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# Nuclear energy — Nuclear fuel technology — Theoretical activation calculation method to evaluate the radioactivity of activated waste generated at nuclear reactors

*Energie nucléaire — Technologie du combustible nucléaire — Méthode théorique de calcul de l'activation pour évaluer la radioactivité des déchets activés produits par les centrales nucléaires*



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# Foreword

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The committee responsible for this document is ISO/TC 85, *Nuclear energy, nuclear technologies, and radiological protection*, Subcommittee SC 5, *Nuclear fuel cycle*.

# Introduction

This International Standard presents guidelines on activation calculation methods for evaluating the radionuclide content of activated waste generated at nuclear reactors.

This International Standard addresses the basic process of planning, executing, and reporting of results for itemized component characterizations (point method) based on neutron source estimation and component elemental compositions and physical parameters and usage in the reactor. This International Standard also introduces the range method that extends the point method to define a radionuclide distribution applicable to a collection of components of similar types and exposure histories that take into account stochastic variations of the input parameters for material composition, neutron fluence rates, and exposure histories applicable to the ranges of these parameters found in the collection.

# Nuclear energy — Nuclear fuel technology — Theoretical activation calculation method to evaluate the radioactivity of activated waste generated at nuclear reactors

## 1 Scope

This International Standard gives guidelines for a common basic theoretical methodology to evaluate the activity of radionuclides in activated waste generated at nuclear reactors using neutron activation calculations.

The evaluation of any additional activity contributed by deposited contamination is not addressed in this International Standard.

## 2 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

**2.1**
**activation calculation**
method of theoretical calculation for determining the radioactivity induced by neutron irradiation



**2.2**
**activated waste**
radioactive waste which contains radioactivity induced by irradiation



EXAMPLE Control rod, channel box, burnable poison, core support structures, reactor internal structures, and materials in close proximity to the reactor core, etc.

Note 1 to entry: It can also contain additional radioactivity in the form of surface contamination.

**2.3**
**difficult-to-measure nuclide**
nuclide whose radioactivity is difficult to measure directly from the outside of the waste packages by non-destructive assay means

[SOURCE: ISO 21238:2007, modified]

EXAMPLE Alpha-emitting nuclides, pure beta-emitting nuclides, and characteristic X-ray-emitting nuclides.

**2.4**
**control index**
index which has a constant relationship with the irradiation conditions affecting the activity concentration of the nuclide contained in the activated waste and enables the calculation of the activity concentration of the target radionuclide by the use of a conversion factor

EXAMPLE Fuel burnup.

**2.5**
**key nuclide**
gamma-emitting nuclide whose radioactivity is correlated with that of difficult-to-measure nuclides and can be readily measured directly by non-destructive assay means

[SOURCE: ISO 21238:2007, modified]

EXAMPLE $^{60}Co$.

 

**2.6**
**parent element**
chemical element which produces a target radionuclide via neutron irradiation

**2.7**
**target radionuclide**
radionuclide of which the activity and/or concentration has to be declared for disposal or transportation of waste packages

**2.8**
**neutron fluence rate**
at a given point in space, the number of neutrons incident on a small sphere in a small time interval, divided by the cross-sectional area of that sphere and the time interval

[SOURCE: ISO 31-10:1992, modified]

# 3 Theoretical evaluation method

## 3.1 General methodology

The following two methodologies can be applied for estimating the radioactivity of the activated waste:

— Point method, a technique applicable to calculate the radioactivity concentration in a representative piece or specific point of an activated waste item;



— Range method, a technique that is an extension of the point method applicable to a class of activated component of similar property and exposure condition to calculate the average radioactivity of a set or collection of activated wastes by evaluating the range of its radioactivity concentrations typical of that set.



## 3.2 Point method

Point method provides the basic structure for performing activation calculations. It is generally performed on an item by item basis using directly applicable or best estimate values for key parameters, including neutron flux and material specification along with specific information on history of usage.

This method can be used for the evaluation of all kinds of activated wastes, including in-core hardware and reactor internals. This method, in general, offers more precision on specific items and can be necessary in the situation where activated wastes are close to the disposal limits. This method is most often applied with corroborative dose rate survey and normalization with dose-based key nuclide estimates.

NOTE See Annex B.

## 3.3 Range method

### 3.3.1 General

The neutron and irradiation conditions of the target activated waste vary depending on the neutron fluence rate at its physical position in the reactor. The total radioactivity of the whole activated item(s) can be estimated by repeating the activation calculation to cover all the necessary conditions of the neutron irradiation among the whole activated item of the specified type. This provides typical or average values and distribution.

The radioactivity concentration of some types of activated waste has a close relationship with the fuel burnup (e.g. components associated with fuel elements). Once equilibrium has been reached, the radionuclides produced in the same part of the same activated waste have constant composition ratios because those parts have the same elemental composition and irradiation conditions.

 

Where reactor components are installed at a fixed location in the reactor (e.g. reactor pressure vessel) with a specified elemental composition, only the neutron fluence rates differ depending on the axial and radial position of this location.

The following three theoretical evaluation methods are applicable as typical range methods:[1]

— Conversion method;

— Correlation method;

— Distribution evaluation method.

NOTE See Annex C.

### 3.3.2 Conversion method

In activated waste such as channel boxes and burnable poison which are used as fuel assembly parts, the induced radioactivity can be closely correlated with some common reactor control parameters such as fuel burnup, since the cases where the items are of similar design and material, remain in the reactor for the same length of time, and are subject to the same neutron fluence as the fuel.

In this method, the relationship (conversion factor) between the control index (such as fuel burnup) and the radioactivity concentration of such fuel assembly parts can be calculated by a series of activation calculations which cover the possible range of burnup variations. The radioactivity concentration of the activated waste can then be estimated by multiplying the control index such as burnup and the conversion factor within its valid range.



NOTE See Annex C.

### 3.3.3 Correlation method



The correlation method can be used if a particular part or individual item of an activated group is observed to have composition ratios of radionuclides produced simultaneously by irradiation that are constant once equilibrium has been reached within a specified range because the elemental composition, neutron, and irradiation conditions (times) of the particular part are very similar.

Therefore, the correlation between the difficult-to-measure (DTM) nuclides in the whole of the activated waste and the key nuclides produced simultaneously is evaluated by a series of activation calculations which cover the elemental composition, neutron, and irradiation conditions of several specific parts of several activated wastes of the same kind. The ratios between the key nuclides and the DTM nuclides are calculated by evaluating this correlation, and the radioactivity concentration of each nuclide in the activated waste can be calculated by multiplying the ratio between the key nuclides and the DTM nuclides by the radioactivity concentration of the key nuclide. Note that the post irradiation decay time should be considered in this method since the ratio between the key nuclides and the DTM nuclides changes over time due to the difference in decay half-life.

NOTE See Annex C.

### 3.3.4 Distribution evaluation method

Fixed reactor components are activated by direct neutron irradiation in the reactor. In the case of such activated wastes, the elemental composition and irradiation conditions (time) can be considered to be similar for all items of the group, and only the neutron fluence rate differs depending on their installation locations in the reactor.

In this method, the radioactivity concentration distribution and range of each radionuclide in all activated wastes can be calculated by a series of activation calculations which completely cover the neutron fluence rate at the installation location of the activated waste. The average radioactivity concentration of each nuclide in the waste can then be calculated based on the resulting radioactivity concentration distribution.

NOTE See Annex C.

# 4 Calculations

## 4.1 General

The basic process for performing activation calculations for the purpose of estimating radionuclide concentrations in activated wastes involves several steps.

a) Establish the context. This defines the purpose of the calculation, the radionuclides of interest, the accuracy and precision required, the basic geometry, and the overall scope of the required calculations. This is an important first step for selecting an appropriate calculation methodology and input parameters (e.g. involved materials, quantity of items, similarity of items, target waste form, accessibility of sampling, etc.).

b) Select the calculation methodology, e.g. point or range method. The selection depends on the context of the calculation and the availability of input data.

c) Select and determine the input parameters. The input parameters and calculation boundary conditions depend on the chosen calculation methodology. Conversely, the availability of data can influence the selection of calculation methodology.



d) Perform the calculation(s) using the selected methodology.

e) Process the raw results of the calculation(s) to determine correlation factors, conversion factors, etc., depending on the chosen methodology.



## 4.2 Selection and determination of input parameters and conditions

### 4.2.1 Input parameters

A general procedure for setting input parameters and conditions can be established to allow point-based or range-based calculation methodologies. Activation calculations require a number of basic input parameters and conditions as listed below:

— elemental composition;

— neutron fluence rates;

— irradiation history (integrated exposure/decay time).

### 4.2.2 Elemental composition

Parent chemical elements are selected based on the context and scope of the calculation and the component materials involved (e.g. steel alloys). Elemental composition data on those parent elements can then be collected from a variety of sources for use in the subsequent activation calculations.

a) Selection of parent elements

The list of parent elements is selected for each kind of activated waste using one or more of the following concepts.

— The initial list of parent elements is assembled from the known basic chemical composition of the material being evaluated (e.g. steel alloys), along with elements which are known or suspected to be present as contaminants or in trace amounts.

 

— The elements which produce radionuclides that are significant in the safety assessment (including those used as key nuclides for scaling other nuclides) should be specifically included in the list of parent elements. Consideration should be given to key nuclides with a sufficiently long half-life, such that the half-life does not significantly affect the ratio between the nuclides over the evaluation timeframe.

The parent elements can be screened out using one or more of the following steps.

— Radioisotopes can be screened out from the original list of parent elements to be used in the activation calculations.

  EXAMPLE Radioisotopes which are produced after activation of material such as Pu, etc.

— Elements which do not produce radionuclides of interest to the context of the calculation can be screened out from the list of parent elements.

— Elements which are demonstrated to be removed during the material refining process can be screened out from the list of parent elements. However, often the element cannot be completely removed and the residual trace amount can still be significant for the activation calculation, depending on the scope and context of the calculation.

— Elements which result in only a very small contribution to the short-term or long-term risk or result in radionuclides of short half-life can normally be screened out from the list of parent elements, depending on the scope and context of the calculation.

b) Collection of elemental composition data



Elemental composition data on the waste can be collected using one (or more) of the following methods, which is selected in consideration of the kind and material of the waste and of the context and scope of the calculation:



— direct elemental analysis of an actual sample of the original material (e.g. one preserved for quality management purposes) or a sample of the same kind of material;

— collection of literature data and mill sheets which show the results of element analysis of the same kind or similar materials;

— collection of elemental composition data given in the material specifications for the original material. (If original material specifications are not available, it would be acceptable to use the national standard material specification or other recognized standard applicable to the material being evaluated.)

c) Selection of input elemental composition

The elemental composition for the material to be evaluated can be set using one of the following methods.

— Set representative values. The representative (or best estimate) values of the chemical element concentrations are set based on the chemical element data collected on the parent elements of the radionuclides to be evaluated. This is normally used for the point method.

— Set a concentration range. The minimum and maximum chemical element concentrations are set in consideration of the concentration distribution based on the chemical element data collected on the parent elements of the radionuclides to be evaluated. This is normally used for the range method.

— Set a concentration distribution. The representative chemical element concentration distribution is set in consideration of the concentration distribution based on the chemical element data collected on the parent elements of the radionuclides to be evaluated. This is normally used for the range method.

NOTE See C.5.

 

#### 4.2.3 Neutron fluence rates

The neutron flux and energy spectrum shall be determined using a suitable neutron transport computer code for the activated material accounting for its position relative to the reactor core. The code should be suitably matched to the requirements of the calculation in context of modelling detail and overall accuracy. Alternative methods including Monte Carlo simulation of the transport process can be justified in instances where additional detail or corroboration is required.

NOTE See C.6.

#### 4.2.4 Irradiation history

The irradiation time and non-irradiation time during the calculation timeframe under consideration (e.g. reactor operating time and post-irradiation decay time) can be set in either of the following two methods for the activated waste to be evaluated. The overall calculation timeframe could involve several cycles of irradiation and non-irradiation time.

a) Setting a detailed irradiation history individually for each waste

   The irradiation history is set in detail for each activated hardware item, based on its individual history. This is normally used for the point method.

b) Setting a representative irradiation history

   Irradiation history, which is considered to be adequate or conservative for a group of activated materials, are set based on the irradiation history of a representative or limiting item of the group.



When the irradiation history is used as input to further calculations by the Conversion method, Correlation method, or Distribution evaluation method, a range of the irradiation conditions can be set which are representative of several activated materials, instead of setting detailed conditions for individual materials.



This is normally used for range method.

NOTE See C.7.

### 4.3 Activation calculations

#### 4.3.1 Calculation code

The activation calculation code should be verified in accordance with the user's quality management system. Users should understand and be familiar with the methodology and appropriately trained in the use of the program and its limitations.

EXAMPLE ORIGEN code, etc.

#### 4.3.2 Setup input data

The input data for activation calculation listed below (for point or range method) are required for each theoretical calculation method to be applied. In accordance with 4.2, these data are set for each kind of activated waste to be evaluated:

— elemental composition;

— neutron fluence rates;

— irradiation history (integrated exposure/decay time).

When the range method is applied, input data for each individual calculation and condition can be selected at random within the range of the input data distribution in 4.2 and can be set as the input conditions for the activation calculation. Alternatively, input data representative of each condition can be set as the input conditions for the activation calculation.

#### 4.3.3 Determining the number of calculations

The number of calculations can be determined by one of two methods:

a) Point method

The required calculation number should be determined case by case.

(e.g. for a large or complex object, it is necessary to divide it into several segments for calculations or use an average or representative value, if the neutron fluence or materials can vary in different parts of the object.)

b) Range method

When the range method is applied, the number of activation calculation results obtained should be adequate for their use as evaluation data for determining the radioactivity concentrations. Whether their number is adequate or not can be judged in consideration of the number of the activation calculations made and the changes in the stability of the statistical values obtained from these activation calculation results.

### 4.4 Validation and uncertainties

#### 4.4.1 Validation



Validation involves determining the accuracy and applicability of the software results with respect to its intended application. Only validation can evaluate such things as the level of accuracy of physical approximations, the applicability of physical correlations, the appropriateness of numerical method approximations, etc.



Validation should be performed using software that is under configuration management and has a clear version number. It is normally performed by the user of the software for a specific application.

Validation confirms that a calculation can be consistently and correctly conducted by demonstrating (with objective and documented evidence) that the calculation code and calculation routine of the theoretical calculation method produce the expected results for a given input. This can be done, for example, by applying the calculation code to known test cases, or by comparing the results with those of an alternate calculation method that has been previously validated or has a known analytical solution.

NOTE 1 It is important to make a distinction between software “verification” and “validation”. Verification is the step where the software is checked against its specifications. This is normally done by the developer of the software prior to delivery to the user.

NOTE 2 See A.4.

#### 4.4.2 Dealing with uncertainties

The allowable level of uncertainty depends on the particular radionuclides and how the waste is ultimately treated in disposal. An estimation of accuracy and uncertainty of the calculation result should be performed in order to quantify the representativeness of the theoretical calculation carried out. Accuracy represents how close the theoretical calculated value is to the real value. As such, it is a measure of the bias, and many times a degree of conservativeness is established to safely guarantee of the limits involved (Waste Acceptance Criteria, radiological protection, transport processes, etc.). Uncertainty represents the variability around the consigned value. A highly precise value is characterized by a low uncertainty and vice versa.

Representativeness can be considered to be a parameter which accounts for both the conservativeness/bias and the uncertainty around a value. It gives an image of distance and variability of the theoretical calculated value to the actual value.

NOTE See Annex D.

## 4.5 Records

Reports should be presented in such a way as to provide a traceable account of the work performed with data sources and assumptions clearly identified. This allows the calculation to be easily reproduced by others for validation purposes.

Results shall be reported in a concise, easy to interpret, manner that allows the result to be understood without additional manipulation. Reporting units should be specified in the record and in any event should be in International System of Units unless specifically directed to use alternative units.

NOTE See Annex E.

# Annex A
(informative)

# Application and example of the theoretical activation calculation method

## A.1 General

Annex A provides explanatory notes and gives examples and practices to assist the understanding or use of this International Standard.

## A.2 Basic application of the theoretical activation calculation method

### A.2.1 General

Activated radioactive waste from reactor core areas generally has significant levels of radioactivity. The empirical evaluation methods, relying on waste sampling and radiochemical analysis, are often limited for such waste by potentially high radiation exposures to involved labour.



The theoretical evaluation method using activation calculations provides a reasonable alternative method for determining the concentrations of radionuclides produced as a result of activation by neutron irradiation inside and near the reactor core. In this method, the types and amounts of the radionuclides are theoretically determined by the use of activation calculations.

Performance of theoretical evaluation depends on the neutron fluence rates local to the subject material and irradiation history of exposure. The radioactivity concentrations of the materials are determined from the calculated results or the evaluation factors determined from those results.

Figure A.1 shows a basic step by step procedure for applying the theoretical evaluation method. These steps are discussed in more detail below.

### A.2.2 STEP 1: Setting the basis for the calculation

The context, scope, and purpose of the calculation need to be established prior to starting the calculations. This assists in determining the radionuclides of interest, the irradiation geometry, parent materials, accuracy and precision required, etc.

The theoretical evaluation of the radioactivity concentrations of activated waste is dependent on knowledge of the reactor operating conditions (irradiation conditions) and the characteristic properties (physical and chemical) of the activated materials being evaluated. This includes the following principal parameters:

— elemental composition of the exposed material;

— neutron fluence rates (including flux and spectrum);

— irradiation history (including irradiation and decay times).

Once the context, scope, and purpose have been determined, the relevant data should be collected. This process is further described in Annex C.

 