact of inaccurate or incorrect assumptions on the calculated results.

# 2.6.1. Physical inputs

Dimensional and material inputs are used to develop the physical models required for use in the particle transport and activity calculations. Physical inputs may be obtained from drawings, component manuals, material data and other sources.

# 2.6.1.1. Drawings

Legible drawings are required, and they need to adequately describe the components of interest. Of particular importance is the availability of 'as-built' drawings, and drawings that show current conditions, particularly with respect to any modifications that may have been performed on a facility. Drawings that provide details of individual components (i.e. reactor internals, beam tubes, the biological shield), and drawings that indicate relationships and interfaces between components are also needed. The importance of reliable drawings to the decommissioning process, including source term assessments, underscores the need for establishing a good document management system at an early stage in the design, construction and operation of a nuclear facility. For example, drawings need to be stored in such a manner that they do not deteriorate over time, and need to be available for review and use (e.g. through the use of a database system) at any time, particularly during decommissioning. Facility specific drawings are preferred to manufacturer 'typical' drawings. Many drawings also identify the materials used in the construction of the component, as well as references to other drawings that help define larger or smaller subcomponents and thereby help identify the dimensional relationships (fit-up) between different components. Special attention needs to be paid to regions of the facility or components where particle streaming or beam loss may occur.

When analysing a reactor facility, fuel assembly drawings for all of the fuel types used over the lifetime of the facility are reviewed for relevant dimensional, material composition and weight information. Compendiums of fuel assembly data [8] may be useful in lieu of, or in addition to facility specific fuel drawings.

# 2.6.1.2. Manuals

Manuals may be available that discuss the fabrication, dimensions and operation of facility components of importance to the activity calculations. Component manuals may have been supplied to the facility during initial construction or during subsequent facility modifications. Manuals may contain information useful for particle transport and activity calculations, such as dimensioned drawings, materials of construction, material specifications, weights and assembly criteria, that may not be available elsewhere. Examples include reactor vessel manuals, reactivity control system manuals and other component or system manuals.

# 2.6.1.3. Material data

The level of quality achieved in modelling the material composition of the SSCs will have a very significant impact on the quality of the results of the activation calculations. This type of data is also frequently the most difficult to find during decommissioning planning, a situation resulting in large part from the fact that it may have been supplied only once, during actual facility construction. This fact further emphasizes the importance of considering decommissioning requirements even at the early stages of a facility lifetime (i.e. ideally during the design phase, but most certainly during the construction phase). In this respect, it can be said that the construction phase is crucial for decommissioning, because information on material compositions, which is of pivotal importance for the determination of the activation source term, is often only available at that stage.

Many drawings reflect the material used in the construction or manufacturing of a component and may reference a material standard. Material standards typically provide limits or ranges for the main material constituents. However, the limits or range values given by a material standard may be too broad for generating useful activation calculation results. Data on an elemental basis for each batch of material used (sometimes referred to as heat or ladle data) for components of interest are preferred to the use of a material standard. However, heat/ladle data also have limitations in their usefulness because the data are often only available for a limited number of elements (i.e. those that are important to material performance, rather than trace impurities). In some cases, values may be assigned to unknown or unmeasured elements based on various assumptions. However, care is required under these circumstances to avoid a situation where a value is assumed to be conservative from the standpoint of, for example, radiation protection but may in fact not be conservative from the perspective of waste acceptance criteria. The above discussion raises an important point that warrants further consideration. While trace impurities or low concentrations of elements in various materials may not be overly important in terms of the properties and performance of that material, if those trace elements have a large nuclear cross-section, the activation products generated from the trace elements could have an appreciable impact on dose rates and whether the material can be accepted into a disposal facility. Therefore, it is important to secure information on the levels of trace elements in materials exposed to particle fluxes, particularly if the calculated results are to be used in predicting doses or assessing disposal options. Compendiums of material data including material standards may be used in lieu of, or to supplement heat/ladle data. NUREG/CR-3474 [9] is one example of a compilation that provides accurate measurements of materials commonly used in nuclear applications.

Mixtures, such as concrete, can be particularly problematic in terms of determining material compositions. Concrete comprises a blend of cement, sand, stone aggregate, water and various additives important to the properties of the final concrete. Variability in the constituents can therefore lead to variability in the composition and homogeneity of concrete structures and thereby cause differences in the levels and types of activation products. Therefore, information concerning mixture constituents, particularly with respect to trace impurities, will play an important role in determining the usefulness of the calculated results. During construction, concrete samples are generally taken and tested to ensure that parameters such as strength, air content and flowability meet specifications. These types of sample may offer an opportunity to assess concrete compositions even after construction is completed.

Before undertaking any programme involving the direct use of chemical and radiochemical analyses to determine material compositions, the programme needs to be carefully designed to optimize its effectiveness by taking into consideration such factors as variability in materials, the constituents of primary concern, data quality requirements and the actual regions or components that will be exposed to the particle flux. For example, because chemical and radiochemical analyses can require significant time and resources, it may be cost effective to determine which regions were not exposed to particle fluxes, as they are unlikely to merit detailed analysis.

In the case of reactors, information on fuel assembly gross weight, enrichment, densities, fissile loads, burnup, overall and nozzle/end fitting dimensions, and materials of construction are required for both the neutron transport and activation calculations.

# 2.6.2. Operational inputs

Details regarding the actual parameters employed in the operation of the nuclear facility are important to the results of both the particle transport and activity calculations. Operational inputs are used to develop the operational history (i.e. a comprehensive description of the ramp-up, operational and decay periods that took place during the entire period that the facility operated). Operational history can be estimated differently depending on the type of facility involved: for reactors it can be estimated by sophisticated analyses of fuel cycle performance; in the case of other nuclear facilities, operating logs can be used.

Larger, commercial reactor facilities normally have records of fuel management and refuelling operations. The fuel and core flux management approach utilized at these facilities forms an important input to neutron transport model development. The core map and layout determines the neutron flux at the boundary of the core. Knowledge regarding changes between 'traditional' and 'partial low leakage' cores is also important to effective modelling.

Smaller research facilities and particle accelerators may only have operational logs for use in identifying periods of operation, beam intensities and other operational data. Both commercial and research facilities may vary operational power over the lifetime of the facility, and such changes need to be identified for inclusion in the development of the model used in the activity calculations. There are a significant number of circumstances where changes to the operational parameters (e.g. operating power and duration, fuel configuration, beam power) will affect the extent of activation. Representative sets of operational parameters need to be identified and employed in the calculations, and at this point in the process of identifying operational inputs, it may be useful to perform sensitivity analyses to gain insight into the effect of changes in operational parameters on the calculated activation results. Based on the sensitivity analyses, it may be beneficial to develop a conservative approach to help guarantee that the decisions about input data made at this stage will not lead to an underestimate of induced activity.

### 2.7. RESULTS

The result of neutron transport calculations is a set of energy and space dependent neutron flux values that apply to a specific reactor configuration. The calculated energy values are divided into discrete ranges or energy groups. The number of energy groups may be as small as three or as large as a few hundred. The activation calculation to determine the total activity and specific activity values is then performed for a specific volume of space at a particular period of time using: (i) the energy levels of the neutrons; (ii) the neutron flux; (iii) the elemental composition of the material in the volume of interest; and (iv) algorithms that account for the radioactive decay of the activation products. The results of activation calculations provide a time dependent description of the specific and total activity for components or regions within the reactor structure. Figure 2 provides an example of typical calculation results. See Annexes I and II for additional examples of output data.

Component: Vessel Wall (<100 cm above/below core				
Component We	eight (kg)	58,385		
Total Activity (E	3q)	1.93E+13		
Total Specific A	Activity (Bq/kg)	3.31E+08		
	Specific	Estimated	Co-60	
Dedienvelide	Activity	Activity	Scaling	
Radionuciide	(Bq/kg)	(вq)	Factors	
Н 3	1.15E+06	6.69E+10	3.01E-02	
C 14	3.40E+04	1.99E+09	8.95E-04	
CL 36	1.96E+03	1.15E+08	5.16E-05	
AR 39	2.58E+03	1.51E+08	6.79E-05	
CA 41	2.73E+01	1.59E+06	7.18E-07	
MN 54	6.49E+05	3.79E+10	1.71E-02	
FE 55	2.84E+08	1.66E+13	7.46E+00	
CO 60	3.80E+07	2.22E+12	1.00E+00	
NI 59	4.83E+04	2.82E+09	1.27E-03	
NI 63	6.29E+06	3.67E+11	1.65E-01	
SR 90	3.15E-06	1.84E-01	8.28E-14	
NB 94	8.61E+02	5.02E+07	2.26E-05	
MO 93	7.20E+03	4.20E+08	1.89E-04	
TC 99	2.06E+03	1.21E+08	5.43E-05	
AG110M	1.97E+02	1.15E+07	5.18E-06	
SB125	2.06E-01	1.20E+04	5.41E-09	
CS134	1.73E+04	1.01E+09	4.56E-04	
CS135	6.17E-05	3.60E+00	1.62E-12	
CS137	2.11E-12	1.23E-07	5.56E-20	
BA133	7.04E+03	4.11E+08	1.85E-04	
SM151	2.19E+04	1.28E+09	5.77E-04	
EU152	3.25E+05	1.90E+10	8.55E-03	
EU154	2.64E+04	1.54E+09 6.94E-04		
EU155	1.46E+02	8.54E+06	3.85E-06	
HO166M	9.06E+02	5.29E+07	2.38E-05	

FIG. 2. Example of activation calculation results for one region of a reactor vessel wall (note that the vessel wall is constructed of carbon steel cladded with stainless steel).

As discussed in previous sections, the decision regarding which model is used to assess the activation source term needs to take into account the purpose for which the results will be used and the quality of the results obtained from that model. The assessment of a source term is crucial to effective decommissioning planning, as it can be used to assess safety, specify end states, select disposal options and develop the details of the decommissioning process itself. To this end, it may be useful to identify the various applications in which the source term will be used, and to also identify which parameters are most important to those applications. This topic is discussed in more detail in Section 5, but as an introduction, some of the applications for which source term information can be used are listed below:

- Radiation protection;
- Decommissioning planning;
- Waste transport;
- Environmental protection;
- Waste management;
- Selection of disposal options;
- Cost estimation;
- Risk management;
- Selection of decommissioning options;
- Development of decommissioning procedures.

In examining each of these applications, it is possible to identify which parameters (generally the type and quantities of radionuclides) are most important to the application. Once this list of key parameters is developed, the characteristics of the results generated by the activity calculations can be examined from the perspective of these key parameters. For example, a sensitivity analysis can be performed to determine if a small change in some of the code input parameters will result in major changes to the levels and types of radionuclides important in the applications. If a high degree of sensitivity is observed, special attention may need to be given to how the results are derived and used.

In summary, to be of value to the decommissioning planning process, the results of the activation calculations need to be evaluated with a knowledge of how the results will be used, and with an understanding of how the usefulness of key parameters in the planning process could be compromised by, for example, an overly high sensitivity to variability in input data.

Figures 3 and 4 show examples of the types of result that can be derived from activation calculations.



FIG. 3. Total activity of the spatial regions in a reactor pressure vessel (RPV) as a function of time after facility shutdown [10].



FIG. 4. Distribution of the specific activities for the major contributing radionuclides for one spatial region in a reactor pressure vessel (RPV) as a function of time after facility shutdown [10].

# 2.8. ASSUMPTIONS AND OTHER CONSIDERATIONS

The purpose of this section is to: (i) examine the circumstances under which general assumptions need to be made in order to undertake the assessment of the activation source term; (ii) provide examples of possible assumptions; (iii) provide insight into where there may be uncertainties or weaknesses in the assumptions; (iv) explore the manner in which the uncertainties or weaknesses could compromise the usefulness of the results; (v) discuss possible actions to reduce the probability or impacts of uncertain assumptions; and (vi) discuss other considerations of importance in undertaking the activity calculations.

#### 2.8.1. General assumptions

In preparation for undertaking a programme to assess an activation source term, it is important to identify the key assumptions that underlie the programme. By carefully considering any uncertainties surrounding these assumptions, and by taking actions to address and evaluate the uncertainties, it is possible to help ensure that the outcomes of the activation source term assessment programme will meet programme objectives. Some of the topics meriting consideration as part of the key assumption identification process include the following:

- The availability and reliability of input data;
- The reliability of the calculated results and their adequacy for the intended applications;
- The extent to which users understand the physical and mathematical models underlying the methodologies;
- The adequacy of the models for providing the required information (e.g. activation products, total activity, specific activity, spatial details);
- The degree to which the results can be effectively assessed for reliability;
- The extent of the spatial region that will require assessment.

The evaluation and selection parameters provided in Table 1 can also be used as 'prompts' to help in identifying the key assumptions.

In line with strategic risk management practices, the degree of uncertainty surrounding each of the key assumptions can be estimated, and if so indicated, it may be appropriate to take actions to reduce the levels of uncertainty. For example, actions could be taken to improve the quality of input information.

Examples of assumptions important to assessing the activation source term are presented below, together with actions that can be taken to assess the level of uncertainty, and to address those uncertainties.

# 2.8.2. Availability and reliability of information

**Assumption:** The information shown on drawings of the structure (i.e. geometry, dimensions, etc.) and for the components being considered in the activation calculations is assumed to be valid and reliable, including details such as penetrations and beam ports. It is further assumed that the structures shown on drawings (sectional views) adequately describe the entire spatial structure.

**Considerations and discussion:** If the reliability of the spatial and dimensional information is questionable owing, for example, to the discovery of contradictory information in drawings, or the inability to obtain drawings that show the actual as-built configurations, a sensitivity or scenario analysis can be performed to determine the effects of the variability found in the inputs on the results of the activation calculations. Under this approach, various scenarios would be examined using sets of input values that bracket the uncertain inputs.

The ability to perform adequate modelling could be compromised if parts of the structure under study are not shown on the drawings, or if some components or structural areas regarded as significant in terms of activation are missing from the documentation (e.g. penetrations, experimental tubes, beam guides, ducts, cavities). As in the case discussed above, a series of scenarios covering a range of possible structural possibilities can be developed and used in the activation calculations. If a decision is taken to adopt a conservative approach in the assessment of the activation source term, it may be useful to determine how that approach affects the various applications being considered for use with the activation calculations. For example, a conservative approach in terms of radiation protection could unrealistically overestimate parameters important for a waste disposal case.

**Assumption:** The information regarding the chemical compositions of the structures being exposed to particle fluxes is assumed to be valid.

**Considerations and discussion:** In most cases, the information available on the chemical composition of metals, concretes and other material comes from manufacturer specifications. If the information source provides tolerance ranges, a conservative approach would involve performing a sensitivity analysis whereby the activation calculations are carried out using chemical concentrations at both extremes of the range. If specific information is not available on chemical composition, then it may be possible to use generally accepted values (e.g. that the concentration of cobalt in stainless steel alloys is 0.2%). A second option in dealing with the lack of chemical composition data is to actually analyse materials from, for example, non-irradiated archived samples, spare components or similar components. In those cases where chemical analysis is being planned, it is important to ensure that the analysis methods are capable of detecting certain trace elements which can be particularly important in terms of neutron activation products.

An example that demonstrates the influence of the material composition on the results of activation calculations is given in Fig. 5. A model of a graphite moderated reactor was analysed using three different types of graphite. The induced activity in graphite can differ by several orders of magnitude depending on the material composition used in the activation calculations.

# 2.8.3. Radionuclides considered in the analysis and their origin

**Assumption:** In the case of a reactor vessel, it is generally assumed that the radionuclides listed in Table 2 are the ones that are most appropriate for consideration when performing activation calculations for thermal reactor facilities (i.e. those radionuclides that are typically present in appreciable quantities in a reactor vessel following irradiation).

**Considerations and discussion:** Decisions can be made to either exclude some of the nuclear reactions and radionuclides given in Table 2, or alternatively, to include other radionuclides not specifically listed. However, careful consideration is needed before a decision is made to exclude certain nuclear



FIG. 5. Induced activity in a nuclear reactor moderator as calculated for graphite of three different compositions from three different reactors [11].

reactions (and therefore certain radionuclides). A more conservative approach is to perform the activation calculations for all reactions and then decide which radionuclides will be irrelevant for the intended applications. This approach may be particularly advisable if there is uncertainty about how the calculated activity results will be used.

In the case of nuclear reactors, the activation products are generated by neutrons produced in the nuclear fission reactions occurring within the reactor core. The interactions (nuclear reactions) of the neutrons with the different materials surrounding the core produce radionuclides at levels that depend on neutron energy, material composition and flux levels.

Material	Radionuclide	T <sub>1/2</sub>	Material	Radionuclide	T <sub>1/2</sub>
Stainless	<sup>14</sup> C	5 730 y	Carbon	<sup>51</sup> Cr	27.7 d
steel	<sup>51</sup> Cr	27.7 d	steel	<sup>54</sup> Mn	312.2 d
	<sup>54</sup> Mn	312.2 d		<sup>55</sup> Fe	2.73 y
	<sup>55</sup> Fe	2.73 y		<sup>59</sup> Fe	45.1 d
	<sup>59</sup> Fe	45.1 d		<sup>58</sup> Co	70.88 d
	<sup>58</sup> Co	70.88 d		<sup>60</sup> Co	5.271 y
	<sup>60</sup> Co	5.271 y		<sup>59</sup> Ni	76 000 y
	<sup>59</sup> Ni	76 000 y		<sup>63</sup> Ni	100 y
	<sup>63</sup> Ni	100 y		<sup>93</sup> Mo	3 500 y
	$^{108M}$ Ag	418 v		<sup>94</sup> Nb	24 000 v
	6			<sup>99</sup> Tc	213 000 y
Concrete	<sup>3</sup> H	12.33 v	Graphite	<sup>3</sup> H	12.33 v
	<sup>152</sup> Eu	13.5 v	1	$^{14}C$	5 730 v
	<sup>154</sup> Eu	8.59 v		<sup>36</sup> Cl	301 000 v
	<sup>55</sup> Fe	2.73 v		<sup>46</sup> Sc	83.81 d
	<sup>59</sup> Fe	45.1 d		<sup>54</sup> Mn	312.2 d
	<sup>54</sup> Mn	312.2 d		<sup>59</sup> Fe	45.1 d
	<sup>60</sup> Co	5.271 v		<sup>60</sup> Co	5.271 v
	<sup>41</sup> Ca	102 000 v		<sup>124</sup> Sb	60.2 d
	<sup>45</sup> Ca	162.7 d		<sup>131</sup> Ba	11.8 d
	<sup>134</sup> Cs	2.064 8 y	7	<sup>133</sup> Ba	10.51 y
	<sup>182</sup> Ta	114.4 d		<sup>152</sup> Eu	13.5 v
	<sup>65</sup> Zn	243.8 d		<sup>154</sup> Eu	8.59 y
	<sup>95</sup> Zr	64.02 d			

TABLE 2. TYPICAL RADIONUCLIDES PRODUCED DURING THE NEUTRON INDUCED ACTIVATION PROCESS FOR REACTOR FACILITIES [9]

The inventory and the specific activities of the radionuclides found in the irradiated material of accelerators differ considerably from those found in nuclear reactors because the activation mechanisms and activating particles are generally different. Several nuclear processes contribute to the activation process in high energy accelerators, with the most important being direct hadron interaction (spallation), neutron induced nuclear processes and photonuclear reactions.

Protons and other ions with energies exceeding a given reaction threshold will produce radionuclides upon interacting with matter. In some special cases, radionuclides can be produced by incident particles at much lower energies as a result of exothermic nuclear reactions that either produce radionuclides directly or emit neutrons capable of inducing radioactivity through their secondary interactions. For high energy proton and ion accelerators, the accuracy of activation calculations may be compromised if processes such as spallation are neglected. The number of radionuclides that can be produced increases as the beam energy is increased because more reaction thresholds are exceeded. As a general rule, at high energies (1 GeV or greater), all radionuclides in the periodic table with mass numbers less than that of the material exposed to the particle beam may be produced. However, many of these radionuclides are of little significance owing to short half-lives and small production cross-sections.

The level of residual activity in the components of electron accelerators is typically lower compared with the level found in the components of hadron accelerators. The majority of the radionuclides are produced by photonuclear (gamma, n) reactions, or in the case of high energy electron accelerators, via (gamma,  $p_xn_x$ ) reactions. Secondary particles, such as protons and neutrons, can also contribute to activation.

Medium and long lived activation products typically found in the materials that generally make up the components of accelerators are listed in Table 3.

Tables 2 and 3 are based on the assumption that decommissioning will not begin immediately after the shutdown of a facility. For Table 2, radionuclides with a half-life of less than 20 days have been omitted. For Table 3, radionuclides with a half-life of less than 1 day have been omitted. The difference in half-life criteria reflects the length of time that might reasonably be required to prepare a facility (e.g. reactor or accelerator) for decommissioning. As a general rule, it is assumed that after 10 half-lives a radionuclide will have decayed to negligible levels. Therefore, based on the decision to exclude radionuclides with a half-life of 20 days, a reactor might typically be expected to require at least 200 days to be prepared for decommissioning activities. Using the same line of reasoning, an accelerator could be expected to require 10 days. Both of these values are viewed as reasonable. If longer or shorter decay periods are anticipated, the list could be modified. The medium and long term hazards of waste are largely defined by the longer lived radionuclides (i.e. with half-lives longer than a year).
Material Radionuclide		T <sub>1/2</sub>	Material	Radionuclide	T <sub>1/2</sub>			
Stainless	<sup>46</sup> Sc	83.81 d	Carbon steel	<sup>44m</sup> Sc	2.44 d			
steel	$^{48}V$	15.97 d		<sup>46</sup> Sc	83.81 d			
	<sup>51</sup> Cr	27.7 d		<sup>47</sup> Sc	3.35 d			
	<sup>52</sup> Mn	5.6 d		<sup>48</sup> Sc	1.82 d			
	<sup>54</sup> Mn	312.2 d		$^{48}V$	15.97 d			
	<sup>55</sup> Fe	2.73 y		<sup>51</sup> Cr	27.7 d			
	<sup>59</sup> Fe	45.1 d		<sup>52</sup> Mn	5.6 d			
	<sup>56</sup> Co	77.3 d		<sup>54</sup> Mn	312.2 d			
	<sup>57</sup> Co	271.8 d		<sup>55</sup> Fe	2.73 y			
	<sup>58</sup> Co	70.88 d		<sup>59</sup> Fe	45.1 d			
	<sup>60</sup> Co	5.271 y		<sup>56</sup> Co	77.3 d			
	<sup>95</sup> Nb	34.9 d		<sup>57</sup> Co	271.8 d			
	<sup>14</sup> C	5 730 y		<sup>60</sup> Co	5.271 y			
	<sup>55</sup> Fe	2.73 y		<sup>58</sup> Co	70.88 d			
	<sup>59</sup> Ni	76 000 y		<sup>59</sup> Ni	76 000 y			
	<sup>63</sup> Ni	100 y		<sup>63</sup> Ni	100 y			
	<sup>108m</sup> Ag	418 y		<sup>93</sup> Mo	3 500 y			
	U	5		<sup>94</sup> Nb	24 000 y			
				<sup>99</sup> Tc	213 000 y			
Aluminium	<sup>7</sup> Be	53.22 d	Tungsten	<sup>182</sup> Ta	114.4 d			
	<sup>22</sup> Na	2.6 y	U	<sup>183</sup> Ta	5.1 d			
	<sup>54</sup> Mn	312.2 d		$^{181}W$	121.2 d			
				<sup>185</sup> W	75.1 d			
Concrete	<sup>3</sup> H	12.33 y	Graphite	<sup>3</sup> H	12.33 y			
	<sup>22</sup> Na	2.6 y		<sup>14</sup> C	5 730 y			
	<sup>41</sup> Ca	102 000 y		<sup>36</sup> Cl	301 000 y			
	<sup>45</sup> Ca	162.7 d		<sup>46</sup> Sc	83.81 d			
	<sup>54</sup> Mn	312.2 d		<sup>54</sup> Mn	312.2 d			
	<sup>55</sup> Fe	2.73 y		<sup>59</sup> Fe	45.1 d			
	<sup>59</sup> Fe	45.1 d		<sup>60</sup> Co	5.271 y			
	<sup>60</sup> Co	5.271 y		<sup>124</sup> Sb	60.2 d			
	<sup>65</sup> Zn	243.8 d		<sup>131</sup> Ba	11.8 d			
	<sup>95</sup> Zr	64.02 d		<sup>133</sup> Ba	10.51 y			
	<sup>134</sup> Cs	2.064 8	y	<sup>152</sup> Eu	13.5 y			
	<sup>152</sup> Eu	13.5 y		<sup>154</sup> Eu	8.59 y			
	<sup>154</sup> Eu	8.59 y						
	<sup>182</sup> Ta	114.4 d						
			Plastics	<sup>3</sup> H	12.33 y			
			and oils	<sup>7</sup> Be	53.22 d			

# TABLE 3. TYPICAL RADIONUCLIDES PRODUCED IN VARIOUSTYPES OF MATERIALS IRRADIATED IN ACCELERATORS [9, 12]

TABLE 3. TYPICAL RADIONUCLIDES PRODUCED IN VARIOUS TYPES OF MATERIALS IRRADIATED IN ACCELERATORS [9, 12] (cont.)

Material	Radionuclide	T <sub>1/2</sub>	Material	Radionuclide	T <sub>1/2</sub>		
Lead	<sup>105</sup> Ag <sup>122</sup> Sb <sup>124</sup> Sb <sup>203</sup> Hg <sup>202</sup> Tl <sup>202</sup> Pb <sup>204</sup> Tl	41.3 d 2.7 d 60.2 d 46.6 d 12.2 d 53 000 y 3.78 y	Copper	<sup>51</sup> Cr <sup>52</sup> Mn <sup>54</sup> Mn <sup>56</sup> Co <sup>57</sup> Co <sup>58</sup> Co <sup>60</sup> Co <sup>63</sup> Ni <sup>65</sup> Zn	27.7 d 5.6 d 312.2 d 77.3 d 271.8 d 70.88 d 5.271 y 100 y 243.8 d		

For the special case of medical accelerators operating at energies above 10 MeV, while the use of electron linear accelerators may result in neutron activation in the walls of the treatment room and in the radiation head of the linear accelerator, such activation is rarely found to be a problem at the time of decommissioning. Concerns about activation products are more relevant to radiation protection considerations during any maintenance of the linear accelerator head that is carried out shortly after patient treatment. However, regardless of the circumstances, the possibility of neutron induced activity always needs to be considered when planning for decommissioning [13].

For electron accelerators with energies below 35 MeV, it is normally only reactions of the  $(\gamma,n)$ ,  $(\gamma,p)$ ,  $(\gamma,np)$  and  $(\gamma,2n)$  type that are considered relevant. For more complicated types of photonuclear reactions that are characterized by higher reaction thresholds, cross-sections are too small for there to be a meaningful contribution to induced activation. Data showing the saturation activity in various target materials as a function of electron energy are given in table XIX of Ref. [6].

#### 2.8.4. Spatial extent of the model used for activation calculations

Assumption: Assumptions are required concerning the spatial extent of the models being used in the activation calculations. In a reactor environment, it is assumed that the neutron flux diminishes as a direct function of distance from the source of neutrons, and that this assumption applies to all spatial directions (horizontally and vertically, or in the case of systems with cylindrical symmetry, in all radial and axial directions). Beyond a certain distance, it is assumed that the neutron flux values drop to such low values that activation is no longer a

primary concern. In the case of nuclear power plants, it is assumed that the external boundaries of the biological shield represent appropriate boundaries for the spatial extent of the activation calculations.

**Considerations and discussion:** Cases may exist where there is significant activation outside the biological shield as a result of the streaming of particles through penetrations in the biological shield. Such penetrations could be the result of modifications for experimental equipment, beam guides or irradiation channels, and this possibility needs to be explicitly considered and analysed as part of the decommissioning planning process.

When modelling small facilities, such as research and training reactors, or accelerators, the particle source (i.e. reactor core or accelerator target) may be surrounded by very complex structures such as those associated with experimental facilities, equipment or irradiation sites. Under these circumstances, the application of  $S_n$  methodologies and three dimensional modelling will in itself require careful model development and careful analyses of the results to help ensure the required quality in the results.

## 2.8.5. Objectives and requirements for activation calculations

In the context of this report, the results of the activation calculations need to be considered in terms of parameters such as:

- Statistical variability;
- Quality;
- Probability distribution type (e.g. normal, log normal).
- Accuracy;
- Spatial resolution;
- Parameter sensitivity;
- Energy resolution;
- Scope of radionuclides provided by the activity calculations.

Before undertaking activation calculations, it is important that any requirements in terms of the parameters identified above be specified, particularly with regard to the end use of the calculations. Results with, for example, too much variability, insufficient spatial resolution, or an incomplete suite of radionuclides may be of limited use for the intended applications. Any requirements in terms of data quality can be included in documentation discussing the calculations and their results.

## 2.8.6. Quality, limitations and uncertainties in results

From the perspective of this report, the 'quality' of results refers primarily to the statistical parameters discussed in Section 2.3. Quality may also include such parameters as spatial resolution as it relates to the level of detail required for use with the components being studied. If the objective of the calculations is a rough estimate of the total radionuclide inventory of activated components, the method for activation calculations can rely on a simplified approach, and have less demanding requirements in terms of the quality of the input data. If more demanding requirements exist for specific activity values for various parts of the components, more sophisticated calculations might be needed. To this end, all of the assumptions and quality requirements as they relate to the activation calculations need to be carefully documented, including any assumptions that have been made about the final use of those calculations. As is the case with any project, the preparation of a project plan for the assessment of an activation source term may provide an opportunity to formally address and document the various issues discussed above.

The uncertainties in the results obtained from activation calculations arise from two major sources: (i) uncertainties in the input data (i.e. spatial model, material composition, nuclear data, etc.) and (ii) uncertainties in the results of the particle transport calculations that have their origin in the statistical nature of the calculation methods.

The quality of the calculated results is primarily dependent on the quality of the data used as input to the calculations. Adequately detailed geometric models can only be constructed if the technical drawings of each component or subcomponent are available. If any part of the documentation is missing or not available, simplifying assumptions can be made, but this will likely lead to a more restricted model. A second major source of uncertainties in the quality of the calculated results can be attributed to unknowns about material composition. It is essential to have information about the material compositions that is as accurate and precise as possible if rigorous requirements have been established for the quality of the results. Conversely, less accuracy and precision may suffice if scoping calculations are being performed. The facility operating history (irradiation time, operating power, beam energy, etc.) will also include critical parameters that will affect the quality of the calculated values of residual activity. As discussed above, it is generally advisable to document any simplifying assumptions that have been made as part of the calculation process, as these assumptions may restrict the applicability of the results.

A sensitivity analysis is designed to provide information on how variability in input parameters affects the variability of output parameters. For those parameters that are considered uncertain, performing a sensitivity analysis can be important. A sensitivity analysis is particularly useful in those cases where: (i) imprecise data exist for the elemental composition of the components under study; and (ii) there is missing information concerning the spatial dimensions of the structure being modelled owing to the unavailability of, for example, technical drawings and documentation. Sensitivity analyses related to other parameters, such as the hydrogen content of the biological shield concrete structures or the densities of certain materials, may also be useful.

## 2.9. COMPUTER CODES

This section provides a general description of computer codes that can be used in determining particle induced activation source terms.

#### 2.9.1. Particle transport codes for use with nuclear reactor facilities

## 2.9.1.1. General

The neutron activation calculation process involves two major steps. The first is to use a neutron transport code to calculate the neutron flux in various areas and components of the structure being assessed. The second step uses an activity calculation code which takes the energy dependent neutron flux values from the transport calculations together with the material composition data to determine the nature and levels of neutron activation products in the structure under study.

For the neutron transport calculations, a model of the neutron source, the surrounding metal structures and the biological shield has to be developed. In the case of a nuclear power plant or research reactor, the neutron source is the reactor core. After selecting the applicable structural cross-sections of the reactor from drawings and manuals, a neutron transport calculation can be performed. The result of this calculation is a description or model of the space and energy dependent neutron flux. Depending on the type of model, code or approach used, the neutron flux can be determined with varying degrees of resolution (i.e. coarse to fine) in terms of both spatial and energy distributions.

Basically, there are two types of neutron transport codes to be considered; one is based on a Monte Carlo (probabilistic) methodology, and the other is based on  $S_n$  (deterministic) methods. Those codes utilizing the neutron diffusion method have limited applicability for the assessment of the induced activity source term for decommissioning purposes, and so they are not discussed in this report.

## 2.9.1.2. Monte Carlo codes

The activation of different components can be calculated by using a general purpose Monte Carlo transport code. Monte Carlo codes allow the detailed modelling of the geometrical and material parameters, and the simulation of neutron physics transport processes. An example of a Monte Carlo model set-up can be seen in Fig. 6.

By applying Monte Carlo codes, detailed descriptions of complex geometries (e.g. spatially complicated arrangements, repeated structures, embedded lattices) are possible, and modelling of the exact material composition of the different structures and components can be performed. Another important feature of such codes is the use of continuous energy cross-section libraries, which allows the program to calculate exact energy values instead of quantizing energy changes. The ability to simulate the particle transport processes by (i) using highly detailed cross-section libraries and (ii) applying continuous energy models allows a very realistic calculation of the energy and spatial distributions of the particles.



FIG. 6. Vertical section of a Monte Carlo model of a reactor assembly and concrete biological shield [10].

By utilizing the Monte Carlo method, codes can simulate the transport of different types of particles (e.g. neutrons). Various characteristics of the modelled system (such as neutron flux, reaction rates) are determined statistically by following the parameters of these particles during their transport processes through the defined spatial areas. The variance of the results depends on the variance reduction techniques applied and the number of particles simulated. Monte Carlo codes may have several options for variance reduction.

In the input file for the Monte Carlo code, the geometrical structure, the material compositions of the different components, the distribution of the source and the operating parameters for the facility need to be specified. The geometry of the components can be modelled by dividing the components into smaller sections or cells, which are then described with defined materials having known initial nuclide compositions and density. Complex structures can be simulated using, for example, the union or intersections of the regions defined by the cells. Although the application of such a comprehensive method enables the construction of detailed and complex geometries, it understandably requires highly elaborate, precise and sometimes time consuming modelling. More detailed descriptions of the features of Monte Carlo codes can be found in the code manuals.

Monte Carlo codes may be used for the determination of both the energy and space dependent neutron flux values as well as the reaction rate values for activation reactions in every material region of interest.

Users of Monte Carlo codes can select from different nuclear data libraries containing evaluated cross-section tables. The cross-section sets represent the physics of the particle interactions; therefore, applying the appropriate data library is important to the validity of the calculations. For general purposes, code developers normally include numerous cross-section libraries in the program package. The reason for the existence of multiple cross-section libraries for reactions of a given nuclide lies in the fact that the libraries are generated by different evaluators from experimentally determined data combined with calculated results. The user can make special purpose cross-section libraries using the processing code NJOY [14] and Evaluated Nuclear Data File (ENDF) formats.

Examples of Monte Carlo codes widely used for neutron transport modelling are listed and described below:

— MCNP (version 5-1.60) [15] is "a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron or coupled neutron/ photon/electron transport" [16], including the capability to calculate eigenvalues for critical systems. The MCNP code treats an arbitrary three dimensional configuration of materials in geometric cells bounded by first and second degree surfaces and fourth degree elliptical tori. Pointwise cross-section data are used. For neutrons, all reactions given in a particular cross-section evaluation (such as ENDF/B) are accounted for. Thermal neutrons are described by both the free gas and  $S(\alpha,\beta)$  models. For photons, the code accounts for incoherent and coherent scattering, the possibility of fluorescent emission after photoelectric absorption, and absorption in electron-positron pair production. Electron/positron transport processes account for angular deflection through multiple Coulomb scattering, collisional energy loss with optional straggling, and the production of secondary particles including Ka X rays, knock-on and Auger electrons, bremsstrahlung and annihilation gamma rays from positron annihilation at rest. Electron transport does not include the effects of external or self-induced electromagnetic fields. Photonuclear physics is available for a limited number of nuclides. Important standard features that make MCNP very versatile and easy to use include a powerful general source, criticality source and surface source, both geometry and output tally plotters, a rich collection of variance reduction techniques, a flexible tally structure, and an extensive collection of cross-section data.

- MCNPX (MCNP eXtended) [17, 18] is a general purpose Monte Carlo radiation transport computer code that simulates transport of many types of particles over a broad range of energies. MCNPX is a production computer code that models the interaction of radiation with matter. The depletion/ burnup capability is based on CINDER'90 and MonteBurns. MCNPX depletion is a linked process involving steady state flux calculations in MCNPX and nuclide depletion calculations in CINDER'90. Currently, the depletion/burnup/transmutation capability is limited to criticality problems. Physics improvements include new versions of Cascade-Exciton Model (CEM) and Los Alamos Quark-Gluon String Model event generator, and a substantial upgrade to fission multiplicities. Current physics modules include the Bertini and ISABEL models taken from the LAHET Code System, CEM 03, and INCL4. Many new tally, source and variance reduction options have been developed. MCNPX is released with libraries for neutrons, photons, electrons, protons and photonuclear interactions. In addition, variance reduction schemes (e.g. secondary particle biasing) and new tallies have been created specific to the intermediate and high energy physics ranges. The 'mesh' and 'radiography' tallies were included for two and three dimensional imaging purposes. Energy deposition received a substantial reworking based on the demands of charged particle high energy physics. The code may be run in parallel at all energies via Parallel Virtual Machine (PVM) or Message Passing Interface (MPI).
- MCNP6 [19] is a general purpose, continuous energy, generalized geometry, time dependent, Monte Carlo radiation transport code designed to track

many particle types over broad ranges of energies. MCNP6 represents the culmination of a multi-year effort to merge the MCNP5 and MCNPX codes into a single product comprising all features of both. Expanded or new tally, source and variance reduction options are available to the user as well as an improved plotting capability. The capability to calculate  $k_{\rm eff}$  eigenvalues for fissile systems remains a standard feature.

- MCBEND [20] is a general purpose radiation transport code that can calculate neutron, gamma ray and charged particle transport in subcritical systems; coupling of the different radiation types is also possible. MCBEND models the transport of individual particles accurately by using a very fine energy group representation of nuclear data and a flexible geometry modelling package. MCBEND has versatile source description options and automatic acceleration options for maximum productivity. Nuclear data libraries exist for MCBEND from a variety of sources, including the United Kingdom Nuclear Data Library (UKNDL), the Joint Evaluated Fission and Fusion Library (JEFF), ENDF/B and the Japanese Evaluated Neutron Data Library (JENDL). MCBEND is validated for an extensive range of applications. The validation database covers many of the materials and geometries that are encountered in the nuclear industry and is subject to ongoing review and enhancement.
- TRIPOLI-4 [21] solves the linear Boltzmann equation for neutrons and photons, with the Monte Carlo method, in any three dimensional geometry. The code uses ENDF format continuous energy cross-sections from various international evaluations, including JEFF, ENDF/B, JENDL and the Fusion Evaluated Neutron Data Library (FENDL). Its official nuclear data library for applications, named CEAV, is mainly based on the European evaluation JEFF. TRIPOLI-4 solves fixed source as well as eigenvalue problems. It has advanced variance reduction methods to address deep penetration issues. Calculations are performed on multicore single units, heterogeneous networks of workstations, and massively parallel machines. Additional productivity tools, graphical as well as algorithmic, allow the user to efficiently set its input decks.

#### 2.9.1.2.1. Limitations and capabilities

Monte Carlo codes are capable of modelling nuclear reactors, including their core, steel components and biological shields, with a high degree of reliability. If the calculations are performed by applying appropriate variance reduction schemes, thus reducing the statistical uncertainties to negligible values, the determining factor in the quality of the calculation will be modelling error and uncertainties related to input and nuclear data. Calculations for large components such as single massive pieces may lead to results which characterize the neutron flux as a single averaged value over the total volume of the component. In the subsequent activity calculations, this will result in specific activities which are the same for the entire component. However, components generally have regions and parts which are in the immediate vicinity of the source (i.e. within tens of centimetres) as well as other parts or regions that are remote from the source (i.e. at distances of up to many metres). Under these circumstances, the single specific activity value obtained for the component will not show a difference in specific activity between regions located very close to or remote from the source. Therefore, even though modelling can be carried out with large contiguous volumes describing entire components, for the source term activity calculations it is advisable to divide the geometry into smaller sections or cells that more realistically simulate different regions of interest. Figure 7 provides an example of how the geometry of a very large component can be segmented into smaller spatial regions.

Another method to achieve optimum results for calculations for large components is to use the mesh tally capability available in some Monte Carlo codes. This technique allows the calculation of a spatial distribution for the neutron flux over the geometric model. In Monte Carlo calculations, the user has two options for dividing the geometry into segments: (i) creating a number of smaller cells; or (ii) leaving the cells intact but creating a superimposed spatial mesh, which can have either Cartesian (*x*-*y*-*z*) coordinates or cylindrical (*r*- $\theta$ -*z*) coordinates. The physical quantities, such as neutron flux, can be calculated as volume averaged values both for the cells and for the spatial mesh intervals.

In applications involving reactors with large cores (i.e. greater than 2 m in height or diameter), Monte Carlo calculations can give biased results for neutron flux values in the vicinity of the boundaries. This concern and its resolution have been described in the relevant literature [22].

## 2.9.1.2.2. Code assumptions

The use of the Monte Carlo codes assumes: (i) model regions adequately reflect the physical dimensions, densities and power density parameters corresponding to the actual reactor regions; (ii) flux levels do not change at region boundaries; (iii) flux levels change within regions; and (iv) microscopic cross-section libraries correspond to the physical state of the system being analysed.



FIG. 7. Spatial regions (segments) defined for use in the induced activation calculations for a reactor pressure vessel (RPV) [10].

## 2.9.1.2.3. Model applicability

Monte Carlo codes can be applied to a very large range of facility types. Monte Carlo codes are generally very flexible in their applicability in terms of geometry, material composition and source types.

In the case of research reactors, material testing reactors and critical assemblies, the development of a Monte Carlo model might, at first, seem relatively straightforward based on considerations of reactor size and power alone. However, these types of facility are often highly complex, and therefore, developing the spatial description of the beam tubes, ports, irradiation equipment, and so on may require a substantial amount of work. However, notwithstanding the work required, the Monte Carlo method may represent the only viable option for assessing an activation source term given that it can address fine details and irregularities in the small reactor structures.

Supporting tools exist to assist users in setting up models for the Monte Carlo codes. Some of these help in visualizing (in two or three dimensions) the model geometry, while others may be used to convert computer aided design (CAD) models to Monte Carlo code inputs.

# 2.9.1.2.4. Hardware and software requirements

Generally, the hardware and software requirements for the particle transport codes described above can be found in the code manuals.

# 2.9.1.2.5. Uncertainty and sensitivity

If all of the required data are available, the operating history and the fuel management strategies can be used in modelling the particle source for the activation calculations. Relevant data about the operational history of a facility include the daily or monthly average power distribution as well as information about the fuel assemblies, including type, enrichment and burnable poisons. Of equal importance is information about the fuel load patterns used with each fuel cycle. In those cases where nuclear reactor facilities have used multiple core configurations during their operating history (e.g. research reactors), reasonably conservative assumptions can be applied in order to develop configurations that are representative of those used during the lifetime of the facility in terms of time and operating power.

## 2.9.1.2.6. Code availability

The codes described in Section 2.9.1.2 are normally available from the developers or from the Radiation Safety Information Computational Center (RSICC) (http://rsicc.ornl.gov) or the Data Bank at the Nuclear Energy Agency of the Organisation for Economic Co-operation and Development (OECD/NEA) (www.oecd-nea.org/databank).

# 2.9.1.2.7. Results

Monte Carlo codes can be used to calculate the energy dependent neutron flux in a predefined spatial structure. The output of the code will comprise neutron flux values for each energy group as averaged over a specified cell volume for the entire spatial region defined in the code. These flux values are subsequently used as input for the activity calculation program. The number of energy or flux groups provided by the neutron transport modelling code will generally be dictated by the input requirements of the activity calculation code. Some examples for the spatial distribution of the neutron flux obtained for different nuclear installations can be found in Ref. [23].

Most Monte Carlo codes can also be used to calculate reaction rates for all of the nuclear reactions of interest. If this option is employed, the result of the calculations will be a list of reaction rates for all the spatial regions identified as being of interest.

# 2.9.1.3. Discrete ordinate $(S_n)$ neutron transport codes for nuclear reactor facilities

Another type of neutron transport code employs the deterministic  $S_n$  method. With the use of  $S_n$  codes, models can: (i) be less complicated to develop; (ii) be easier to troubleshoot; (iii) be quicker to run; and (iv) require less advanced computer hardware than do the three dimensional Monte Carlo models.  $S_n$  models generate energy grouped neutron flux levels at locations of interest in fixed energy groups. Good correlation has been observed between the results from  $S_n$  models and those from three dimensional Monte Carlo models.

Examples of  $S_n$  neutron transport codes that are widely used for neutron transport modelling are listed and described below:

- DOORS3.2a [24] includes the most recent versions of ANISN, TORT, DORT, as well as other codes, and various utility programs. ANISN solves one dimensional neutron/photon transport, while DORT and TORT solve two and three dimensional neutron/photon transport problems, respectively. ANISN solves the one dimensional Boltzmann transport equation in deep penetration problems for neutrons or gamma rays in slab, sphere or cylinder geometries in which energy dependent angular flux values are calculated in detail using the S<sub>n</sub> method. The neutron source may be fixed, fission or a combination of the two. Cross-sections may be weighted using the space and energy dependent flux generated in solving the neutron transport equation. ANISN also includes a technique for handling general anisotropic scattering and pointwise convergence criteria.
- DORT is used in one or two dimensional geometric systems. The principal application is for the deep penetration transport of neutrons and photons. Reactor eigenvalue problems can also be solved.
- TORT is used in two or three dimensional geometric systems, and calculates the flux or fluence of particles from either external or internal sources.

The problem dependent cross-sections needed for calculations with TORT, DORT or ANISN may be developed using codes available in SCALE [25].

ATTILA [26] is a software suite developed to provide fast and accurate solutions to demanding radiation transport applications. ATTILA leverages an advanced Boltzmann equation solver with an intuitive graphical user interface (GUI) with CAD integration, enabling users to rapidly and reliably perform complex calculations. ATTILA is well suited for applications dominated by large attenuations, such as those associated with radiation shielding. The ATTILA solver combines deterministic solution methods on a computational domain of unstructured tetrahedral elements enabling ATTILA to accurately and efficiently calculate solutions through many orders of magnitude of attenuation. ATTILA calculates the solution everywhere, not just at predefined tally locations. ATTILA also provides tight integration with the MCNP6 Monte Carlo code. ATTILA can produce a CAD based computational model directly usable by the new MCNP6 Embedded Unstructured Mesh Hybrid Geometry feature. Additionally, ATTILA supports the GUI setup of complete MCNP6 calculations and efficient adjoint solutions for highly optimized weight windows variance reduction. Furthermore, GUI driven activation and depletion calculations are fully integrated with ATTILA.

#### 2.9.1.3.1. Limitations and capabilities

If consideration is being given to the use of a graded approach to the assessment of the activation source term, the user needs to define the objectives of the calculations. If the objective is to assess the magnitude and spatial distribution of the activity of the components and structures responsible for the majority of the total activity, simplified models can be used. One, two and three dimensional  $S_n$  neutron transport calculations are capable of calculating neutron flux values in reactor facilities that range from the core to the biological shield.

One or two dimensional  $S_n$  calculations can give adequate neutron flux values in specified directions, with added advantages: (i) the calculations only require very short running times; and (ii) it is relatively easy to set up the model. In certain regions located at larger distances from the particle source (i.e. near boundaries, in penetrations and ducts, or at transition zones between different material regions), three dimensional calculations yield significantly better results, but longer times may be required to perform the calculations. Certain effects, such as the streaming of neutrons in the cavity between the pressure vessel and biological shield of a nuclear power plant, can be best accommodated using the three dimensional calculations.

For  $S_n$  codes, the geometry of the system under study needs to be adapted to either a Cartesian (*x-y-z*) or a cylindrical (*r-\theta-z*) coordinate system. Normally, a set of spatial mesh boundaries is applied. Within each mesh, the program assumes homogeneous cross-sections (i.e. a homogeneous mixture of material).

For each region or cell, homogenized group neutron cross-sections are required. At this point, there are two options: either the user applies a pre-collapsed and self-shielded cross-section library [22], or the cross-sections applied for the actual neutron flux calculation are created in a sequence of calculations.

One limitation associated with the  $S_n$  methodology arises from inherent simplifications in most of the  $S_n$  codes whereby material regions need to be defined in terms of either planes or cylindrical surfaces, and therefore it may be difficult to describe the actual shapes of the system structure and components. In addition, if the nuclide composition of the structures change suddenly as a function of spatial coordinates, this will also make modelling more difficult based on the  $S_n$  code limitations discussed above.

The choice of the number of spatial cells and energy groups is important. With a large number of groups and appropriate cell intervals, a more detailed description of the flux and activation conditions in the structure can be expected from the calculations. However, convergence problems may arise depending on the iteration scheme and the convergence acceleration methods used.

For nuclear power plants, the neutron flux levels outside of the biological shield are, by design, so low as to make hazards from activation products minimal.

For nuclear power plant applications, a precise calculation of the neutron flux distribution requires knowledge of the different fuel management strategies that were employed throughout the operational history of the facility, including: (i) the fuel types used (with all of the important parameters such as dimensions and enrichment); (ii) the use of low leakage cores; and (iii) the different core load patterns used with the various types of fuel. Developing models for all of these configurations can be very time consuming and may lead to extremely complex models.

## 2.9.1.3.2. Code assumptions

The assumptions that apply to the  $S_n$  codes are the same as those that apply to the Monte Carlo codes. In addition, the assumption is made that region specific macroscopic cross-sections are a function of the physical, power and microscopic cross-sections.

#### 2.9.1.3.3. Model applicability

S<sub>n</sub> transport models are applicable to reactor facilities.

## 2.9.1.3.4. Hardware and software requirements

Generally, the hardware and software requirements for the particle transport codes described above can be found in the code manuals.

## 2.9.1.3.5. Code availability

The codes described in Section 2.9.1.3. are normally available from the developers or from the RSICC (http://rsicc.ornl.gov) or the OECD/NEA Data Bank (www.oecd-nea.org/databank).

## 2.9.1.3.6 Results

Annex 1 provides an excerpt of an ANISN output showing neutron data from 68 groups in one region.

# 2.9.2. Particle transport codes for use with accelerator facilities

## 2.9.2.1. General

The use of general purpose particle interaction and transport Monte Carlo codes is one of the most effective ways of assessing the source term in accelerator facilities. In the case of accelerators, the main sources of secondary particles are normally either targets (patients in the case of medical applications) or areas where beams collide, as would be the case with colliders. In addition, lower intensity sources of secondary particles are found around beam loss areas.

The direct Monte Carlo calculation methodology is particularly appropriate for large and complex items such as accelerators. Prior to the application of a Monte Carlo code, it can be useful to examine the various factors that will be involved in undertaking a simulation (e.g. geometry or spatial input, material compositions, computational time, data analysis) and to determine if there is an optimal mix of these factors.

The activation calculations are performed in two steps as illustrated in Fig. 8. The particle transport calculation is done using Monte Carlo codes, and deterministic activation codes are then used for the calculation of induced activity. This methodology takes into account the unique aspects of accelerator facilities, and incorporates the capability to address:

- Activation by particles other than neutrons;
- Particle energies higher than 25 MeV.

The results of the Monte Carlo step provide: (i) the particle flux in the accelerator components for neutrons and photons with energies below 25 MeV; and (ii) the yields of radionuclides produced by neutrons and photons above 25 MeV, as well as by all other particles at all energies. This information is subsequently used as input for the activation calculation module.

## 2.9.2.2. Monte Carlo models and codes

For Monte Carlo models and codes, the user can select from two options to simulate particle interactions with materials. The first option uses evaluated cross-section libraries, and the second option is based on calculated cross-sections using nuclear reaction models. The basis for the selection of the option generally involves considerations concerning operational history, the material composition of the components exposed to the beam, and the energy of the beam. An analysis also needs to be performed in order to identify those nuclear reactions that will act as the major sources for activation products. Having selected the most prevalent nuclear reactions important to the activation processes, it is important to further analyse those reactions in terms of the capability of the code to simulate them. In view of the diversity of the nuclear reactions that may be involved, validation of the results against experimental data is warranted.

An example of the importance of performing a validation test prior to the Monte Carlo calculations is demonstrated in Fig. 9, where the cross-section for deuteron induced <sup>65</sup>Zn production in a copper target is calculated by different models and compared to experimental values. Significant discrepancies can be



*FIG. 8. Activation calculations for accelerator facilities (ENDF, JEFF, FENDL, JENDL and EAF are nuclear data libraries).* 

identified, which in several cases could lead to an underestimation of the value of the <sup>65</sup>Zn production rate and consequently of the induced activity.

In some cases, none of the calculation capabilities available in Monte Carlo codes can properly simulate the nuclear reactions of interest. Under these circumstances, the cross-sections need to be calculated by an appropriate independent program, such as the TALYS code [28]. The resulting cross-section values can then be input into the Monte Carlo model and the transport calculations performed.

Several codes are available for modelling the interaction of radiation with matter. A thorough, general description of the Monte Carlo method as used for particle transport, including some aspects of biasing techniques and the applicability of the method, is given in Ref. [29]. For a comparison of some of the more widely used codes for particle transport, see Refs [30, 31]. Short descriptions of the most common Monte Carlo codes utilized for this purpose are provided in the following paragraphs:

— FLUKA [32, 33] is a general purpose particle interaction and transport code with a wide range of applications, including for proton and electron accelerator shielding as well as for assessing the quantities of radionuclides produced in high energy accelerators. The production of radionuclides is



FIG. 9. Example of a code validation study where the capabilities of various codes to simulate nuclear reactions is compared with experimental results [27].

based directly on the types of nuclear interaction. The calculation starts with the implementation of the system geometry and the simulation of the material activation for any incoming particle, target nucleus and energy. The cross-sections are calculated at run time by means of nuclear models, with the only exception being low energy neutrons (below 20 MeV), for which the calculations rely on nuclear data libraries.

The simulations for transport of neutrons with energies below 20 MeV are performed by a multigroup algorithm based on evaluated cross-section data (ENDF/B, JEFF, JENDL, etc.) binned to 260 energy groups, 31 of which are in the thermal energy region.

The module for hadronic interaction (PEANUT — PreEquilibrium Approach to Nuclear Thermalization) consists of a phenomenological description of high energy interactions (up to 20 TeV), generalized intranuclear cascade and pre-equilibrium emission models as well as models for evaporation, fragmentation, fission and de-excitation by gamma emission.

Many variance reduction techniques are available in FLUKA, including weight windows, region importance biasing, leading particle interaction and decay length biasing.

— GEANT4 [34, 35] is a free object oriented software package for simulating the passage of particles through matter. It was developed through worldwide collaboration at the European Organization for Nuclear Research (CERN) and other high energy physics research organizations.

To handle the interactions of particles with matter, the GEANT4 toolkit includes an abundant set of physics models, including electromagnetic, hadronic and optical processes, as well as a large set of long lived particles, materials and elements with energies ranging from 250 eV up to the TeV range.

The experienced user can construct stand alone applications or applications built upon another object oriented framework. The toolkit provides the abstract interface for eight user classes, of which three are mandatory (material/geometry setup, physics processes, and primary vertices/particles) and five are optional. This enables the user to customize GEANT4 to specific situations.

— MARS15 [36, 37] is a set of Monte Carlo programs for the simulation of hadronic and electromagnetic cascades, and muon, heavy ion and low energy neutron transport in accelerator, spacecraft, shielding and detector studies. It covers an energy range from a fraction of an electron volt up to 100 TeV.

The system consists of a set of Monte Carlo programs for a detailed simulation of the hadronic and electromagnetic cascades in an arbitrary three dimensional geometry. Hadronic interaction can be simulated with either an inclusive or exclusive event generator. MARS15 has five geometry options, some of which can be coupled to FLUKA or MCNP geometry descriptions.

Different variance reduction techniques, such as inclusive particle production, weight windows, particle splitting and Russian roulette, are available in MARS15.

— The Particle and Heavy Ion Transport code System (PHITS) [38, 39] is among the first general multipurpose codes to simulate the transport and interaction of heavy ions in a wide range of energies (10 MeV up to 100 GeV per nucleon). Two simulation codes, Jet AA Microscopic Transport Model (JAM) [40] and JAERI Quantum Molecular Dynamics (JQMD) [41] (JAERI refers to the Japan Atomic Energy Research Institute) have been developed for intermediate and high energy nuclear reactions. JAM is a simulation code based on the INC (intra-nuclear cascade) model, which explicitly treats hadron–nucleus interactions through the production and decay of resonances, while at higher energies (up to 200 GeV), inelastic hadron–nucleus collisions are simulated by the formation of strings.

In PHITS, neutron transport is modelled using thermal energies up to 200 GeV. For the energy range from thermal neutrons to 20 MeV, neutrons are described in the same manner as in the MCNP code. For neutron energies above 20 MeV, the simulation model JAM is applied.

Electromagnetic interactions are based on the ITS code in the energy range between 1 keV and 1 GeV. Several variance reduction techniques, including weight windows and region importance biasing, are available in PHITS.

One of the advantages of PHITS is its ability to model the transport of nuclei in materials. Below 10 MeV per nucleon, only the ionization process for the nucleus transport is taken into account. Above that momentum, the JQMD code describes nucleus collisions up to 100 GeV per nucleon. PHITS is also able to simulate light and heavy ion trajectories in simple magnetic fields.

MCNP6 and MCNPX codes can also be applied for modelling accelerators. For the description of these codes, see Section 2.9.1.2. Other Monte Carlo methods for calculations related to material activation are described in the literature. A non-exhaustive list includes the following codes:

- PENELOPE 2011 [42, 43] is a code system for Monte Carlo simulations of electron and photon transport.
- ALEPH2 [44] is a Monte Carlo depletion code as applied to neutron and proton induced reactions.

— EGS4 [45] is a general purpose package for the Monte Carlo simulation of the coupled transport of electrons and photons in an arbitrary geometry for particles with energies from a few keV up to several TeV.

## 2.9.2.2.1. Limitations and capabilities

Among the main Monte Carlo codes, MCNPX, MCNP6 and FLUKA allow particle transport and residual activity calculations to be performed in a single run. All other codes (MCNP5, PHITS, MARS15, GEANT4) need to be coupled with activation programs to calculate induced activation in accelerator components.

Computer clusters are useful for decreasing the time required for Monte Carlo calculations. Some codes (MCNPX, PHITS, GEANT4) can be run in parallel, while FLUKA does not have this type of functionality.

Neutron cross-sections in the FLUKA low energy libraries are available for "about 200 materials or isotopes, temperature, and self-shielding combinations" [46]. All other particle interactions and transport are based on models and are not restricted by any material related parameters. The upper energy limit for hadron–hadron and hadron–nucleus interactions and transport is 10 PeV. For nucleus–nucleus interactions and transport, the upper energy limit is 10 PeV/n when the interface with the model DPMJET-2.5 or DPMJET-3<sup>1</sup> is activated, but it is 100 TeV otherwise. Electron, positron and photon interactions and transport can be modelled for energies between 1 keV and 10 PeV.

GEANT4 defines no default geometry or physics process. Even the particle transport process needs to be defined by the user in the form of GEANT4 specific C++ language; otherwise, GEANT4 will not model the transport of any particle. However, this feature does provide flexibility in that the user can readily switch the transport mechanism or physics process without influencing other processes or the behaviour of GEANT4. As an alternative to the provision of defaults, GEANT4 provides various examples.

In the collision process, PHITS can simulate the elastic and inelastic interactions as well as the decay of particles. The total reaction cross-section or the lifetime of the particle is an essential quantity in the determination of the mean free path of the transport particle. Based on the mean free path, PHITS chooses the next collision point using the Monte Carlo method. Special features of PHITS include the event generator mode [47] and the microdosimetric function [48].

<sup>&</sup>lt;sup>1</sup> DPMJET is a Monte Carlo model for sampling of hadron-hadron, hadron-nucleus, nucleus-nucleus and neutrino-nucleus interactions at accelerator and cosmic ray energies according to the two-component dual parton model.

The availability of an event generator mode enables PHITS to determine the profiles of all secondary particles generated from a single nuclear interaction taking both momentum and energy conservation into account. This capability is even possible using nuclear data libraries. PHITS cannot be used for microscopic track structure simulation because PHITS adopts the continuous slowing down approximation for the ionization process of a charged particle.

## 2.9.2.2.2. Model applicability

Monte Carlo codes provide a very flexible and versatile method for the assessment of the activation source term in accelerator facilities. Monte Carlo methods can be employed for simulating radiation fields and the activation products that would result from exposure to those simulated radiation fields. This capability is particularly useful in those cases where nuclear attenuation data cannot be used (e.g. neutron attenuation data cannot be used to estimate the attenuation of electromagnetic radiation). An example of the effectiveness and usefulness of the Monte Carlo codes is demonstrated by the ability of these codes to model the streaming of radiation through ducts, cavities and labyrinths. Issues surrounding the streaming of radiation through cavities can be particularly problematic in that it can both cause unexpected activation and constitute a radiation protection issue. However, such circumstances can be effectively simulated by Monte Carlo codes, with the ability to reliably simulate the geometrical and angular distribution of the radiation source, as well as its position with respect to the entrance of the maze.

Several benchmarking studies can be found in the literature comparing the capabilities of the different Monte Carlo codes presented in the previous paragraphs, see for example Refs [48, 49].

## 2.9.2.2.3. Hardware and software requirements

Generally, the hardware and software requirements for the particle transport codes described above can be found in the code manuals.

#### 2.9.2.2.4. Uncertainty and sensitivity

Most of the uncertainty in the calculated results for an accelerator source term arises from the diversity of the nuclear reactions involved in the production of radionuclides. This diversity of nuclear reactions has its origins in: (i) beam interactions with accelerator components; and (ii) interactions of secondary neutrons and photons. Cross-sections obtained from physics models may also be a source of uncertainties. A careful sensitivity analysis needs to be performed to assess the effects of variability in the nuclear reaction cross-section values available in the Monte Carlo codes. It can also be beneficial to expand the sensitivity analysis to include:

- Source term strength;
- Material composition;
- Structural dimensions;
- Structural features;
- Material densities;
- Trace element concentrations;
- Hydrogen content of the biological shield.

As noted in Section 2.3, the results of a sensitivity analysis may also provide important insight into the usefulness of an activation methodology to a particular application. For example, if the results for a particularly important parameter are found to be very sensitive to variability in input parameters, it may be necessary to consider the use of a different assessment methodology.

# 2.9.2.2.5. Code availability

The codes described in Section 2.9.2.2. are normally available from the developers or from RSICC (http://rsicc.ornl.gov) or the OECD/NEA Data Bank (www.oecd-nea.org/databank).

# 2.9.2.2.6. Results

There are several ways for evaluating the source term via FLUKA. If region based information is required, a scoring of the track length spectra can first be obtained and the results subsequently combined with the cross-sections and irradiation and decay pattern as a postprocessing step. This method can be automated by a specific code [43]. The advantage of this method is that the postprocessing is relatively easy; however, the correct spatial resolution needs to be defined from the beginning of the process because the results are based on the regions established at the beginning of the FLUKA simulation. A second method for evaluating the source term via FLUKA involves scoring the region based on production yields, and then postprocessing the results with an offline time evolution program that allows for radioactive decay.

A region independent method involves scoring the yield per primary particle at the production point (using the scoring tool USERBIN) and then postprocessing the results by applying a special binning that allows computation of the yield per bin. This method has the advantage of being nuclide specific and region independent, with the added benefit that the binning can be adjusted even after the FLUKA simulation is run to provide more detailed information on specific points. The disadvantages are that the postprocessing is quite complex and a specific program needs to be written by the user.

For other Monte Carlo codes (MCNPX, GEANT4, PHITS), the flux values for neutrons and photons below 25 MeV are provided in specific predefined energy groups. Additional results available from Monte Carlo calculations include the radionuclide production rates from neutrons and photons with energies greater than 25 MeV as well as from other particles. An example of this capability is provided in Fig. 10, where the production rates of various nuclides resulting from the interaction of 200 MeV protons with an alloy made of copper, zinc and lead are shown.

Similar results can be obtained for each region of the geometric model defined for transport calculations.

## 2.9.3. Activation codes

The activation codes discussed in this section are applicable to both reactor and accelerator facilities. The application of the activation codes is the second step in the process for assessing the activation source term.



FIG. 10. Results of a typical set of PHITS simulated radionuclide production rates by 200 MeV proton induced nuclear reactions.

The objective of the activation source term calculations is to determine the total radionuclide activity and specific activity in each component and subcomponent of importance to the decommissioning planning process. The activity calculation uses three sources of data: (i) the energy dependent neutron flux values from the transport calculations; (ii) the material composition data for various components (i.e. mass percentage of elements and densities); and (iii) the operating history of the facility.

The activation codes require flux values, and under some circumstances, radionuclide production rates derived from Monte Carlo codes as inputs to the activation calculations. In addition, the activation codes require physical, operational and measurement data. The activation code calculates the radionuclide distribution in those regions and components where a neutron flux or radionuclide production rate was determined as part of the transport calculations.

#### 2.9.3.1. Codes and their limitations and capabilities

The activation codes use the outcome of the transport calculations to: (i) determine the radionuclide production rates; (ii) establish the total quantity of activation products resulting from facility operations; and (iii) perform radioactive decay calculations to determine radionuclide inventories as a function of time after facility shutdown.

Activation codes are capable of calculating both radionuclide production and decay in essentially any material in any component in any facility. Radionuclide generation and depletion modelling is relatively common and can be performed by a number of software programs:

- ORIGEN [50] is a computer code system for calculating the buildup, decay and processing of radioactive materials using the matrix exponential method to solve a large system of coupled, linear, first order ordinary differential equations with constant coefficients. ORIGEN incorporates simple reactor models, cross-section libraries, fission product yields, decay data and decay photon data when solving the equations. ORIGEN's ability for variable dimensions allows the user to tailor the size of the executable module to the problem size and/or the available computer space. The ORIGEN code calculates the activation based on neutron flux values using three energy groups that are sufficient for most light water reactor calculations. ORIGEN is not normally suitable for accelerator activation calculations.
- CINDER'90 [17] is used to calculate the inventory of radionuclides in an irradiated material. Utilizing a self-contained nuclear data library, CINDER'90 calculates the atom density (atoms per unit volume) and activity density (e.g. becquerels per unit volume) of each radionuclide

present at a specified time. The code is identified as a transmutation nuclide inventory code because the code follows all paths of nuclide transmutation (i.e. the conversion of nuclides to different radionuclides by particle absorption and radioactive decay). The CINDER'90 library of 63 energy group cross-sections describes 3400 nuclides in the range  $1 \le Z \le 103$ . The code requires a multigroup neutron flux for neutron energies up to 20 MeV and radionuclide production rates for reactions at higher neutron energies or for additional particles. Although developed for accelerator based problems, the code is applicable to any transmutation problem for which simulation calculations of particle reactions are available. The 63 energy groups are sufficient in most cases to calculate the activities.

- DCHAIN-SP2001 [51] estimates the radionuclide inventories and radiation environment of high energy accelerator related facilities and was designed to resolve issues regarding spallation neutron utilization facilities. DCHAIN-SP2001 is an update of DCHAIN-SP. For analysing the decay and buildup characteristics of spallation products, DCHAIN-SP was developed on the basis of CCC-370/DCHAIN2 by revising the decay data and implementing the neutron cross-section data. The decay data are newly processed from the data libraries of version 3.1 of the European Activation File (EAF 3.1), FENDL/D-1 and the Evaluated Nuclear Structure Data File (ENSDF). The neutron cross-section data taken from FENDL/A-2 are also prepared to take account of the transmutation of nuclides by the neutron field at the produced position. DCHAIN-SP solves the time evolution of decay and buildup of radionuclides in every decay chain by the Bateman method. It can calculate the radionuclide inventory, activity, decay heat and gamma ray energy spectra on the basis of the radionuclide production rate calculated by the nucleon-meson transport code NMTC/ JAERI97. The DCHAIN-SP2001 code calculates the activation based on neutron flux values given in 175 energy groups. The use of this code allows the treatment of very complicated neutron spectra such as in the case of spallation reactions associated with accelerators.
- FISPACT [52] is an inventory code that has been developed for neutron, proton and deuteron induced activation calculations. FISPACT-2007 uses external libraries of nuclear data for all relevant nuclides to calculate the number of atoms of each species at a specified time during irradiation or after a decay period following shutdown. The various species are formed either by a direct reaction on a starting material (by a series of reactions, some of which can be on radioactive targets) or by a decay reaction or series of decay reactions. The basic equations solved by the FISPACT code are those giving the rate of change of nuclide number density with time (i.e. the Bateman equation). The method of solution used is basically that

of Sidell (i.e. a numerical solution). The number densities are calculated by the Taylor series expansion in a modified form. The quality of the calculated inventory is dependent on the quality of the input nuclear data (i.e. the cross-sections and decay properties). The EAF is one source of data for the calculations. FISPACT is able to use up to 351 energy groups, and may be the most suitable code for accelerator and fusion device activation calculations.

A combined neutron transport calculation and activation calculation can be performed by applying MCNP6 [19] or MCNPX [17]. These codes can be used for the direct determination of the integral activation values. By applying these codes in this manner, the requirement to couple the neutron flux calculation with the activation calculation can be avoided.

In order to calculate the activity of each predefined region, MCNPX calculates the energy and space dependent neutron flux distribution and the reaction rate of the relevant nuclear reactions. By applying these values, the so called CINDER'90 [17] submodule of MCNPX calculates the radionuclide composition in the predefined regions at the end of a specified time period.

#### 2.9.3.2. Activation model assumptions

The power history of a reactor or the beam strength of an accelerator is approximated by converting the history into discreet periods (e.g. a histogram structure), and it is assumed that this approximation will adequately describe the actual operations. A second assumption is that the activation results are homogeneous over the volume being calculated.

#### 2.9.3.3. Model applicability

Activation models are applicable to all facilities, materials, systems and components/subcomponents where material is being activated by energized particles.

## 2.9.3.4. Hardware and software requirements

Generally, the hardware and software requirements for the activation codes described above can be found in the code manuals.

## 2.9.3.5. Code availability

The codes described in Section 2.9.3.1 are normally available from the developers or from the RSICC (http://rsicc.ornl.gov) or the OECD/NEA Data Bank (www.oecd-nea.org/databank).

# 2.9.3.6. Results

The reaction rates can be postprocessed in the manner discussed below. Based on the neutron flux and neutron induced activity calculations, specific activity values are provided for each specified radionuclide and for every predefined region or cell as a function of time elapsed after the (presumed) final shutdown of the facility. Data are usually obtained in a simple ASCII file format, which can be postprocessed by virtually any data handling software. An example of such a data file can be seen in Fig. 11.

Providing the results in this type of format allows the user to consider various possibilities for subsequent evaluations. A typical progression of evaluations could be as follows:

- (1) The specific activity and total activity of each radionuclide for each region is calculated based on inputs that include geometric, spatial and material composition data of an appropriate quality.
- (2) The total activity in specific components is derived based on the total activity of the predefined regions as determined in the previous step.
- (3) Based on the total activity of each component included in the model, estimations can be made of the total volume and mass of the various activated regions and components.

Assessments of the depth of the activation can also be performed. The total activity values can then, for example, be used as a basis for radiation protection

NPP unit: Material: Region: Density: Volume: Activation time-span:	1 region_1 7.85 2.986E+04 12.2	(Stainless g/cm <sup>3</sup> cm <sup>3</sup> years	steel)															
Specific activity (Bq/g	g) of acivation	products																
Isotope	0.0833333	0.25	0.5	1	. 2	5	10	20	30	50	0 70	10	200	500	1000	2000	5000	10000
C-14	3.441E+04	3.441E+04	3.441E+04	3.441E+04	3.441E+04	3.439E+04	3.437E+04	3.433E+04	3.429E+04	3.421E+04	3.412E+04	3.400E+04	3.359E+04	3.239E+04	3.048E+04	2.700E+04	1.877E+04	1.023E+04
Cr-51	6.063E+08	1.322E+08	1.345E+07	1.394E+05	1.495E+01													
Mn-54	1.356E+07	1.185E+07	9.673E+06	6.449E+06	2.866E+06	2.516E+05	4.364E+03	1.312E+00	3.947E-04									
Fe-55	5.811E+08	5.570E+08	5.228E+08	4.604E+08	3.572E+08	1.668E+08	4.686E+07	3.699E+06	2.920E+05	1.820E+03	1.134E+01	5.581E-03						
Fe-59	1.396E+07	5.479E+06	1.346E+06	8.133E+04	2.967E+02	1.440E-05												
Co-58	2.806E+07	1.547E+07	6.336E+06	1.062E+06	2.985E+04	6.626E-01	1.162E-08											
Co-60	3.249E+07	3.179E+07	3.076E+07	2.880E+07	2.525E+07	1.702E+07	8.819E+06	2.368E+06	6.356E+05	4.581E+04	3.302E+03	6.389E+01	1.243E-04					
Ni-59	2.079E+05	2.079E+05	2.079E+05	2.079E+05	2.079E+05	2.078E+05	2.078E+05	2.078E+05	2.078E+05	2.078E+05	2.077E+05	2.077E+05	2.075E+05	2.069E+05	2.060E+05	2.041E+05	1.986E+05	1.897E+05
Ni-63	2.338E+07	2.335E+07	2.331E+07	2.323E+07	2.307E+07	2.259E+07	2.182E+07	2.036E+07	1.900E+07	1.654E+07	1.440E+07	1.170E+07	5.848E+06	7.309E+05	2.284E+04	2.231E+01	2.077E-08	
Total	1.299E+09	7.773E+08	6.078E+08	5.204E+08	4.086E+08	2.068E+08	7.771E+07	2.664E+07	2.013E+07	1.679E+07	1.461E+07	1.190E+07	6.055E+06	9.379E+05	2.288E+05	2.041E+05	1.986E+05	1.897E+05

FIG. 11. Example of an output file from an activation calculation code.

calculations, which will play a pivotal role not only during the decommissioning implementation activities, but also as an important input into the planning, design and construction of any shielding structures. In addition to important input into radiation protection initiatives, the total activity values can allow a preliminary estimate of the mass and volume of radioactive wastes that will be produced during the decommissioning, and as a corollary, provide input into the decommissioning cost estimation process.

The calculated results for the total activity in each component of interest can provide important input into the decommissioning planning process, particularly in terms of providing a basis for estimating the quantities of radioactive waste in different waste classifications as a function of time after facility shutdown. The waste classification process can be performed in accordance with either national regulations (where available) or international standards [53].

Annex II provides an example of an ORIGEN output showing radionuclide data in one region at two different points in time.

# 3. SOFTWARE AND DATA VERIFICATION AND VALIDATION

#### 3.1. SOFTWARE

The discussions in this section concern the verification and validation of software being utilized in the assessment of an induced activation source term. The discussions apply to both particle transport and activation codes.

# 3.1.1. General

Software verification is the process of determining whether a computational model correctly implements the intended conceptual model or mathematical model. Software validation is the process of building confidence that a model adequately represents a real system for a specific purpose. In general, it is assumed that the software codes used for the transport and activation calculations are validated. Additional information on software verification and validation can be found in Ref. [54], and although this reference focuses on nuclear power plant instrumentation and control software, the basic principles are applicable to software designed for activation source term calculations.

## 3.1.2. Verification

All of the codes discussed in this report are verified by the developers before release, and independent verification reports are available for some codes (e.g. see Ref. [55]). The verification process performed by the software developers normally consists of a thorough analysis of comparisons between benchmark values and the corresponding calculated results.

Notwithstanding the above, the user is generally instructed to calculate a set of test cases (often supplied by the developers) and to compare the results with those provided by the developers in order to help ensure that the actual user installed version of the code conforms to the verification standards established by the developers. Verification processes are carried out before every release of new versions of the code by comparing code versions, compilers, platforms and parallel options.

## 3.1.3. Validation

Models are normally validated by comparing calculated results to a set of physical measurements made on or in the facility under study. The nature and extent of the measurements made for validation will in large measure be dictated by the nature of the nuclear facility. Some of the physical parameters that can be measured for validation purposes include dose rates, particle flux or fluence, and radionuclide concentrations in samples taken at specific locations within the facilities. Generally, the robustness and usefulness of the validation process can be improved by: (i) increasing the number of measurements and sampling points; and (ii) optimizing the measurement process to help ensure that the parameters being measured are those best suited to validating any parameters that are of particular importance to the intended use of the source term (e.g. validating results for those radionuclides that are important to a disposal safety assessment case). When the measured and computed quantities agree within a predefined confidence interval, the model is considered validated.

The activation source term calculations can be validated by a quantitative analysis of the specific activity of key radionuclides using gamma spectrometry. With the use of appropriate statistical methods, the validation process may be able to provide important information about various factors: (i) the statistical uncertainties inherent in the simulation methodology; (ii) the extent of variability in material compositions; (iii) the accuracy of the spatial parameters used to describe the irradiation conditions and component dimensions; (iv) details on irradiation conditions; and (v) the uncertainties in the gamma spectrometry measurements. As part of the validation exercise, criteria can be established as to what constitutes acceptable agreement between experimental results and calculated results. These criteria will need to consider, for example, that uncertainties in the gamma spectrometry analyses can normally be controlled to less than 30%. In general, once the validation process has been acceptably completed using gamma spectrometry, it can be assumed that the calculated results for the non-gamma emitting radionuclides are correct. However, it is generally beneficial to remain diligent for circumstances or results that might indicate that the extrapolation from gamma emitting species to non-gamma emitting species is not valid.

A further validation of the calculated activation source term can be obtained by comparing actual dose rate measurements with dose rates calculated from the activation calculations. As an example of a validation process for FLUKA, a benchmark experiment was carried out at the CERN–EU High-Energy Reference Field (CERF) facility [55, 56]. The experiment was conducted to confirm that the models implemented in FLUKA for the description of nuclear reactions allow precise predictions of individual radionuclides. A further objective was to confirm the premise that if the elemental composition of a material is known with a high degree of certainty, then FLUKA can reproduce the complete radionuclide inventory. This benchmarking experiment included most of the materials typically found in high energy accelerators (aluminium, copper, stainless steel, iron, concrete, etc.). The results of these studies show an agreement within 20–30% [57] between the measured and calculated values, confirming that FLUKA is a suitable particle transport and activation code for calculating induced radioactivity in high energy accelerators.

Measurements important to validation studies are further discussed in the sections that follow.

# 3.1.3.1. Measurements of flux/fluence of neutrons and other particles

Many facilities have a variety of techniques for measuring flux/fluence of neutrons and other particles at certain locations. Neutron instrument data used during operation and radiochemical analyses of samples taken during operation may be used to measure the flux/fluence of neutrons and other particles. Power reactors may have surveillance capsule or coupon analysis reports, and research or non-power facilities may have experimental data. Particle accelerators often have neutron and gamma detectors for radiological protection as well as devices used during operations to measure beam parameters. During operations, it is important to properly archive such types of data for subsequent use in decommissioning planning and for the purposes of validation.

#### 3.1.3.2. Dose rate measurements

Dose rate measurements at locations of interest can be useful in validating the transport and activation calculations. It is important to know the precise date, locations and circumstances of the dose rate surveys. Similarly, it is important to record the conditions surrounding the survey, including: (i) accurate measurements as to the location of the survey relative to the component being measured; (ii) the locations of other components relative to the measured component; (iii) the type of dose rate detector employed; and (iv) the nature of any fluid or material surrounded the component and the detector. This level of careful record keeping is necessary to help ensure that the influence of multiple source regions can be modelled, as it may not be possible to isolate the dose rate for a specific component from other dose contributions, particularly in a low background environment. The survey is also best carried out at an optimum time after power operations have ceased (i.e. after a period of time that will allow the decay of short lived gamma emitting radionuclides while still permitting good measurements to be made of key gamma emitting radionuclides such as <sup>60</sup>Co). The usefulness of dose rate surveys is reduced if too much time elapses between power or beam operation and dose rate measurements.

#### 3.1.3.3. Scaling calculations

As discussed in Section 3.1.3, gamma spectrometry can be employed as a tool in the validation of activation source term calculations. There are, however, other methods that can also be employed to make activity measurements that can be used for validation purposes. For example, the scaling factor method is widely applied to evaluate difficult to measure radionuclides. The scaling factor method is based on a correlation between easily measurable gamma emitting nuclides and difficult to measure radionuclides, such as <sup>3</sup>H, <sup>99</sup>Tc, <sup>129</sup>I, <sup>55</sup>Fe, <sup>63</sup>Ni and transuranic material (see Refs. [58–60]).

# 3.2. QUALITY MANAGEMENT — DATA VERIFICATION AND VALIDATION

The terms data verification and data validation, as used in this section, refer to the use of quality management processes to evaluate whether data needed for source term calculations (e.g. dimensions, material compositions/densities, nuclide concentrations, nuclear data libraries) have been generated in accordance with required specifications, satisfy acceptance criteria and are appropriate and consistent with their intended use. The United States Environmental Protection Agency (EPA) has issued a document providing guidance on the verification and validation of environmental data [61]. The topics of data verification and validation are part of the EPA Quality System and fit into the category of project level tools. This category of tools includes systematic project planning, project implementation in the field and analytical laboratory, and the assessment phase, where data are evaluated and prepared for use.

Although the scope of verification and validation may be broader when taken in the context of quality management, the initiatives surrounding code verification and validation clearly form part of the process. The extent to which Member States may require explicit procedures to ensure the defensibility of results (scientifically, legally, etc.) will clearly depend on specific situations.

# 3.2.1. Definition of data verification

The EPA guidance document [61] provides the following definition of data verification:

"For the purposes of this guidance, the term 'data verification' is the process of evaluating the completeness, correctness, and conformance/compliance of a specific data set against the method, procedural, or contractual requirements. Again, the goal of data verification is to ensure and document that the data are what they purport to be, that is, that the reported results reflect what was actually done."

## **3.2.2.** Definition of data validation

The EPA guidance document [61] defines data validation as follows (footnote omitted):

"For the purposes of this guidance, the term 'data validation' is an analyteand sample-specific process that extends the evaluation of data beyond method, procedural, or contractual compliance (i.e., data verification) to determine the analytical quality of a specific data set. Data validation criteria are based upon the measurement quality objectives developed in the QA Project Plan or similar planning document, or presented in the sampling or analytical method. Data validation includes a determination, where possible, of the reasons for any failure to meet method, procedural, or contractual requirements, and an evaluation of the impact of such failure on the overall data set. Data validation applies to activities in the field as well as in the analytical laboratory."

# 4. OTHER SOURCE TERMS

#### 4.1. GENERAL

For a comprehensive assessment of the radiological source term in nuclear facilities that have been shut down, contributions in addition to the activation source term may need to be included. These additional contributions can come from: (i) corrosion products that are generated as activated systems and components age; (ii) additional activation products resulting from reactions in the corrosion products; (iii) fuel debris; (iv) naturally occurring radioactive material; (v) radioactive items brought into the facility (e.g. waste brought in for storage); (vi) waste generated during maintenance on activated components; and (vii) samples resulting from the planned irradiation of samples (e.g. samples analysed using neutron activation analysis).

In general, the major components that make up a radioactive source term include:

- Particle induced activation products;
- Loose or fixed radioactive contamination;
- Spent fuel elements, operational waste and other radioactive sources.

Completing an assessment of a radioactive source term that includes all of the above components may not always be readily attainable in all Member States, particularly with respect to the activation source term. While this report focuses on the activation source term, a brief discussion of the assessment processes for the other two source term components seems warranted for the sake of completeness. The evaluation of the latter two source term components requires activities such as radiological surveys, sampling and analysis, and an examination of historical records and operating reports. Standard practices for use in determining these two source terms can be found in other IAEA publications [62]. An overview of the contribution of contaminated material to the radionuclide inventory of a facility, as well as a list of relevant radionuclides and typical contaminated components found in nuclear reactors that have been shut down, is given in the IAEA publication Radiological Characterization of Shut Down Nuclear Reactors for Decommissioning Purposes [3].

The removal of spent fuel, operational waste and disused sealed radioactive sources is generally considered to be a prerequisite for decommissioning a facility. However, for a variety of reasons, it is recognized that this may not be the case for all facilities. Depending on the type of facility (e.g. medical, research), contamination arising from poorly confined radioactive materials such as gases, liquids and powders can contribute significantly to the overall source term.

# 4.2. IDENTIFICATION AND EVALUATION OF OTHER SOURCE TERMS

A brief discussion of other source term components, in addition to that component arising from particle induced activation, is provided in the sections that follow.

## 4.2.1. Loose or fixed radioactive contamination

The major contributor to a source term, other than particle induced activation products, is radioactive contamination. Contamination can be generally categorized as loose material capable of being removed by simple mechanical means or as fixed material requiring more aggressive methods for removal.

Radioactive contamination can be deposited on internal and external component surfaces as a result of the movement or leaching of radioactive corrosion, erosion, fission and actinide products during facility operation. Some of the radioactive contamination products may be a result of the activation process, particularly in the case of corrosion and erosion products.

Contamination can generally be found throughout a nuclear facility where radioactive material has been used, manufactured or processed. In a reactor facility, it can often be found near the nuclear fuel discharging equipment, inside primary systems and components, in fuel or component storage pools and at the processing and storage facilities used for radioactive effluents and waste. At accelerators, contaminated areas can be found both in and outside of the beam line in those components in contact with cooling media, or from deteriorated structural material surrounding the beam tube.

In order to determine the contribution of contamination to the source term, radiological surveys using on-site measurements together with sampling and analysis campaigns are needed. For the estimation of surface contamination in the primary heat transport system of a nuclear power plant, modelling can be used to calculate the transport and deposition of corrosion products in the system. An example of a computer code capable of this type of modelling is PACTOLE [63].

## 4.2.2. Spent fuel elements, operational waste and other radioactive sources

As noted previously, the removal of spent fuel is normally completed during the operational phase of a facility. However, there are cases where a reactor may have experienced abnormal operational events, such as a major fuel element failure, in which case residues of these materials will likely remain in the systems and will need to be included in the decommissioning source term inventory.

Operational waste can form part of the facility source term if it has not been removed as part of operational activities. It may be possible to characterize operational waste if the source of the waste is well known and understood. For example, if the waste is a well characterized by-product from a processing facility, then its characteristics can often be assigned with a reasonable degree of certainty. Wastes from unknown sources or which have been poorly documented will likely require chemical and radiochemical analyses. Other radioactive material might also include sealed sources, laboratory chemicals or research materials. Useful information on the decommissioning of small medical, industrial and research facilities can be found in Ref. [13].

# 4.3. ASSESSMENT OF OTHER SOURCE TERMS

In addition to performing activation calculations, other methods for determining decommissioning source terms include in situ measurements together with sampling and analysis programmes to improve understanding of the radiological conditions that will be encountered during decommissioning.

Types of measurement that can be considered for use in assessing source terms include:

- Dose rate measurements;
- Direct surface contamination measurements;
- Measurement of radionuclide activities by spectrometry;
- Measurement of total activity using gross gamma detectors.

In undertaking a programme of surveying, sampling and analysis (including in situ measurements), the use of methodologies such as those embodied in the Radiation Survey and Site Investigation Process used in the Multi-Agency Radiation Survey and Site Investigation Manual (MARSSIM) [64] may warrant consideration. The purpose of MARSSIM is to provide a standardized approach to demonstrating compliance with a dose based or risk based regulation. This can be particularly important if the goal of a decommissioning project is to provide evidence that approved cleanup criteria have been met, and that the facility licence
can be terminated. MARSSIM also provides guidance in optimizing surveying and sampling programmes, and incorporates the use of statistical considerations. In all cases, particular attention needs to be paid to ensuring that the methods of measurement take into account the geometry, the surface conditions and the nature and extent of the radioactive contaminants. Survey procedures need to consider the physical limitations of the measurement equipment and techniques. The assessment of the decommissioning source terms is usually followed by dose assessments, which include evaluating the possible exposures from both internal and external sources. A discussion of dose assessment is not included in this report.

## 5. APPLICATION OF RESULTS

#### 5.1. GENERAL

The decommissioning source term drives much of the decommissioning planning process, and as a consequence, the quality and reliability of the source term data can play an important role in determining the success of a decommissioning project. Furthermore, this source term can play an important role in demonstrating the capability for and feasibility of decommissioning a facility, a demonstration that may need to be completed before initial criticality or before facility operation commences [65].

Many of the discussions in this report concern the importance of such parameters as material composition, component geometry, spatial data, beam strength and particle flux to the ability to effectively assess the particle induced activation source term, as well as other source terms. For this reason, it can be very beneficial to measure (or establish the means for measuring) parameters important to determining the decommissioning source term prior to initial criticality or facility operation. Similarly, it may be beneficial to calculate the predicted source term prior to facility operation, and then to use this information as a benchmark for actual measurements taken during facility operations. Differences between the predicted and measured results observed during the operational lifetime of a facility can then be used to refine the source term model and thereby the quality of the source term data. The source term information generally sees substantial use throughout the decommissioning planning process, and provides important inputs into such tasks as developing safety assessments; determining waste management requirements; selecting decommissioning options; developing radiation protection programmes to ensure the safety of the workers, public and the environment; and estimating the decommissioning costs. Some of these aspects are discussed in the sections that follow, which are intended to provide a brief description of the role that the source term plays in these applications.

#### 5.2. SAFETY ASSESSMENT

The decommissioning safety assessment process uses input from the source term data to determine, for example, the levels of possible radioactive releases that could occur as the result of an abnormal event taking place during the decommissioning process.

Decommissioning activities generally differ from those normally performed during a facility's operational phase. These differences primarily arise from the fact that during decommissioning, areas and materials are being exposed and processed that would not normally be accessed during routine operations. A prime example of such a situation would be the removal of the concrete biological shield of a reactor, where the inner portion is activated from the neutron flux and the outer surface may be contaminated. Such an operation would be extremely unusual as part of the operational phase of a facility, but represents a relatively common activity in decommissioning processes. The removal of the activated concrete can involve the generation of large quantities of contaminated dust and rubble. An upset scenario could include the loss of localized containment, with the resulting release of dust to the immediate work area or the environment. The consequences of such a release could be the uncontrolled contamination of workers or the general public. In order to evaluate the impact of such a scenario in terms of, for example, dose commitment, the levels and types of radionuclides present in the concrete must be known, and it is the data from the source term calculations that can provide the information required for these analyses and assessments.

#### 5.3. WASTE MANAGEMENT

A first step in the management of the waste generated during decommissioning is to classify the waste in a manner that will allow the final disposition routes to be determined. The classification of waste is based on the types of radionuclides within the material, the properties of the waste and the specific activities of the radionuclides. The classification of the waste is generally based on national requirements. Guidance on how to determine waste classification is given in Ref. [53]. The results of the source term assessment can

be used to estimate the form and extent of radioactive material in a facility, and this in turn helps in selecting appropriate removal techniques, and in estimating the quantities of waste that will be generated. It may bear noting that although the volume of waste resulting from the contamination source term discussed above may exceed the volumes that result from the activation source term, the total activities generated by activation are typically orders of magnitude higher than those arising from contamination.

#### 5.4. RADIATION PROTECTION

The results of the activation source term calculations have a major role in the management of the radiation protection issues [66] associated with the decommissioning process. However, given the importance of radiation protection, it is generally advisable to have a means of independently confirming the values generated by the calculations, particularly for any potentially problematic radionuclides.

Based on the source term, important radiation safety requirements can be established, requirements that may specifically call for shielding, personal protective equipment, monitoring equipment, dosimetry programmes including internal dosimetry, and the fabrication of specialized equipment to reduce doses.

Although the topic of dose assessment as it relates to decommissioning is not in the scope of this report, the process of handling large radioactively contaminated components can have a significant impact on the dose to the workers. On the one hand, sectioning large components into discrete pieces makes it possible for various regions and subcomponents having different levels of activation products to be isolated and handled individually. On the other hand, the process of cutting and segmenting may lead to higher worker doses than those that would result if the component were to be handled intact for shipping and disposition. In view of the complexities associated with the waste arising from decommissioning activities, it is generally important to establish a waste management programme as well as a safety assessment programme to examine these issues and to support decommissioning activities [1].

While the detection of radiation fields (e.g. gamma radiation) is relatively straightforward with modern radiation surveying instrumentation [62], the identification and quantification of the radionuclides in a source term by chemical and radiochemical means may be technically challenging and time consuming, and may require statistically based sampling procedures if the material being analysed is highly variable and non-homogeneous. Furthermore, the measurement of some types of radionuclides may simply not be possible owing to factors such as detection limits, matrix effects and background radiation levels. Under these

circumstances, theoretical inventory predictions may represent the only practical option for developing a comprehensive assessment of the decommissioning source term.

#### 5.5. COST ESTIMATION

In order to ensure that adequate resources are available to successfully complete a decommissioning project, a cost estimate is generally required. In broad terms, the cost of performing decommissioning depends on the type and quantity of labour required to perform the work, the equipment needed to support the activities, and the types and quantity of waste being generated. Each of these issues is, in turn, largely dependent on the decommissioning source term.

The activation source term serves to identify the location and quantity of activated material requiring removal, and these data can, in turn, be used to develop an estimate of the personnel resources needed to remove this material. Based on the type of material being removed (i.e. concrete or metal) and the radionuclide levels in the materials, it is then possible to estimate factors such as dose rates, quantity of material to be removed and equipment requirements. Based on the staffing and equipment needs, a project schedule can be prepared and the costs estimated. An important component in a decommissioning cost estimate is the cost for the disposition of waste. This cost is largely driven by the waste volumes predicted for various waste classifications, which in many applications can be determined by considering the activity calculations. An internationally accepted method for preparing decommissioning cost estimates has been developed by the IAEA, OECD/NEA and European Commission [67].

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#### Annex I

## **EXAMPLE OF ANISN CODE OUTPUT**

Figure I–1 contains an example of ANISN output showing neutron data for 68 groups in one region.

GRP.	FIX-SOURCE	FISS-SOURCE	IN-SCATTER	SLF-SCATTER	OUT-SCATTER	ABSORPTION	LEAKAGE	BALANCE	RT-BDY-FLUX	RT-BDY-J+	RT-BDY-J	RT-LEAKAGE	LFT-LEAKAGE	FISS-RATE	TOTAL-FLUX	DENSITY
1	0.00E+00	0.00E+00	0.00E+00	4.30E-09	5.48E-09	8.01E-10	-6.28E-09	1.00E+00	7.78E-11	6.36E-11	6.30E-11	6.05E-08	6.68E-08	0.00E+00	4.99E-08	4.99E-08
2	0.00E+00	0.00E+00	6.72E-10	2.28E-08	2.30E-08	3.75E-09	-2.60E-08	1.00E+00	3.38E-10	2.69E-10	2.63E-10	2.53E-07	2.79E-07	0.00E+00	2.16E-07	2.16E-07
3	0.00E+00	0.00E+00	2.63E-09	1.11E-07	1.02E-07	1.38E-08	-1.13E-07	1.00E+00	1.39E-09	1.12E-09	1.10E-09	1.06E-06	1.17E-06	0.00E+00	8.92E-07	8.92E-07
4	0.00E+00	0.00E+00	1.15E-08	2.57E-07	2.18E-07	2.35E-08	-2.30E-07	1.00E+00	2.81E-09	2.25E-09	2.21E-09	2.12E-06	2.35E-06	0.00E+00	1.80E-06	1.80E-06
5	0.00E+00	0.00E+00	2.99E-08	5.14E-07	4.13E-07	3.48E-08	-4.18E-07	1.00E+00	5.05E-09	3.98E-09	3.89E-09	3.74E-06	4.16E-06	0.00E+00	3.24E-06	3.24E-06
6	0.00E+00	0.00E+00	7.64E-08	1.44E-06	1.11E-06	6.83E-08	-1.10E-06	1.00E+00	1.31E-08	1.01E-08	9.78E-09	9.41E-06	1.05E-05	0.00E+00	8.41E-06	8.41E-06
7	0.00E+00	0.00E+00	2.07E-07	2.01E-06	1.60E-06	6.50E-08	-1.45E-06	1.00E+00	1.80E-08	1.29E-08	1.23E-08	1.18E-05	1.32E-05	0.00E+00	1.15E-05	1.15E-05
8	0.00E+00	0.00E+00	4.92E-07	3.26E-06	2.23E-06	6.35E-08	-1.80E-06	1.00E+00	2.72E-08	1.73E-08	1.56E-08	1.50E-05	1.68E-05	0.00E+00	1.75E-05	1.75E-05
9	0.00E+00	0.00E+00	6.55E-07	2.05E-06	1.49E-06	2.43E-08	-8.63E-07	1.00E+00	1.86E-08	1.01E-08	8.37E-09	8.05E-06	8.91E-06	0.00E+00	1.18E-05	1.18E-05
10	0.00E+00	0.00E+00	6.12E-07	1.30E-06	1.0/E-06	1.19E-08	-4./1E-0/	1.00E+00	1.29E-08	6.94E-09	5.52E-09	5.31E-06	5.78E-06	0.00E+00	8.16E-06	8.16E-06
11	0.00E+00	0.00E+00	7.16E-07	1.55E-06	1.14E-06	9.44E-09	-4.38E-07	1.00E+00	1.42E-08	7.06E-09	5.21E-09	5.01E-06	5.45E-06	0.00E+00	8.92E-06	8.92E-06
12	0.00E+00	0.00E+00	5.19E-07	5.28E-07	7.42E-07	3.72E-09	-2.2/E-0/	1.00E+00	6.9/E-09	3.53E-09	2.63E-09	2.53E-06	2.75E-06	0.00E+00	4.3/E-06	4.3/E-06
13	0.00E+00	0.00E+00	1.65E-07	4.08E-08	2.09E-07	9.12E-10	-4.48E-08	1.00E+00	1.74E-09	9.15E-10	6.99E-10	6.72E-07	7.1/E-U/	0.00E+00	1.08E-06	1.08E-06
14	0.0000000	0.000+00	6.51E-07	0.54E-07	7.97E-07	4.29E-09	-1.50E-07	1.000+00	8.55E-09	4.002-09	2.63E-09	2.72E-06	2.8/E-06	0.000+00	5.50E-06	5.502-00
15	0.00E+00	0.00E+00	1.29E-06	2.18E-06	1.39E-06	6.59E-09	-1.0/E-0/	1.00E+00	2.11E-08	8.78E-09	5.15E-09	4.95E-06	5.06E-06	0.00E+00	1.30E-05	1.30E-05
10	0.0000000	0.00E+00	1.55E-00	2.165.06	1.21E-00	5.10E-09	1.08E-07	1.00E+00	2.10E-08	0.285.00	2 19E 00	2.055.06	3.40E-08	0.00E+00	1.51E-05	1.316-05
10	0.000,000	0.000+00	2.215.05	4.910.00	1.340-00	0.402-03	4.492-07	1.000.+00	2.000-00	1 1 2 0 0	0.000 10	0.000-00	2.010-00	0.000000	2.525.05	2.525.05
10	0.000+00	0.000+00	1 205 06	4.81E-00	1.10E-00	9.02E-09	6.29E.07	1.00E+00	4.24E-08 2.60E.08	6.625.00	3.00E-10	9.23E-07	-2.78E-07	0.00E+00	1 605.05	1 605 05
20	0.00E+00	0.00E+00	1.01E-06	1.67E-06	7.432-07	3 71E-09	2.44E-07	1.00E+00	1 29E-08	3.52E-09	4 74F-10	4 565-07	2 12F-07	0.00E+00	7.80E-05	7.80E-05
20	0.000+00	0.005+00	1.010-00	2.045.06	6.055.07	0.525.00	0.575.07	1.000+00	2.495.00	6 90E 00	2 515 00	2 295 06	4 245.06	0.000+00	2.025.05	2.025.05
21	0.00E+00	0.00E+00	1.376-00	3.455-06	6 51E-07	7.09F-09	5.76E-07	1.00E+00	2 77E-08	5.81E-09	-3.31L-03	-3.38L-00	-4.34E-00	0.00E+00	1.63E-05	1.63E-05
23	0.00E+00	0.00E+00	1.31E-06	5.44E-06	5.20E-07	7.80E-09	7.78E-07	1.00E+00	3.07E-08	6.56E-09	-2.17E-09	-2.09E-06	-2.87E-06	0.00E+00	1.80E-05	1.80E-05
24	0.00E+00	0.00E+00	9.38E-07	3.75E-06	3.65E-07	7.49E-09	5.66E-07	1.00E+00	2.92E-08	5.29E-09	-3.85E-09	-3.70E-06	-4.26E-06	0.00E+00	1.69E-05	1.69E-05
25	0.00E+00	0.00E+00	9.66E-07	7.10E-06	6.19E-07	1.18E-08	3.36E-07	1.00E+00	3.82E-08	8.73E-09	-1.65E-09	-1.59E-06	-1.93E-06	0.00E+00	2.28E-05	2.28E-05
26	0.00E+00	0.00E+00	9.03E-07	6.89E-06	4.21E-07	1.15E-08	4.71E-07	1.00E+00	3.46E-08	7.49E-09	-2.22E-09	-2.14E-06	-2.61E-06	0.00E+00	2.04E-05	2.04E-05
27	0.00E+00	0.00E+00	5.60E-07	6.53E-06	2.95E-07	1.23E-08	2.53E-07	1.00E+00	2.41E-08	5.92E-09	-2.78E-10	-2.68E-07	-5.21E-07	0.00E+00	1.46E-05	1.46E-05
28	0.00E+00	0.00E+00	3.63E-07	4.82E-06	3.49E-07	1.02E-08	4.45E-09	1.00E+00	1.96E-08	4.96E-09	3.92E-11	3.77E-08	3.33E-08	0.00E+00	1.20E-05	1.20E-05
29	0.00E+00	0.00E+00	3.68E-07	2.29E-06	5.55E-07	7.93E-09	-1.94E-07	1.00E+00	6.89E-09	2.01E-09	4.73E-10	4.55E-07	6.50E-07	0.00E+00	4.45E-06	4.45E-06
30	0.00E+00	0.00E+00	5.67E-07	5.92E-06	6.63E-07	7.46E-09	-1.04E-07	1.00E+00	3.68E-09	1.17E-09	4.42E-10	4.25E-07	5.29E-07	0.00E+00	2.88E-06	2.88E-06
31	0.00E+00	0.00E+00	6.67E-07	5.97E-07	3.96E-07	4.90E-09	2.67E-07	1.00E+00	8.34E-09	1.01E-09	-1.82E-09	-1.75E-06	-2.02E-06	0.00E+00	4.75E-06	4.75E-06
32	0.00E+00	0.00E+00	4.01E-07	4.09E-07	2.42E-07	6.93E-09	1.52E-07	1.00E+00	5.06E-09	1.04E-09	-3.39E-10	-3.26E-07	-4.78E-07	0.00E+00	2.95E-06	2.95E-06
33	0.00E+00	0.00E+00	2.54E-07	2.68E-06	5.44E-07	6.82E-09	-2.97E-07	1.00E+00	1.03E-08	2.89E-09	5.11E-10	4.91E-07	7.88E-07	0.00E+00	6.52E-06	6.52E-06
34	0.00E+00	0.00E+00	5.71E-07	9.52E-06	6.95E-07	2.77E-08	-1.52E-07	1.00E+00	1.79E-08	5.31E-09	1.47E-09	1.41E-06	1.56E-06	0.00E+00	1.18E-05	1.18E-05
35	0.00E+00	0.00E+00	7.01E-07	1.32E-05	5.29E-07	2.99E-08	1.42E-07	1.00E+00	2.03E-08	5.54E-09	8.03E-10	7.72E-07	6.30E-07	0.00E+00	1.29E-05	1.29E-05
36	0.00E+00	0.00E+00	5.31E-07	8.49E-06	4.35E-07	3.95E-08	5.67E-08	1.00E+00	1.91E-08	5.39E-09	1.07E-09	1.03E-06	9.69E-07	0.00E+00	1.21E-05	1.21E-05
37	0.00E+00	0.00E+00	4.36E-07	1.53E-05	4.89E-07	1.43E-07	-1.95E-07	1.00E+00	3.06E-08	8.64E-09	1.63E-09	1.57E-06	1.77E-06	0.00E+00	1.95E-05	1.95E-05
38	0.00E+00	0.00E+00	4.89E-07	9.70E-06	4.98E-07	2.61E-08	-3.48E-08	1.00E+00	1.78E-08	5.08E-09	1.10E-09	1.06E-06	1.09E-06	0.00E+00	1.14E-05	1.14E-05
39	0.00E+00	0.00E+00	4.98E-07	1.03E-05	5.21E-07	3.93E-08	-6.20E-08	1.00E+00	1.88E-08	5.19E-09	8.19E-10	7.87E-07	8.49E-07	0.00E+00	1.19E-05	1.19E-05
40	0.00E+00	0.00E+00	5.21E-07	1.41E-05	5.24E-07	8.11E-08	-8.36E-08	1.00E+00	2.51E-08	6.92E-09	1.04E-09	1.00E-06	1.09E-06	0.00E+00	1.59E-05	1.59E-05
41	0.00E+00	0.00E+00	5.24E-07	1.74E-05	5.16E-07	1.76E-07	-1.68E-07	1.00E+00	3.08E-08	8.53E-09	1.36E-09	1.31E-06	1.48E-06	0.00E+00	1.95E-05	1.95E-05
42	0.00E+00	0.00E+00	5.16E-07	9.98E-06	5.01E-07	1.68E-07	-1.52E-07	1.00E+00	1.78E-08	5.04E-09	9.7/E-10	9.40E-07	1.09E-06	0.00E+00	1.14E-05	1.14E-05
43	0.00E+00	0.00E+00	5.UIE-U/	1.2/E-U5	4.74E-07	3.29E-07	-3.02E-07	1.00E+00	2.22E-08	6.41E-09	1.48E-09	1.42E-06	1.72E-06	0.00E+00	1.44E-05	1.44E-05
44	0.0000000	0.000+00	4.74E-07	8.84E-00	4.43E-07	3.3/E-U/	-3.25E-07	1.000+00	1.322-08	4.305-09	1.55E-09	1.302-06	1.035-06	0.000+00	0.405.05	1.012-05
40	0.0000000	0.00E+00	4.42E-07	0.22E-00 2.21E.0E	4.11E-07	4.62E-07	-4.50E-07	1.00E+00	2.525.08	4.55E-09	1.55E-09	£ 20E 06	0.205.06	0.00E+00	9.40E-00	9.40E-06
40	0.00E+00	0.00E+00	9.20E-07	1.77E-04	1.64F-09	4.45E-05	-4.36E-05	1.00E+00	2.35E-07	9.49F-08	6.06E-08	5.83E-06	1.02F-04	0.00E+00	1.92E-04	1.92E-04
48	0.00E+00	0.00E+00	8.45E-10	2 72F-11	1.41E-09	4.61E-13	-5.67E-10	1.00E+00	9.09E-17	5.82F-12	5.43E-12	5.23E-00	5.79F-04	0.00E+00	6.08E-09	6.08F-09
49	0.00E+00	0.00E+00	1.14E-05	1.25E-06	4.32E-05	1.81E-08	-3.18E-05	1.00E+00	2.75E-07	1.88E-07	1.87E-07	1.80E-04	2.12E-04	0.00E+00	1.89E-04	1.89E-04
50	0.00E+00	0.00E+00	2.20E-05	2.05E-06	7.85E-05	4.00E-08	-5.66E-05	1.00E+00	5.09E-07	3.33E-07	3.21E-07	3.09E-04	3.65E-04	0.00E+00	3.45E-04	3.45E-04
51	0.00E+00	0.00E+00	1.03E-05	9.37E-07	3.72E-05	2.29E-08	-2.69E-05	1.00E+00	2.39E-07	1.67E-07	1.65E-07	1.59E-04	1.86E-04	0.00E+00	1.61E-04	1.61E-04
52	0.00E+00	0.00E+00	1.23E-05	2.19E-06	5.39E-05	3.93E-08	-4.16E-05	1.00E+00	3.44E-07	2.52E-07	2.49E-07	2.39E-04	2.81E-04	0.00E+00	2.30E-04	2.30E-04
53	0.00E+00	0.00E+00	1.70E-05	4.73E-06	9.46E-05	8.78E-08	-7.77E-05	1.00E+00	5.82E-07	4.47E-07	4.43E-07	4.26E-04	5.04E-04	0.00E+00	3.89E-04	3.89E-04
54	0.00E+00	0.00E+00	3.13E-05	1.62E-05	2.06E-04	2.58E-07	-1.75E-04	1.00E+00	1.21E-06	9.61E-07	9.55E-07	9.18E-04	1.09E-03	0.00E+00	8.14E-04	8.14E-04
55	0.00E+00	0.00E+00	7.77E-05	1.71E-04	1.59E-03	3.12E-06	-1.52E-03	1.00E+00	8.07E-06	6.26E-06	6.25E-06	6.01E-03	7.53E-03	0.00E+00	5.58E-03	5.58E-03
56	0.00E+00	0.00E+00	3.41E-04	1.13E-04	8.80E-04	2.48E-06	-5.41E-04	1.00E+00	4.14E-06	3.15E-06	3.14E-06	3.02E-03	3.56E-03	0.00E+00	2.76E-03	2.76E-03
57	0.00E+00	0.00E+00	6.19E-04	3.01E-04	1.37E-03	6.63E-06	-7.58E-04	1.00E+00	5.90E-06	4.29E-06	4.27E-06	4.10E-03	4.86E-03	0.00E+00	3.93E-03	3.93E-03
58	0.00E+00	0.00E+00	5.66E-04	1.42E-04	9.70E-04	7.10E-06	-4.12E-04	1.00E+00	3.36E-06	2.27E-06	2.23E-06	2.15E-03	2.56E-03	0.00E+00	2.24E-03	2.24E-03
59	0.00E+00	0.00E+00	4.37E-04	6.45E-05	6.74E-04	6.78E-06	-2.44E-04	1.00E+00	2.05E-06	1.31E-06	1.28E-06	1.23E-03	1.48E-03	0.00E+00	1.37E-03	1.37E-03
60	0.00E+00	0.00E+00	5.74E-04	1.02E-04	8.44E-04	1.18E-05	-2.82E-04	1.00E+00	2.45E-06	1.48E-06	1.43E-06	1.37E-03	1.65E-03	0.00E+00	1.64E-03	1.64E-03
61	0.00E+00	0.00E+00	2.10E-03	9.85E-04	2.75E-03	9.26E-05	-7.43E-04	1.00E+00	8.53E-06	4.15E-06	3.53E-06	3.39E-03	4.13E-03	0.00E+00	5.71E-03	5.71E-03
62	0.00E+00	0.00E+00	4.43E-03	4.84E-03	4.98E-03	1.03E-03	-1.57E-03	1.00E+00	1.73E-05	6.34E-06	3.45E-06	3.32E-03	4.89E-03	0.00E+00	1.22E-02	1.22E-02
63	0.00E+00	0.00E+00	5.68E-03	1.02E-02	4.09E-03	9.13E-03	-7.54E-03	1.00E+00	1.61E-05	6.38E-06	3.63E-06	3.49E-03	1.10E-02	0.00E+00	1.43E-02	1.43E-02
64	0.00E+00	0.00E+00	4.09E-03	2.64E-03	7.08E-04	1.04E-02	-7.07E-03	1.00E+00	1.28E-06	4.09E-07	8.47E-08	8.14E-05	7.15E-03	0.00E+00	2.90E-03	2.90E-03
65	0.00E+00	0.00E+00	7.16E-04	1.28E-04	5.41E-06	1.96E-03	-1.25E-03	1.00E+00	2.24E-08	1.10E-08	8.88E-09	8.54E-06	1.26E-03	0.00E+00	1.06E-04	1.06E-04
66	0.00E+00	0.00E+00	9.15E-06	5.61E-07	5.00E-08	4.98E-05	-4.0/E-05	1.00E+00	4.99E-11	1.41E-11	-1.81E-13	-1./5E-10	4.0/E-05	U.UUE+00	4.51E-07	4.51E-07
60	0.000+00	0.000+00	3.74E-Ub	1.000-08	2.19E-10	3.94E-06	-1.95E-07	1.000+00	7.245-05	3.000-12	7.02E-13	2.055.02	1.905-07	0.00E+00	7.295-09	7.295-09

*FIG. I–1.* Example of ANISN code output. Summary for Zone 8 by group including sum for all groups in line 68 volume = 1.09097E+04.

#### Annex II

# **EXAMPLE OF ORIGEN CODE OUTPUT**

# TABLE II–1. EXAMPLE OF ORIGEN OUTPUT SHOWING ISOTOPIC DATA FOR ONE REGION

1	OUTPUT UNIT = 6	PAGE 18
ORIGEN2 V2.1 (8-1-91), Ru * Activation of vessel clad — Power = 0.00000E+00 MW, I Nuclide table: Activity, curies	n on 08/24/10 at 19:38:21 thermal flux activation product Burnup = 0.00000E+00 MWD, 1 s material composition based on	s Flux = 3.94E+13 N/CM**2-SEC 0.10% Co SS304
	1/1/2013	7/1/2011
H-1	0.000E+00	0.000E+00
Н-2	0.000E+00	0.000E+00
Н-3	4.576E-04	4.205E-04
H-4	0.000E+00	0.000E+00
He-3	0.000E+00	0.000E+00
He-4	0.000E+00	0.000E+00
He-6	0.000E+00	0.000E+00
Li-6	0.000E+00	0.000E+00
Li-7	0.000E+00	0.000E+00
Li-8	0.000E+00	0.000E+00
Be-8	0.000E+00	0.000E+00
Be-9	0.000E+00	0.000E+00
Be-10	0.000E+00	0.000E+00
Be-11	0.000E+00	0.000E+00

1	OUTPUT UNIT = 6	PAGE 18		
B-10	0.000E+00	0.000E+00		
B-11	0.000E+00	0.000E+00		
B-12	0.000E+00	0.000E+00		
C-12	0.000E+00	0.000E+00		
C-13	0.000E+00	0.000E+00		
C-14	1.297E-04	1.296E-04		
1	OUTPUT UNIT = 6	PAGE 32		

TABLE II–1. EXAMPLE OF ORIGEN OUTPUT SHOWING ISOTOPIC DATA FOR ONE REGION (cont.)

ORIGEN2 V2.1 (8-1-91), Run on 08/24/10 at 19:38:21

\* Activation of vessel clad — thermal flux activation products

Power = 0.00000E+00 MW, Burnup = 0.00000E+00 MWD, Flux = 3.94E+13 N/CM\*\*2-SEC

	1/1/2013	7/1/2011	
Н-3	4.576E-04	4.205E-04	
Fe-55	2.306E-01	1.544E-01	
Co-60-3	1.675E-01	1.374E-01	
Ni-59	7.868E-04	7.868E-04	
Ni-63	9.347E-02	9.241E-02	
SUMTOT	4.928E-01	3.854E-01	
TOTAL	4.931E-01	3.856E-01	

# TABLE II–2. ACTIVITY, CURIES MATERIAL COMPOSITION BASED ON 0.10% Co SS304

#### Annex III

## LESSONS LEARNED IN THE DETERMINATION OF AN ACTIVATION SOURCE TERM

The information contained in this annex is based on lessons learned during the process of determining the source term for facilities that either have undergone decommissioning or for which decommissioning is being planned. The information is designed to provide practical examples.

#### III-1. GENERAL LESSONS LEARNED

#### III-1.1. Model input

The quality of the input data used in the activation calculations will affect the quality of the calculated results.

#### III-1.2. Physical model inputs

Several important input parameters are required in establishing an appropriate model for calculating the activation reactions for different steel components and biological shield structures in nuclear reactors. To create the geometric model of the structures, properly detailed technical drawings are necessary.

The configuration of a facility can undergo significant changes over its operational lifetime. For this reason, the implementation of a document management system at an early stage in the lifetime of a facility can be very useful in terms of subsequent decommissioning activities. The document management system can provide a process for cataloguing and protecting documents such as original construction drawings as well as those drawings and documents that provide information on facility modifications. The document management system might, for example, also require that records of these types be retained on the site to help ensure their long term availability.

The documentation used for physical model inputs needs to represent the facility configuration as it is at the time of decommissioning. The use of earlier or obsolete configurations could jeopardize the quality of the source term assessment results.

If drawings and manuals have been lost, it may be possible to obtain documentation from manufacturer or installation contractors, but the quality and applicability of the information may not be as good as the original on-site documentation. In other cases, the degradation of documents and drawings may make it difficult to read dimensions and other important details, and under these circumstances it may be necessary to estimate or infer the dimensions of interest from other locations on the drawing, or even from legible dimensions of the same item on a different drawing.

Employees who are approaching or considering retirement may warrant particular attention. It is not uncommon for long term operational staff to be aware of facility changes that may not have been formally recorded, or of upset conditions that may have occurred during the facility operation. In these circumstances, it is generally good to have personnel with this type of useful operational information document their knowledge.

#### III-1.3. Material data

It is not unusual to see the amount and distribution of impurities vary from component to component in the same nuclear facility. This situation may arise if the origin of the various components changes during the lifetime of the installation. For example, in the case of an accelerator, the origin for the magnets could change, and as a consequence the level of <sup>60</sup>Co in the stainless steel could vary from magnet to magnet owing to differing amounts of elemental cobalt in the original magnet castings. This variability could affect the reliability of the source term assessment, and for this reason either it needs to be recognized in the input data, or actual survey measurements need to be taken at the start of the decommissioning process to check for such possibilities.

#### III-1.4. Transport/activation modelling: lessons learned

At the point in the preparation of a final decommissioning plan where details about actual operational activities are being developed (e.g. component cutting procedures), there may be a requirement for more detailed activation data. Similarly, if there is a requirement on the part of the decommissioning operator to better determine the extent of those regions where the levels of activation products are significant, it may be that more advanced models and calculation methods are required. This could include, for example: (i) the use of more sophisticated computer codes (e.g.  $S_n$  or Monte Carlo) rather than codes based on diffusion approximations; and (ii) the subdivision of the geometry into more spatial regions.

#### III-1.5. Interpretation of results and conclusions

It can generally be assumed that activity calculations, if performed appropriately, can provide specific activity values with uncertainties and errors sufficiently low to allow their use in estimating the amount (mass and volume) of waste that will be produced during decommissioning, and that the calculated results can also be used for classification of the waste. However, the calculated results are best treated as a preliminary estimate and will not normally substitute for a thorough characterization of the wastes at the time of disposal.

#### III-1.6. Validation of results

It can be particularly useful to collect samples during the construction of a facility, or during the manufacturing of components, particularly for those structures and components that may later be exposed to activation processes during facility operations. These preoperational samples can then be analysed for various constituents, including trace impurities. The samples need to be correctly identified, stored and maintained during the lifetime of the facility so they can be analysed when needed. They also need to be maintained in a radiologically and chemically clean environment where they will not be subject to activation or contamination during facility operation.

# III–2. LESSONS LEARNED FROM APPLICATIONS TO NUCLEAR REACTORS

#### III-2.1. Material data

Besides the characteristics of the neutron flux to which components and structures are exposed, the nature and extent of activation primarily depends on the material composition of the exposed SSCs. Therefore, careful analysis and/or an examination of available data concerning material composition can be indispensable. Based on experience, trace elements and low percentage constituents such as cobalt or europium may be responsible for approximately 90% of the total activity in the irradiated structures and components. It also needs to be emphasized that the quality of the calculated results primarily depends on the quality of the data on material composition.

The results of activation calculations for those radionuclides important to waste classification (and subsequent cost estimates) can be very sensitive to actual and assumed elemental impurity levels. In order to generate high quality results, the direct use of chemical and radiochemical analyses of metals and other materials needs to be combined with a thorough understanding of the variability of the materials, their locations within the facility or component, and the neutron flux developed at the various locations. For example, the results of an in situ radiochemical analysis of biological shield concrete constituents can vary substantially from the data presented in NUREG/CR-3474 [III–1] owing to batch specific differences in the concrete and aggregate amounts, and the sources of the constituent materials, as well as differences in the batches of reinforcing steel. Quality assurance/control documentation for concrete is typically oriented towards material properties, and contains less information that is applicable to activity calculations than is the case with documentation for the metals used in structural and component construction.

#### III-2.2. Transport/activation modelling lessons learned

Input data for use by a transport or activation software package can be subject to typographical errors such as "O" versus zero (0) that are difficult to detect and that can result in a failure in the execution of the software run, or cause erroneous results. Software based two and three dimensional plots of the combinatorial geometry can be a useful tool for verifying/validating the spatial input data.

Although some of the codes yield information on the reliability of the results, the information generally only applies to the statistical reliability.

It is important to ensure that the data for the components and the corresponding material locations are correct for the intended model. Failure to correctly model absorber or void regions can lead to inaccurate results.

If a mesh is being employed in the model, it is important to ensure that the mesh is appropriate for the components of interest as well as for any transitions between regions and components.

If performing an  $S_n$  transport analysis, ensure that the microscopic cross-section library is appropriate for the type of system being analysed.

The appropriate selection of the boundaries which define the region where the activation process needs to be considered is also very important. Based both on previous experience on the part of the authors and on data in the international literature, it is considered advantageous to have the geometric boundaries of the calculation defined in such a way that all of the system structures and components that will be exposed directly to neutron irradiation are covered in detail in the model, for example, the reactor assembly with all of its components (i.e. the reactor pressure vessel, baffle/former, basket, and all the equipment for instrumentation and control), as well as those regions of the biological shield which are exposed to a neutron flux. Experience also shows that in some regions of the biological shield, backscattered neutrons can also cause activation through neutron streaming, and in particular that this may occur in the cavity between the pressure vessel and the biological shield. Therefore, as part of the modelling process, it may also be advisable to consider those components and regions which are not directly exposed to neutron irradiation.

Owing to the inhomogeneous nature of the neutron flux distribution in a reactor, it may be advisable to subdivide the modelled geometry into hypothetical spatial regions to facilitate the determination of the spatial distribution of the reaction rates. A properly chosen subdivision of the geometry can also be advantageous in handling the radioactive waste arising from the activation of different reactor elements and biological shield structures.

#### **III–2.3.** Interpretation of results and conclusions

Analyses of different activation calculation results show that the radionuclides which are responsible for the vast majority of the activity found in the stainless steel reactor structures shortly after shutdown (within a year) are produced from the original Fe, C, Co, Ni, Cr and Mn content of the structural materials. In the case of other steel structures (primarily the pressure vessel), the original Nb and Mo content plays a significant role as well, but the effect of the original C content is practically negligible (<sup>14</sup>C is produced from nitrogen). If the time dependence of the total activity is also considered, then it is important to note that the information about the original Fe, Co and Ni content of the materials is of very high importance because the radionuclides resulting from the neutron activation of these original constituents will largely determine the total activity of the structures in the period of 1 to 100 years after shutdown.

For the case of the biological shield structures, Fe, the main constituent of the reinforcing steel, has a definite contribution to the total activity within the first 100 years following the final shutdown. Other important radionuclides which can affect the manner in which waste is classified include various radionuclides of Co, Ca and Eu. Uncertainties in the concentrations of these radionuclides can limit the quality of the results for total activity.

The results for total and specific activity can be an important input to optimization planning, where comparisons can be made in terms of undertaking activities at different points in time. For example, estimates can be made of the expected dose rates at a pool surface as a function of time after facility shutdown where those exposures could originate from the convection of secondary waste particles during underwater plasma arc segmentation operations.

#### III-2.4. Validation of results

Typically, metal and concrete structures within the biological shield can be adequately characterized through activation calculations. In some cases (e.g. if the biological shield is extremely thick, i.e. on the order of several metres), it may be acceptable to limit the activation calculations to distances that lie within the actual physical boundary of the biological shield, but only as long as sample analysis is subsequently used to validate the calculations. However, for facilities having significant irregularities in the biological shield (e.g. penetrations) or experimental devices (e.g. beam ports, medical irradiation stations), the boundaries of the activation calculations may need to be extended beyond the external limits of the primary biological shield.

It is important that the distances used in dose rate measurements be accurately and precisely known. For example, in a reactor environment, dose rate surveys are frequently performed underwater, where substantial differences in shielding can occur with only a few millimetres difference in the location of the measurement. A light gauge plastic or non-shielding metal 'standoff' affixed to the detector can be helpful in ensuring that the detector is at a known and constant distance from the components of interest. The selection of survey locations needs to be considered in the context of transport code strengths and limitations as well as the components of interest.

#### III-2.5. Dose modelling lessons learned

It is important to consider and account for all source and shielding regions associated with in situ measurements and estimates. To the extent practical, it is best to obtain dose rate measurements being used for characterization purposes in a low background area.

The activity calculations can be used to estimate the potential doses to workers during the implementation of decommissioning activities, and include both direct exposures as well as any internal exposures resulting from ingestion or inhalation. The calculated results are important in assessing the dose rate levels in the vicinity of activated components. The calculations can also provide source term data for use in the development of safety analysis reports, and for addressing any unplanned events or upset conditions. For example, the specific activity values can provide input data for the determination of radioactive material dispersion models. The ability to estimate both external and internal dose values based on the source term is vital to being able to assess and manage the potential hazards that could arise from the activated materials. For example, the use of predicted external dose rate values is fundamental to selecting appropriate waste handling methods. Similarly, the shielding arrangements and other radiation protection measures for workers handling pieces of activated waste can be planned as well. Finally, cutting techniques, transport methods/casks, and long term storage requirements can be optimized based on these data.

# III–3. LESSONS LEARNED FROM APPLICATION OF SOURCE TERM ASSESSMENTS TO ACCELERATOR FACILITIES

During the planning phases of decommissioning, a preliminary or scoping assessment of the radiological committed dose can be calculated through the use of  $\omega$  factors [III–2] to develop an 'order of magnitude' estimate. The  $\omega$  factors give the dose rate per inelastic interaction above a certain threshold (e.g. 50 MeV) on contact with an extended and uniformly irradiated object, assuming uniform activation. This estimate does not include the contribution to the induced activity from thermal neutron activation.

To establish the source term for high energy accelerators, it is necessary to understand the possible mechanisms leading to induced radioactivity. In general, there are two predominant sources of activation: localized beam losses and distributed beam losses. Localized beam losses are mainly caused by the interaction of the beam with the materials of the beam line, and this occurs mainly at restrictions in the beam pipe aperture (e.g. collimators, beam detecting systems), or where machine elements intercept a fraction or the totality of the beam (e.g. targets, dumps). Distributed beam losses occur in any part of the accelerator and result from the interaction of the beam with the residual air particles in the vacuum chambers, or with the other beam particles in the case of colliders. These two main radiation sources can be augmented by less important, but more specific, phenomena characteristic of the type of accelerator. An example is described in the study in Ref. [III-3], where the source term for the LEP (Large Electron Positron Collider, an accelerator at CERN decommissioned in 2000) was assessed. In this electron collider, apart from the first two radiation sources, two other phenomena contributed to the radiation field that was responsible for material activation: the synchrotron radiation and the high energy X rays emitted by the superconducting radiofrequency system. The methodology used in this case to establish an a priori source term was to establish conversion coefficients from unit beam power lost in the material to induced specific activity at saturation. These conversion coefficients were evaluated for the most common materials in the accelerator (aluminium, copper, lead, stainless steel, and laminated iron and concrete). These conversion coefficients were validated by a specific experiment conducted on appropriately activated samples of the different materials and applied to predict the specific activity induced in the accelerator materials for a typical beam loss scenario. This method can be used in other

cases as long as good logging of the beam losses and a good understanding of the activation phenomena is available.

Activation in concrete is dominated by <sup>24</sup>Na (short decay times) and <sup>22</sup>Na (longer decay times). These radionuclides can be produced by either low energy neutron reactions (on elemental sodium) or by spallation reactions on silicon, calcium or other components. At longer decay times, other radionuclides increase in importance in the radionuclide inventory (i.e. <sup>60</sup>Co, <sup>152</sup>Eu, <sup>154</sup>Eu and <sup>134</sup>Cs). These radionuclides are produced by (n, $\gamma$ ) reactions on natural traces of cobalt, europium and caesium. Thus, the knowledge of the exact composition of the concrete in the facility, particularly with respect to trace elements, is key to having complete information on the source term.

#### **REFERENCES TO ANNEX III**

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#### Annex IV

# EXAMPLE OF THE VALIDATION OF NUMERICAL SIMULATIONS OF NEUTRON ACTIVATION

#### IV-1. BACKGROUND

As Electricité de France (EDF) is the only operator of French nuclear power plants, under French law, EDF is responsible for dismantling and decommissioning its plants. There are nine first generation plants which have been shut down, some for more than 20 years. These can be placed in four categories: six natural uranium gas cooled reactors, one heavy water reactor, one pressurized water reactor and one fast breeder reactor.

About 186 000 tonnes of radioactive waste will be produced from the dismantling and decommissioning of the first generation plants.

In France, five classes of nuclear waste are defined, with each class based on a particular level of activity and radiotoxicity: very low activity, low activity short life, low activity long life, intermediate activity long life and high activity long life.

Currently, the National Radioactive Waste Management Agency operates two disposal sites, one for very low activity waste and another for short life waste. However, two new sites will be required, one for graphite and the other for fission products, actinides and long life waste.

The distinction between 'long life' and 'short life' waste is based on a list of specific activity limits for 40 radionuclides. If one of these 40 specific activity limits is exceeded, the waste is classified as long life waste. If none of these limits are exceeded, a weighted specific activity level is used to separate very low activity and low activity short life waste. The weighted specific activity value is obtained by taking into account the levels of specific activity together with the levels of radiotoxicity for 143 radionuclides.

Numerical simulations are used to calculate the levels of neutron activation products, which in turn are used to predict the requirements for the dismantling processes and for radioactive waste management.

# IV–2. NUMERICAL SIMULATION METHODOLOGY FOR NEUTRON ACTIVATION

The methodology used by EDF for calculating activation by neutrons was developed by its Engineering Centre for Dismantling and the Environment (EDF-CIDEN), and is divided into four steps (see Fig. IV–1):

- (1) Development of a three dimensional multigroup neutron flux map. The mapping of the neutron flux is based on neutron propagation calculations. The codes used are MCNP [IV–1], developed by Oak Ridge National Laboratory in the United States of America, or TRIPOLI [IV–2], developed by the French Alternative Energies and Atomic Energy Commission. Both codes solve the transport equation, which is also referred to as the Boltzmann equation. The input data includes the microscopic cross-sections, the three dimensional geometry, the chemical compositions (without impurities) and a computed model of the neutrons emitted by the fuel assemblies. The neutron flux map is calculated at the nominal power rating conditions, and each flux is homogenized in a limited number of energy groups.
- (2) Calculation of the activities. The activities are calculated for each component or subcomponent of interest. The code used is DARWIN-PEPIN [IV-3] (developed by the French Alternative Energies and Atomic Energy Commission), which solves a system of Bateman equations. The input data include the three dimensional neutron flux map calculated in step one, the microscopic cross-sections, radioactive decay constants, the chemical compositions (with impurities) and the history of irradiation resulting from the daily power production. The output is the radioactive inventory for each component or subcomponent of interest based on a list of 143 radionuclides.
- (3) Waste classification. Based on the radioactive inventory of each component or subcomponent together with the waste classification criteria, an estimate of the quantities of waste that will be generated in each waste classification can be made. The classification process is primarily based on the levels of specific activity found for the 143 radionuclides.
- (4) Comparison between calculated and measured results. The completion of this step requires: (i) samples; (ii) the results of radiochemical analyses of those samples; and (iii) a tabulation of the measured results and the corresponding calculated results. Comparisons are then made by calculating the ratio of the calculated results to the measured results. A value of greater than 1 corresponds to an overestimated calculation, and a value of less than 1 corresponds to an underestimated calculation. Depending on the comparison of calculated to measured results, the input

data may be adjusted to create a revised simulation that better reflects the measured results.

#### IV-2.1. The Boltzmann equation

The Boltzmann equation (see Eq. (IV-1)) is used to simulate the propagation of neutrons from the fuel assemblies in order to build the three dimensional multigroup neutron flux map.

$$\vec{\Omega} \cdot \vec{\nabla} \Phi(\vec{r}, \vec{\Omega}, E, t) = Q(\vec{r}, \vec{\Omega}, E, t) + \int_{0}^{4\pi} \int_{0}^{\infty} \Sigma_{s}(\vec{r}, \vec{\Omega}' \to \vec{\Omega}, E' \to E)$$

$$\cdot \Phi'(\vec{r}, \vec{\Omega}', E', t) \cdot d\Omega' \cdot dE' - \Sigma_{t}(\vec{r}, E) \cdot \Phi(\vec{r}, \vec{\Omega}, E, t)$$
(IV-1)

The Boltzmann equation is a seven parameter equation which includes: the neutron flux, the three dimensional coordinates for a position in the geometry under study, the direction, the energy and the time. In reality, however, the time parameter is not considered because the propagation simulation corresponds to a time stable condition.

Without going into detail, there are four major components to the equation: (i) the transport operator; (ii) a term corresponding to the production of neutrons emitted by fission; (iii) a term corresponding to the scattering process



FIG. IV-1. EDF-CIDEN calculation methodology.

which results in a change in neutron direction and a loss of energy; and (iv) an absorption term.

A Monte Carlo method is used to solve the Boltzmann equation whereby a random series of numbers are used to simulate the behaviour of millions of neutrons. The code follows each neutron individually, from its initial emission to its disappearance as a result of leakage, absorption or fission.

#### IV-2.2. The Bateman equations

A Bateman equation (see Eq. (IV–2)) is used to simulate the evolution of the isotopic compositions. This is a multiparameter equation which includes the multigroup neutron flux, isotopic concentrations, radioactive decay constants and absorption cross-sections. The Bateman equation also includes parent and daughter nuclides.

$$\frac{\partial N_{i}}{\partial t} = -\left[\lambda_{i} + \sum_{j} \left[\sigma_{i \to j}(E) \cdot \Phi(E, t)\right]\right]$$

$$\cdot N_{i} + \sum_{k} \left[\lambda_{k \to i} + \sigma_{k \to i}(E) \cdot \Phi(E, t)\right] \cdot N_{k}$$
(IV-2)

This equation simulates both the neutron absorption reactions and the radioactive decay reactions. Figure IV–2 shows the 10 main neutron absorption reactions, and the seven main radioactive decay reactions. Depending on the nuclear library used, all of these reactions are taken into account in the Bateman equations.



FIG. IV-2. Main neutron absorption and radioactive decay reactions.

The system of differential equations is solved by the Runge–Kutta method, resulting in successive iterations using approximate solutions for each step.

## IV-3. CHOOZ A SIMULATIONS

Chooz A is a 300 MW(e) pressurized water reactor plant (shut down since 1993). Figure IV–3 provides an illustration of the underground facilities and structures (i.e. the cavern).

## IV-3.1. Input data

A three dimensional geometry was used in the Monte Carlo code to calculate the mapping of the neutron flux. Furthermore:



FIG. IV–3. Chooz A underground structures and facilities.

- The peripheral fuel assemblies were described pin by pin, whereas the internal fuel assemblies were represented as being homogeneous.
- All of the internal structures were fully described, including the different plates, the control rods, the guide tubes and the in-core instrumentation.
- The concrete vessel wall was modelled to a depth of 1 m.

The neutron sources as calculated with a core code were provided on a pin by pin basis with axial distributions.

The control rods were not included as part of the fuel assemblies.

Three temperatures were defined for the primary water: one for the core inlet, a second for the fuel assembly zone and a third for the core outlet.

For the propagation calculations used in calculating the neutron flux, values for isotopic compositions were limited to those of the major chemical constituents because impurities do not affect the propagation process. However, for the activation calculations, it is necessary to use the complete chemical compositions, including those impurities which can directly impact the parameters important in waste classification (i.e. specific activity and radionuclide).

The neutron flux map is calculated at the nominal power rating conditions, while the isotopic generation rates resulting from activation use the history of irradiation. The irradiation history was, however, simplified to a limited number of steps (see Fig. IV–4).

#### IV-3.2. Results of the calculations

The neutron propagation was computed three dimensionally using a continuous energy scale. The flux was then homogenized into a limited number of energy groups (315) and a limited number of tallies (150). Figure IV–5 illustrates this step.

For each of the tallies, the radioactive inventory was calculated taking into account the history of the operating conditions.



FIG. IV-4. Chooz A irradiation history.



FIG. IV–5. Chooz A three dimensional neutron flux mapping by numerical simulation.

Using these radioactive inventories together with the waste classification criteria, the Chooz A vessel can be depicted in terms of waste categories (i.e. very low level activity shown in blue, low activity shown in green and intermediate activity shown in red). Figure IV–6 depicts Chooz A in terms of waste classifications.

#### IV-4. VALIDATION OF THE CHOOZ A SIMULATIONS

To make comparisons between calculated and measured values, EDF-CIDEN uses calculated to measured (C/M) ratios. The reason for using C/M ratios is that each tally and each radionuclide has the same weight. As a consequence, the comparisons are not affected by the level of the flux or the level of the activity.

However, there are some difficulties in validating the simulations, including the following:

- The radionuclides result from the activation of both major and minor chemical elements.
- The uncertainties in the concentrations are different for the major and minor chemical elements.



FIG. IV-6. Chooz A calculated classification of irradiated waste.

- Information on the levels of impurities in the steel is generally not available from the suppliers.
- Different parents can produce the same daughter radionuclides.

In view of these difficulties, EDF-CIDEN supports the use of a general validation process for the numerical simulation schemes which utilizes the activation of 'standard' chemical elements. A variety of criteria need to be satisfied in order for chemical elements to qualify as standard, including the following:

- A high concentration level;
- A low degree of uncertainty in the concentration values;
- A good energy band cross-section range;
- An activation process that results in the production of radionuclides with significant half-lives;
- No significant problems in the measurement of the activated radionuclides.

For steel, the iron can be used as a standard, and for stainless steel, iron and nickel can be used as standards. Table IV–1 gives the average concentrations of these standard chemical elements along with the corresponding activation reactions and the radionuclides produced.

# TABLE IV–1. AVERAGE CONCENTRATIONS OF 'STANDARD' CHEMICAL ELEMENTS IN STEEL AND STAINLESS STEEL, AND THE ASSOCIATED ACTIVATION REACTIONS AND ACTIVATION PRODUCTS

Standard chemical element	Material	Average chemical concentration	Activation reaction	Radionuclide produced	Energy band cross-section	Half-life of radionuclide produced
	Steel	~ 98%	54E ( )55E	F 55	10 X/20 M X	2.7
Fe	_ Stainless steel	~ 68%	Fe(n,γ) <sup></sup> Fe	Fe-35	10 µe v/20 Me v	2.7 y
Ni		~ 11%	$^{62}\mathrm{Ni}(n,\gamma)^{63}\mathrm{Ni}$	Ni-63	10 μeV/20 MeV	100 y

## IV-4.1. Activation of 'standard' chemical elements

Figure IV–7 presents the C/M values calculated using the standard chemical elements (as defined in Section IV–4). The flux decreases in going from the internal components to the vessel coating, the vessel, and finally the external biological shield.

An analysis of Fig. IV–7 shows that:

- The numerical simulation produces an overestimation of the radioactive inventories.
- The extent of the overestimation is different in the different components being analysed.
- The extent of the overestimation increases with increasing distance from the fuel.

The overestimations can be attributed to:

- Measurement uncertainties;
- Nuclear data uncertainties;
- Monte Carlo statistical uncertainties;
- The assumptions, hypotheses and simplifications employed in the computational model.



FIG. IV–7. Calculated to measured ratios for the 'standard' chemical elements (as defined in Section IV–4).

Notwithstanding the above, these overestimations are considered reasonable and acceptable because the waste classifications are not based on the overestimated values.

#### IV-4.2. Activation of minor chemical elements and impurities

Figure IV–8 presents the C/M values calculated for the minor chemical elements and the impurities. Measured concentrations for the minor elements and impurities were averaged for use in calculating the radioactive inventories resulting from the activation process.

An analysis of Fig. IV-8 shows that:

- The numerical simulation produces an overestimation of the radioactive inventories.
- The extent of most of the overestimations is comparable to those found with the standard chemical elements.
- For some radionuclides, such as <sup>14</sup>C or <sup>3</sup>H, the C/M ratios are significantly different from those observed for the standard chemical elements.

For the most part, the C/M variability for the minor chemical elements is directly related to the variability in their concentrations. Based on this observation, the use of average values for concentrations based on multiple measurements of different samples would appear to be a good option.

As in the case of the standard chemical elements, these overestimations are considered acceptable because they do not affect the waste classifications. In fact, the waste classification is primarily based on the level of <sup>63</sup>Ni, which has its source in the activation of a standard chemical element.



FIG. IV-8. Calculated to measured ratios for minor chemical elements and impurities.

#### IV-5. CONCLUSION

This annex discusses the use of numerical simulations to model the activation of components irradiated by a neutron flux. EDF-CIDEN uses such simulations in planning for dismantling and radioactive waste management activities as applied to decommissioning.

To calculate the radioactive inventories resulting from neutron activation, EDF-CIDEN has developed a calculation methodology which comprises: (i) three dimensional mapping of the neutron flux; (ii) calculation of the activated radionuclide inventories; (iii) a waste classification methodology; and (iv) a comparison of calculated and measured values.

As an example, this annex focused on Chooz A, a 300 MW(e) pressurized water reactor plant. The comparisons between calculated and measured values show that the calculation methodology slightly overestimates the radioactive inventories produced by neutron activation.

The overall validation of the numerical calculation methodology is based on the activation of standard chemical elements. The results obtained for the activation of minor chemical elements and impurities indicated that the use of average measured compositions represents a valid approach.

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#### Annex V

#### **EXAMPLE OF A GRAPHITE ACTIVATION ASSESSMENT**

#### V-1. INTRODUCTION

This annex contains an example originating in part from the work done by the Lithuanian Energy Institute (LEI) for the IAEA coordinated research project on Treatment of Irradiated Graphite to Meet Acceptance Criteria for Waste Disposal (2010–2014). LEI activities for this project were mainly focused on the modelling of the spatial distribution of radionuclides in the RBMK-1500 reactor graphite components, and on sensitivity analyses.

The example presents the results of the modelling of the spatial distribution of neutron fluxes in the reactor RBMK-1500 graphite blocks, and the results for the axially (longitudinally) induced activity distribution in these graphite components. Modelling was performed for both Ignalina nuclear power plant (NPP) RBMK-1500 reactors, taking into account their individual operational histories.

#### V-2. BACKGROUND

Ignalina NPP, located in Lithuania, contains two RBMK-1500 reactors (Units 1 and 2). Unit 1 was commissioned in 1984 and went into final shutdown in December 2004. Unit 2 was commissioned in 1987 and went into final shutdown in December 2009. The RBMK-1500 is water cooled graphite moderated channel-type nuclear power reactor with a design power of 4800 MW(th). It has a graphite block structure (stack) that functions as the neutron moderator with fuel channels passing vertically through it. The reactor can be visualized as a vertical cylinder made up of 2488 graphite columns, constructed from graphite blocks of different heights.

#### V-3. ASSESSMENT METHODOLOGY

The assessment of neutron induced radionuclide activity levels requires, as a first step, knowledge of the spatial and energy distributions of the neutron flux throughout the system. The neutron flux is then used to calculate the activity levels in specific components based on the known initial concentrations of the elements in the material from which the component is manufactured, together with the mass of the components. The general methodology involved in the inventory calculation of activation products is diagrammatically represented in Fig. V–1.

The neutron flux modelling and subsequent inventory calculations (activation modelling) were performed using the MCNP5 and SCALE 5 (ORIGEN-S) computer codes.

The cross-section of the Ignalina NPP RBMK-1500 reactor vault is presented in Fig. V–2 [V–2]. The cross-sectional model developed for the neutron flux modelling and subsequent neutron activation calculations is labelled 12 in Fig. V–2.



FIG. V-1. General methodology for neutron induced activity calculations [V-1].



FIG. V-2. Cross-section of RBMK-1500 reactor vault [V-2].

#### V-3.1. Initial material composition

Neutron activation and the axial distribution of induced activity were modelled and estimated for the graphite blocks. The chemical compositions and elemental concentrations (main elements and impurities) for these reactor graphite components were based on the data presented in available scientific and technical literature for the specific material used (GR-280 grade graphite). It was assumed that the isotopic composition of each chemical element corresponded to the naturally occurring isotopic levels. Information on the material composition of the graphite blocks used in the Ignalina NPP reactors was lacking, and therefore a maximum level of impurities was assumed for neutron activation modelling purposes.
#### V-3.2. Modelling of the spatial and energetic distribution of neutron flux

The MCNP5 computer code was chosen for neutron flux modelling, as this code successfully solves neutron transport problems for almost any three dimensional geometry and material configuration. Various input data for the RBMK-1500 reactor were used in developing the MCNP model. The input data included the geometric configurations of the reactor components, material compositions and densities, and reactor operational parameters. These data were based on the information provided in various documents [V–2 to V–4]. One lattice segment model was developed in this example assuming that the fuel channel was loaded with UO<sub>2</sub> fuel with an average burnup of ~10 MW·d/kgU, and with 2.4% <sup>235</sup>U enrichment and 0.41% burnable  $Er_2O_3$  absorber.

A view of the cross-section of one lattice segment model ( $25 \text{ cm} \times 25 \text{ cm}$ ) of the RBMK-1500 reactor (labelled 12 in Fig. V–2), as developed with MCNP5 code, is presented in Fig. V–3.

The radionuclide inventory of the nuclear fuel was modelled using the computer code SAS2 from the SCALE 5 computer code system. It was assumed that a fuel assembly, consisting of two fuel bundles with UO<sub>2</sub> fuel ( $2.4\%^{235}$ U enrichment and 0.41% burnable Er<sub>2</sub>O<sub>3</sub> absorber) with a burnup of ~10 MW ·d/kgU is placed in a fuel channel. The parameters for the reactor components and the operating conditions (temperatures, dimensions, etc.) were set to correspond to



FIG. V-3. Cross-section of the modelled segment of the RBMK-1500 reactor (through the fuel bundle).

the conditions in the fuel channel at an average power level of  $\sim 2.61$  MW, which corresponds to that found for a nominal 4200 MW(th) reactor power.

The actual model developed (i.e. the vertical cut), including the graphite column with internal elements, the shield and support plates, and the top and bottom metal structures with the serpentine structures, together with geometric data, is presented in Fig. V–4. This model of one reactor lattice cell segment, using periodic boundary conditions for the side walls of the segment, corresponds to an infinite lattice made up of segments, and is suitable for modelling the neutron fluxes in the graphite components of the central (in radial direction) core (plateau). However, this approach is conservative because the impacts of the surrounding fuel channels and control rods in the vicinity of the segment are not considered.

In order to evaluate the characteristics of the neutron flux, particularly in terms of differences and variability, the separate reactor elements were modelled (bottom, central and top fuel channel parts, column of graphite blocks, shield and support plates, etc.), and then each of these elements was further subdivided into several separate zones along the reactor's axial direction. By calculating the neutron flux in this manner, and then analysing the variations in the flux characteristics, it is possible to optimize the second part of the induced activity calculations. The optimization is achieved by properly dividing the reactor structure into different zones, with each zone having specific activation conditions. This approach helps ensure a proper evaluation of the activation processes.

The neutron fluxes estimated with MCNP were grouped into three energy groups:

- Thermal neutrons, with energies up to 0.625 eV;
- Resonance neutrons, with energies in the range of 0.625 eV to 1 MeV;
- Fast neutrons, with energies above 1 MeV.

The neutrons were grouped into these energy groups because the activation modelling was to be performed with the ORIGEN-S computer code, which uses these groups.

#### V-3.3. Modelling of the neutron activation in the reactor materials

The ORIGEN-S computer code (SCALE 5 code system) was used for the neutron activation modelling. The code considers radioactive disintegration and neutron absorption (capture and fission) and enables the identification of isotopic content, activities and concentrations of neutron activated radionuclides. The ORIGEN-S code was used as a standalone program and the neutron flux input data required for the neutron activation modelling were taken from the neutron



- 1 Central part of fuel channel
- 2 Top part of fuel channel
- 3 Bottom part of fuel channel
- 4 Graphite blocks
- 5 Steel shield plate (block)
- 6 Steel support plate (block)
- 7 Bottom steel plate of top metal structure
- 8 Top steel plate of bottom metal structure
- 9 Serpentinite filling of top metal structure
- 10 Serpentinite filling of bottom metal structure
- 11 Top steel plate of top metal structure
- 12 Bottom steel plate of bottom metal structure
- 13 Graphite rings/sleeves
- 14 Top fuel bundle
- 15 Bottom fuel bundle
- 16 Centre of the reactor core (zerc mark in axial direction)

FIG. V-4. The analysed segment of the RBMK-1500 reactor, developed with the MCNP code.

flux modelling results (i.e. thermal neutron flux, and weighting factors for fast and resonance fluxes).

The 'yearly basis' operational histories (with a smaller more detailed scale for the last four years) for the Ignalina NPP Unit 1 and Unit 2 reactors were used for the neutron activation modelling (Fig. V–5 presents the operational history of Unit 1; a similar plot was constructed for Unit 2).

The graphite structures of the two Ignalina NPP reactors were modelled separately. These models indicated differences in the activation inventories of the two graphite structures, which, it was determined, result from different operational histories.

# V-4. RESULTS AND DISCUSSION

### V-4.1. Spatial and energetic neutron flux distributions

The axial and radial distributions of the modelled neutron flux in the graphite blocks are presented below. The modelled flux represents reactor operation at a nominal 4200 MW(th) (i.e. at  $\sim$ 2.6 MW(th) for each fuel channel), with the same value being used for both Ignalina NPP reactors. Furthermore, the modelled fluxes, as presented here, are normalized to the maximum value of the neutron flux presented in the figure. The top and bottom 0.5 m thick layers of the graphite stack in the axial direction are called the top and bottom reflectors, respectively, while the remaining 7 m thick portion of graphite is referred to as the active core.



1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997 1998 1999 2000 2001 2002 2003 2004

FIG. V–5. Ignalina NPP Unit 1 reactor operational history data for the period 1984–2004 [V–5].

#### V-4.1.1. Radial (lateral) distribution of neutron fluxes

Neutron fluxes presented in this section are averaged over a 50 cm high section of the modelled segment (i.e. an axial range of -150 cm to -100 cm from the centre of the reactor core (see Fig. V-4 for details)) and show the radial distribution of the longitudinally averaged flux for all of the modelled components in the segment.

The radial distributions of thermal, resonance and fast neutron fluxes calculated in the one cell model (averaged over the axial range of -150 cm to -100 cm from the centre of the core) are presented in Figs V–6, V–7 and V–8, respectively.

Results from the one cell model (see Fig. V–6) clearly show that thermal neutrons are dominant in the graphite block (where moderation of the fast and the resonance neutrons generally takes place). However, the thermal neutron flux is lower in the fuel channel (marked with black circles in Fig. V–6) and in the graphite rings/sleeves (graphite ring/sleeve is represented as  $\sim$ 1.2 cm thick circular region just outside the marked fuel channel). The region beyond the graphite ring/sleeve represents the graphite block. The absorption of thermal neutrons in the fuel elements inside the fuel channel is well modelled, with 18 circular zones visible (fuel elements, see Fig. V–4) where thermal neutron flux is lowest.



FIG. V-6. Radial distribution of the thermal neutron flux in the RBMK-1500 reactor (one cell model).



FIG. V–7. Radial distribution of the resonance neutron flux in the RBMK-1500 reactor (one cell model).



FIG. V–8. Radial distribution of the fast neutron flux in the RBMK-1500 reactor (one cell model).

Figure V–8 presents the radial distribution of the fast neutron flux in the modelled reactor segment. The fast neutron distribution is opposite to that of the thermal neutron flux (i.e. the fast neutron flux is highest in the region of the fuel elements inside the fuel channel, where uranium fuel fission takes place). In moving radially away from the fuel channel, the fast neutron flux decreases. It is lowest at the edges of the modelled segment as a result of the neutron moderation taking place in the graphite components.

The radial distribution of the resonance neutron flux, presented in Fig. V–7, shows no unexpected features when compared to the thermal or fast neutron fluxes. The intensity of the flux is almost uniform in the radial direction of the graphite components, being slightly higher in the graphite rings/sleeves.

Figures showing the radial distributions of the various types of neutron fluxes are useful for visualization (interpretation) of the results, and help confirm that the models are predicting features that are in line with expected features. However, the figures are not directly useful for neutron activation modelling purposes.

# V-4.1.2. Axial (longitudinal) distribution of neutron flux

The neutron fluxes presented in this section are averaged over the whole cross-section of graphite blocks in the lateral (radial) direction. The plots indicate the axial distribution of the laterally averaged fluxes in the column of graphite blocks.

For convenience, the axial distance from the centre of the reactor core is shown on the ordinate (y) axis, with the centre of the core located at y = 0.

The results of the neutron flux modelling show that thermal and resonance neutron fluxes are dominant in the column of graphite blocks; however, the thermal neutron flux is more intense than the resonance neutron flux in some regions (see Fig. V–9).

The fast neutron flux is lower than that of the resonance neutrons, although the fast neutron flux distribution along the axial direction shows the same types of variation as found in the resonance neutron flux. As expected, there are two maxima and one minimum in the distribution profile for both the fast and resonance neutron fluxes, features which correspond with the points at which the fuel bundles are connected to the fuel assembly. In this region, the fast and resonance neutron fluxes are both slightly lower than their maximum values in the axial distribution. At the edges of the graphite block columns (top and bottom reflector blocks), the fast and resonance neutron fluxes are more than an order of magnitude lower than their maximum values.

For the thermal neutron flux, there is only one maximum in the flux distribution, and that maximum is located in the central part of the reactor core. In

moving axially further from the reactor core centre, the thermal fluxes decrease monotonically, and at the graphite column edges (i.e. at the top and bottom reflectors), the flux is several times lower than the maximum value.

# V-4.2. Neutron induced activities

For the neutron activation modelling of the graphite components, the variation in activity along the axial direction of the components was assessed. The assessment process involved: (i) identifying the activation products (radionuclides); and (ii) determining the activity levels at the time of reactor final shutdown (RFS) as well as at various times after RFS. The list of radionuclides found in the graphite block column is presented in Figs V–10 and V–11. The list includes only those radionuclides that show activity levels that are greater than  $10^{-30}$ % of the total specific activity at 2 years after RFS. This approach avoids showing too many of the short lived radionuclides which could interfere with assessing those radionuclides of primary concern in the decommissioning process.

# V-4.2.1. Unit 1 graphite blocks

For the purposes of modelling, the levels of impurities in the graphite blocks were set to maximum levels based on published information for graphite analyses. The resulting model shows that the total specific activity in the graphite



FIG. V–9. Axial distribution of neutron fluxes in the column of graphite blocks.



FIG. V–10. Principal radionuclides and their change in activity levels in the graphite blocks during the 5 year period following reactor final shutdown (Unit 1).



FIG. V–11. Principal radionuclides and their change in activity levels in the graphite blocks during the 5 year period following reactor final shutdown (Unit 2).

blocks at 2 years after RFS (Ignalina NPP Unit 1 reactor) within the top and the bottom reflectors and the active zone is almost the same as that at the time of RFS ( $1.01 \times 10^8$  Bq/g vs  $1.38 \times 10^8$  Bq/g) (see Fig. V–12).

After a cooling period of 5 years, the specific activity decreases by a factor of about 1.5, but the distribution profile stays almost the same. The maximum activity is observed in the central region of the graphite block column (Fig. V–12), but this distribution profile is different from that of the thermal neutron flux (Fig. V–9) (i.e. the total specific activity of the top and bottom reflector blocks is only ~1.3 and ~1.2 times lower, respectively, than the maximum activity in the active core blocks).

The principal radionuclides and their values as averaged over the height of the graphite block column as a function of time after RFS are presented in Fig. V–10.

After a 5 year cooling period, <sup>3</sup>H, <sup>55</sup>Fe, <sup>60</sup>Co, <sup>14</sup>C and <sup>36</sup>Cl are the most prevalent radionuclides in the graphite blocks in terms of radioactivity. The total specific activity is predominantly determined by short lived <sup>3</sup>H and <sup>55</sup>Fe during the 5 year cooling period, while <sup>14</sup>C has the highest activity among the long lived radionuclides.



FIG. V–12. Axial distribution of the total specific activity in the graphite blocks at 2 and 5 years after reactor final shutdown (Unit 1).

#### V-4.2.2. Unit 2 graphite blocks

The behaviour found with the Ignalina NPP Unit 2 reactor graphite blocks is similar to that found with Unit 1, but the induced activities are slightly higher. For the purposes of modelling, the levels of impurities in the graphite blocks were set to maximum levels based on published results for graphite analyses. The resulting model shows that the total specific activity in the graphite blocks at 2 years after RFS (Ignalina NPP Unit 2 reactor) within the top and the bottom reflectors and the active zone is almost the same as that at the time of RFS (1.08 × 10<sup>8</sup> Bq/g vs 1.40 × 10<sup>8</sup> Bq/g) (see Fig. V–13).

After a cooling period of 5 years, the specific activity decreases by a factor of about 1.5, but the distribution profile stays almost the same. The maximum activity is observed in the central region of the graphite block column (Fig. V–13), but this distribution profile is different from that of the thermal neutron flux (Fig. V–9) (i.e. the total specific activity of the top and bottom reflector blocks is only ~1.2 and ~1.1 times lower, respectively, than the maximum activity in the active core blocks).

The principal radionuclides and their values as averaged over the height of the graphite block column as a function of time after RFS are presented in Fig. V–11.



FIG. V–13. Axial distribution of the total specific activity in the graphite blocks at 2 and 5 years after reactor final shutdown (Unit 2).

As was the case with Unit 1, after a 5 year cooling period, <sup>3</sup>H, <sup>55</sup>Fe, <sup>60</sup>Co, <sup>14</sup>C and <sup>36</sup>Cl are the most prevalent radionuclides in the graphite blocks in terms of radioactivity. The total specific activity is predominantly determined by short-lived <sup>3</sup>H and <sup>55</sup>Fe during the 5 year cooling period, while <sup>14</sup>C has the highest activity among the long lived radionuclides.

# V-4.2.3. Comparison of induced activities

In comparing the modelled specific activities of the Unit 1 and Unit 2 graphite components (same assumed compositions for both), the latter have slightly higher activities. This difference can be directly attributed to differences in the operational histories of the units (i.e. Unit 2 operated for a slightly longer time producing higher thermal power).

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