

Qualification of scientific computing tools used in the nuclear safety case – 1st barrier

Produced jointly with
The French Institut de
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Preamble

The ASN collection of guides comprises documents intended for professionals concerned by the nuclear safety and radiation protection regulations (licensees, users or transporters of ionising radiation sources, general public, etc.). These guides can also be issued to the various stakeholders, such as the local information committees (CLIs).

Each guide sets out recommendations with the aim of:

- explaining the regulations and the rights and obligations of the persons concerned by the regulations;*
- explaining the regulatory objectives and, as applicable, describing the practices considered by ASN to be satisfactory.*
- giving practical tips and information concerning nuclear safety and radiation protection.*

This guide was produced jointly by ASN and IRSN and presents the recommendations concerning the qualification of scientific computing tools (SCT) used to verify compliance with the safety criteria applicable to the first barrier, which is the fuel cladding.



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1. INTRODUCTION

1.1. Context and regulatory references

1.1.1. Regulatory references

- [1] The Environment Code, particularly title IX of book V
- [2] Decree 2007-1557 of 2nd November 2007 amended, relative to basic nuclear installations and to the regulation of the transport of radioactive substances in terms of nuclear safety
- [3] Order of 7th February 2012 setting the general rules concerning basic nuclear installations.

1.1.2. Regulatory context

More specifically in its article L. 593-7 the Environment Code requires that the licensee provide the *nuclear safety case*^(*)¹ for its facility. The decree in reference [2] requires that this safety case appear in the facility's safety analysis report and that it be provided in support of creation, commissioning and modification authorisation applications subject to article L. 593-15 of the Environment Code and in the facility's decommissioning file.

Furthermore, the order in reference [3] more specifically states that "*The nuclear safety case is based on computing and modelling tools that are **qualified** for the areas in which they are used.*"

Article L. 593-7 of the Environment Code (extract)

[The creation authorisation for a basic nuclear installation] may only be issued if, on the basis of current scientific and technical knowledge, the licensee can demonstrate that the technical and organisational measures taken or envisaged in the design, construction and operation, as well as the general principles proposed for decommissioning or, with regard to radioactive waste disposal facilities, for their upkeep and monitoring after closure, are such as to prevent or sufficiently mitigate the risks or drawbacks the facility presents for the interests mentioned in article L. 593-1.

Article 3.8 of the order in reference [3]

- I. – The nuclear safety case is based on:
 - up-to-date and referenced data; it more specifically takes account of the available information mentioned in article 2.7.7;
 - appropriate, clearly explained and validated methods, containing hypotheses and rules appropriate to the uncertainties and the extent of the knowledge of the phenomena involved;
 - calculation and modelling tools qualified for the fields in which they are used.
- II. – The licensee specifies and substantiates its criteria for methods validation, computing and modelling tools qualification and assessment of the results of the studies performed to demonstrate nuclear safety.

1.1.3 International reference texts

- [4] NRC Regulatory guide RG-1.203 Transient and accident analysis methods. December 2005
- [5] Deterministic Safety Analysis for Nuclear Power Plants for protecting people and the environment IAEA guide No. SSG-2

¹ The words in italics followed by an asterisk (*) are explained in the glossary at the end of the guide.



1.2. Purpose of the guide

Some of the studies used in the *nuclear safety case*(*) for basic nuclear installations (BNI) are based on the use of *scientific computing tools*(*) (SCT).

Article 3.8 of the order in reference [3] requires the use of “validated”² methods and of SCTs that have been qualified for the performance of these studies. The licensee must thus have adopted formal approaches to establishing the validation of the methods and the *qualification*(*) of the SCT.

The examinations by ASN and IRSN of the file concerning a method and that concerning the *qualification*(*) of an SCT used for application of this method, are generally separate; however, if the method and the SCT are linked, these two files are generally examined jointly. These files are examined prior to the examination of the studies performed using these methods and SCTs.

In this guide, the *qualification*(*) of an SCT implies recognition by the licensee that an SCT is able to provide results that are usable for a *nuclear safety case*(*). This recognition is established on the basis of data produced by *verification*(*), *validation*(*), quantification of *uncertainties*(*) and transposition operations. These operations are part of an overall process described in chapters 3, 4 and 5 ensuring that the SCT is capable of calculating the *variables of interest*(*) with the *uncertainties*(*) appropriate to the requirements, within the *intended scope of utilisation*(*).

This guide presents the ASN and IRSN recommendations for these operations and this process. Its purpose is to provide a coherent set of recommendations to be implemented in order to ensure that an SCT is qualified in accordance with ASN's requirements. It aims to facilitate the preparation and assessment of the files establishing the *qualification*(*) of the SCTs, by specifying the contents of the file to be produced by the licensee for transmission to ASN. It takes account of international reference texts (references [4] and [5]).

1.3. Scope of the guide

In the studies contributing to the *nuclear safety case*(*), this guide applies to the SCT used to demonstrate compliance with the technical acceptance criteria associated with the fuel behaviour in *normal operation*(*) or in the event of incidents or accidents³ affecting pressurised water reactors, research reactors, or spent fuel or fuel storage pools.

The technical areas concerned are fuel neutronics, thermohydraulics, thermomechanics and the physical chemistry of the fuel.

This guide applies to the SCT used in the initial design of basic nuclear installations (BNIs), during their periodic safety reviews, for modifications or in the additional substantiation files, during operation or for shutdown and decommissioning.

1.4. Document status and structure

This guide was produced by ASN and IRSN, with the participation of representatives from industry and the licensees during certain steps. It was submitted for consultation to industry and the licensees and then to the public, from 31st March 2017 to 4th May 2017.

After recalling the context of *qualification*(*) (see chapter 1.2), the guide deals with the following in turn:

- the intended *scope of utilisation*(*) of the SCT in the safety case (chapter 2), which must be

² Methods validation, not covered by this guide, is different from SCT validation mentioned in chapter 1.2

³ Except for severe accidents with fuel melt





- defined before the processes of *verification*, *validation*(*) and transposition subsequently presented;
- the process of *verification*(*) and *validation*(*) (chapter 3) of the SCT, which lies at the heart of *qualification*(*);
 - the process of transposition of the *validation cases*(*) to the intended *scope of utilisation*(*) (chapter 4);
 - the declaration of *qualification*(*) (chapter 5);
 - several particular points concerning certain software (pre- and post-processing, coupling, etc.) and certain uses of the SCT (chapter 6);
 - the description of the content of the *qualification*(*) file to be submitted to ASN (chapter 7).

2. USING THE SCT IN THE INTENDED SCOPE OF UTILISATION

2.1. Description of the intended scope of utilisation

The intended *scope of utilisation*(*) of the SCT is defined as being all the situations or scenarios associated with the *nuclear safety case*(*) studies and that one aims to justify using this tool.

These situations or scenarios can be described with reference to *normal operation*(*) of the facility and the incidents or accidents studied in the safety analysis report.

2.2. Identification and ranking of the principal phenomena

The definition of the *scope of utilisation*(*) of the SCT involves the following four steps. The depth of the analysis performed during each step is proportionate to the consequences and implications.

2.2.1. Identification of variables of interest

The first step is to identify the *variables of interest*(*) to be calculated with the SCT.

2.2.2. Identification of the principal physical phenomena

During the second step, the physical phenomena which influence these *variables of interest*(*) are identified and then ranked in order of importance, in order to identify the principal physical phenomena. The identification and ranking of the physical phenomena involved in the studies in question in the *nuclear safety case*(*) are the result of the analysis of the scope of utilisation and are based on expert assessments, experimental results, validated SCT application results, or the results of sensitivity calculations. The list of principal physical phenomena thus adopted with regard to the intended *scope of utilisation*(*) must thus be confirmed as being sufficient.

2.2.3. Influential parameters

During the third step, the *simulation*(*) input parameters which influence these physical phenomena are identified in turn and ranked in order of importance in order to define the *influential parameters*(*). The *influential parameters*(*) can be parameters of the SCT physical models associated with the physical phenomena. Their identification and classification can be based on expert assessments, or test results, or sensitivity studies. The list of principal *influential parameters*(*) thus adopted with regard to the intended *scope of utilisation*(*) must thus be confirmed as being sufficient.

2.2.4. Utilisation range

The preceding analysis ends with a determination of the variation range of the most influential parameters or of the *variables of interest*(*) which make it possible to specify the *utilisation range*(*) of



the SCT for the intended safety case.

3. PROCESS OF VERIFICATION, VALIDATION AND QUANTIFICATION OF UNCERTAINTIES FOR THE INTENDED STUDY

3.1. Preamble

This chapter describes the process which ensures that an SCT is capable of correctly representing the various physical phenomena it is required to simulate. Application of this process demonstrates the ability of the SCT to provide calculation results that are usable for the *nuclear safety case*(^{*}).

This process concerns an SCT with an identified version. It takes place upstream of the transposition step described in chapter 4.

The process comprises three steps, detailed below.

3.2. Verification

Verification(^{*}) is a formal process to determine whether the equations are solved correctly from both a numerical and data processing viewpoint. *Verification*(^{*}) concerns numerical methods and algorithms, their implementation, the data flow diagrams, the architecture of the IT programmes and compliance with any programming rules defined by the licensee.

In the case of *coupling*(^{*}) of computing tools, *verification*(^{*}) more specifically concerns the design and implementation of the links and interfaces between computing tools.

If the SCT is used on an IT platform (hardware architecture, operating system and compiler) different from that on which *verification*(^{*}) was carried out, it is advisable, to the extent possible, to ensure that this change has no impact on *verification*(^{*}).

3.3. Validation

Here we look at the *validation*^{*} of the SCT in its *scope of utilisation*(^{*}).

Whenever possible, *validation*(^{*}) follows a gradual two-step⁴ process in order to minimise the error compensations:

- the aim of *validation*(^{*}) with separate effects is to validate the physical models of the *scientific computing tools*(^{*}) in conditions in which the principal physical phenomena identified in chapter 2.2.2 are as isolated as possible;
- the purpose of integral *validation*(^{*}) is to verify the overall ability of the *scientific computing tool*(^{*}) to correctly simulate all the physical phenomena and their interactions.

This *validation*(^{*}) is based on the comparison of the calculation results on *validation cases*(^{*}) with respect to:

- measurements taken from experiments or BNI operations:
 - in the case of *validation*(^{*}) with separate effects: tests performed on mock-ups or facilities allowing optimum representation of basic physical phenomena, comparisons with *analytical solutions*(^{*}) when available;

⁴ It may be necessary to supplement these two steps with an “intermediate” validation step, if the scope of utilisation involves numerous coupled physical phenomena.

- in the case of integral *validation*(^{*}): tests performed on mock-ups or facilities allowing simulation of the physical phenomena (fully or partially) representative of the intended utilisation, operating experience feedback of physical tests on a BNI;
 - results from *reference scientific computing tools*(^{*}).

Failing which, if this gradual process cannot be followed (for example, if it was impossible to carry out *validation*(^{*}) with separate effects) or if there are gaps (for example, lack of data to validate certain models), the impact on *qualification*(^{*}) must be evaluated, for example by running the following approach:

- identification of the models concerned;
- sensitivity of the SCT response to these models;
- re-assessment of the *uncertainties*(^{*}) taking account of the gaps in *validation*(^{*}) or evaluation of a penalty to be applied in the methods to cover these gaps.

The justification of the pertinence and adequacy of the *validation cases* (^{*}) adopted with regard to the principal physical phenomena identified (chapter 2) must be provided and documented. This justification should in particular present:

- the description of the physical phenomena studied;
- the description of the variables measured and their variation range, the instrumentation used and the associated measurement *uncertainties*(^{*});
- the aims and the description of the *validation cases*(^{*}) both with separate effects and integral;
- the description of the study, the analysis and the interpretation of the test results;
- the definition of the variation range of the *influential parameters*(^{*}).

The experimental measurements or the data derived from operating experience feedback must, whenever possible, be representative of the *variables of interest*(^{*}) and the *influential parameters*(^{*}) as well as of their *validation*(^{*}) ranges within the *scope of utilisation*(^{*}).

If it is impossible to substantiate the adequacy of the separate effects or integral *validation cases*(^{*}) with respect to the principal physical phenomena, additional separate effects or integral *validation*(^{*}) would need to be provided. In the case of a lack of experimental data, it is necessary to ensure *validation*(^{*}) of the SCT by an appropriate approach proportionate to the issues, such as the alternative approaches mentioned in chapter 6.5.

The consistency of the choices (physical models, spatial mesh, temporal discretisation, numerical schemes, convergence criteria, calculation options, etc.) between the various calculations of the *validation cases*(^{*}) adopted (whether *validation*(^{*}) with separate effects or integral *validation*(^{*})) is to be sought. If there are different choices, the *validation*(^{*}) calculations would need to be revised. Failing which, the impact of these differences on the *qualification*(^{*}) of the SCT would have to be evaluated.

In particular, the spatial and temporal numerical convergence criteria of the *calculation schemes*(^{*}) must be identified and respected. The modelling recommendations resulting from the various calculations of the *validation cases*(^{*}) with separate effects, as well as the *validation range*(^{*}) for each of the models associated with the principal physical phenomena, must be identified and, whenever possible, respected in the integral *validation*(^{*}) calculations. In the event of non-compliance with the *validation*(^{*}) ranges or certain recommendations, the impact of this non-compliance in the *validation*(^{*}) file must be evaluated.



Finally, the use of *adjustments*(*) defined during the separate effects or integral *validation*(*) calculations is acceptable provided that it is explained and justified. The method followed to define these various *adjustments*(*) must be described and justified. In addition, their impact on the predictive nature of the *scientific computing tool*(*) shall be evaluated. This is because:

- *adjustments*(*) are a means of reducing the *uncertainties*(*) of certain *variables of interest*(*) calculated in a given field, but they can also reduce the overall predictive nature of the *scientific computing tool*(*) outside this field;
- the consistency of the *adjustments*(*) between the various *validation*(*) calculations (whether *validation*(*) with separate effects or integral *validation*(*)) is to be sought. The impact of any inconsistencies on the predictive nature of the SCT shall be evaluated.

3.4. Quantification of uncertainties

By comparing the results supplied by the SCT with those of the *validation cases*(*), *validation*(*) should allow evaluation of the various *uncertainties*(*):

- *uncertainties*(*) resulting from *validation*(*) with separate effects, associated with each basic physical model;
- *uncertainties*(*) resulting from integral *validation*(*), associated with SCT prediction of the *variables of interest*(*).

Whenever possible, the assessment of the *uncertainties*(*) resulting from integral *validation*(*) should take account of the *uncertainties*(*) in the basic physical models resulting from the chosen *validation*(*) calculations with separate effects, in order to minimise error compensations.

For those cases in which it would not be possible to compare the results supplied with experimental data or with results obtained using the reference SCT, the evaluation of the *uncertainties*(*) may, if substantiated, rely on comparisons with other SCTs, on expert assessments and on sensitivity studies.

Finally, the quantification methods for the various *uncertainties*(*) shall be described and substantiated.

When it proves particularly complex to determine the various *uncertainties*(*), an alternative “conservative” approach may be used: this approach consists in showing that the application of conservative hypotheses (on the initial or limit conditions, or on the physical models) is a means of obtaining a conservative value for the *variables of interest*(*) in the *validation cases*(*).

3.5. Summary of chapter 3

The implementation of this process contributes to the production of the *qualification*(*) file, with respect to its *scope of utilisation*(*). It is specific to the SCT version considered. On the basis of this file, a *validation range*(*) is defined, in other words the variation range of the characteristic values (pressure, temperature, flowrate, power, enrichment ratio, type of fuel, geometry, etc.), covered by the *validation cases*(*) and for which the SCT results are considered to be satisfactory.

Particular attention must be paid to the definition of the *validation range*(*), which may be delicate in certain cases, notably when some configurations may potentially not be covered by experimentation.

4. TRANSPOSITION FOR USE OF THE SCT IN THE INTENDED SAFETY CASE

The purpose of transposition is to specify how the conclusions of SCT *validation*(*) apply to the intended *scope of utilisation*(*).

Transposition may take place in two steps:

- a first step consisting in identifying the geometrical (scale effect) and physical differences between the *validation cases*(*) (for example experimental mock-ups or data collected on the BNI itself) and the *scope of utilisation*(*) for the facility concerned. The impact of these differences on the principal physical phenomena (list and intensity of the phenomena) and the *influential parameters*(*) is evaluated, notably on the basis of a physical analysis. If the impact is very slight, or even non-existent, this step may be sufficient;
- a second step which, as necessary, consists in assessing the ability of the models to remain predictive (or penalising) taking account of the differences identified between the *validation range*(*) of the SCT and the *utilisation range*(*). This evaluation may be based on additional experimental data, on sensitivity calculations or on expert assessments. It notably includes the justification of the transposition of the *adjustments*(*) and the *uncertainties*(*).

Finally, during transposition, it is important to ensure that the modelling choices in the safety studies (physical models, spatial mesh, temporal discretisation, numerical schemes, convergence criteria, calculation options, etc.) in the intended *scope of utilisation*(*) are consistent with the choices adopted for the *validation cases*(*). In the event of inconsistency, the *simulations*(*) of the *validation cases*(*) must be revised. Failing which, the impact of this inconsistency on the safety studies must be evaluated.

Following transposition, the *validity range*(*) of the SCT is defined.

5. DECLARATION OF QUALIFICATION

The *qualification*(*) of the SCT is declared by the licensee for the intended *scope of utilisation*(*) in the light of the elements obtained by the processes described in chapters 2 to 4.

Qualification(*) is declared if the following conditions are met:

- the SCT is capable of calculating the *variables of interest*(*) for the intended *scope of utilisation*(*) with *uncertainty*(*) values adapted to the needs of the safety studies in which it will be used;
- the *utilisation range*(*) for which *qualification*(*) is declared is within the *validity range*(*) of the SCT.

The licensee may declare *qualification*(*) of an SCT when the approaches described in chapters 3 and 4 have not been followed in full: the licensee then demonstrates that, within the intended *scope of utilisation*(*), the hypotheses and decouplings adopted in the method enable conservative values to be obtained for the *variables of interest*(*) in the safety studies concerned.

The document constituting confirmation of *qualification*(*) must state:

- the SCT version concerned as well as the versions of the pre- and post-processors necessary for performance of the planned studies (see chapter 6.1);
- the *utilisation scope and range*(*) of the SCT;
- as necessary, the *study methods*(*) with which the SCT is to be used (see chapter 6.6).



6. SPECIAL POINTS

6.1. Pre- and post-processing

Most of the time, the calculation of *variables of interest*(*) by the SCT requires data entry⁵ and post-processing (meshing, interpolation of data or results, projections, calculation of derived variables or statistical values, plotting of curves or graphs, etc.) which can end up having an influence on the values of the *variables of interest*(*).

The pre- and post-processing software which need to be used to carry out studies with the SCT and their conditions of use, must be taken into account in the *qualification*(*) approach. In addition, adequate *verification*(*) of these tools is required.

6.2. Chaining and coupling

An SCT may consist of a *chaining*(*) or *coupling*(*) of several SCT. These SCT must then first of all have been verified and validated. There should not in principle be any difference in terms of *qualification*(*) requirements by comparison with the case of a single SCT. Consequently, the *verification*(*), separate effects *validation*(*), integral *validation*(*) and then transposition steps are necessary.

Certain specific aspects must however be taken into consideration:

- during the *verification*(*) step, it is necessary to ensure that the links or interfaces between the SCTs are correctly designed and implemented (functional verification);
- during the *validation*(*) steps, proof must be provided that convergence is managed for the *couplings*(*) (spatial and temporal convergence, but also *coupling*(*) iterations);
- in the case of SCT *chaining*(*), the integral *validation*(*) step may not be necessary, provided that the following have been performed:
 - o an analysis of the pertinence of *chaining*(*), for example by comparison with an SCT *coupling*(*);
 - o functional verification of *chaining*(*);
- in the case of SCT *coupling*(*), integral *validation*(*) may not be necessary if the licensee can demonstrate that the *coupling*(*) of physical phenomena modelled by the various SCTs does not compromise the identification and scope of the principal physical phenomena.

In fact, it must be ensured that the *scope of validity*(*) of each SCT involved in an SCT *chaining*(*) or *coupling*(*) is respected. The data of the various SCTs must be within their respective scopes of validity.

6.3. User-related effect

The results obtained with the SCT by one user may differ from those obtained by another user with the same SCT. Precautions can be taken to mitigate this effect, for example by controlling user access to parameter settings and modelling choices.

6.4. Specialised tools

For certain safety case studies, a specialised SCT may be produced from a general-purpose SCT (neutronics, thermohydraulics, mechanics, etc.).

⁵ For example, the production of data sets with pre-processing software

For this specialised SCT, *qualification*(*) is required only for the intended scopes of utilisation. The processes covered by chapters 3 and 4 can rely on *verification*(*), *validation*(*), quantification of *uncertainties*(*) and transposition elements established for the general-purpose SCT. It is nonetheless necessary to show that these elements are actually pertinent for the intended *scope of utilisation*(*) of the specialised SCT.

6.5. Gaps in experimental data

Validation(*) with separate effects and integral *validation*(*) must whenever possible rely on experimental results or experience feedback that is pertinent for the intended *scope of utilisation*(*). In certain cases, these results are not available (for example because they are not technically achievable). Alternative approaches are then possible.

Thus, *validation*(*) can be carried out on the basis of:

- comparisons with a reference SCT;
- *cross evaluations*(*) with other equivalent SCTs. This alternative is to be used with caution because the models of these SCTs may be similar or even identical, and thus not provide a physical validation of the SCT models.

In addition, the results of the sensitivity studies with regard to the physical models and the modelling choices can be utilised. If these sensitivity studies show that the sensitivity of the *variables of interest*(*) to certain physical models and to the modelling choice is slight, the *validation*(*) step can be adapted. However, for the modelling choices, the pertinence of these sensitivity studies is necessarily limited by the capabilities of the SCT. These results are therefore to be used with the necessary reservations.

Finally, it is possible to cover the gaps in experimental data and thus the corresponding *validation*(*) shortcomings by choosing hypotheses enabling a conservative value to be obtained for the *variables of interest*(*). In this case, the adequacy of these hypotheses must be demonstrated.

6.6. Link with the study methods

The SCTs are generally used in conjunction with *study methods*(*) which, according to the order in reference [3], must be “*appropriate, clearly explained and validated*”.

In certain cases, the SCT may be separate from the *study method*(*). In these cases, the *qualification*(*) of the SCT may be declared without mentioning the *study method*(*).

In other cases, the *study method*(*) is only appropriate and validated for one or more given SCTs, which run the calculations by implementing the approach provided for in this method. In this case, *qualification*(*) of the SCT must mention the *study method* (*) applied.

Validation(*) and transposition may also require additional analyses for use of the SCT in the *nuclear safety case*(*) in the case of application of a *study method*(*). Indeed, certain hypotheses or decouplings introduced into the methods may affect the SCT result. These analyses then supplement the study method files.

Finally, as mentioned in chapter 6.5, in the event of gaps in the experimental data or when the *uncertainties*(*) could not be determined (see chapter 3.4), particular hypotheses can be adopted in the *study methods*(*) in order to ensure the conservative nature of the values of the *variables of interest*(*).

7. COMPOSITION OF THE FILE TO BE SENT TO ASN

The *qualification*(*) file builds on all the knowledge acquired through the various steps described in chapters 2 to 6.

7.1. Case of first qualification of an SCT

For the case of the first *qualification*(*) of an SCT, elements associated with the description of the SCT (see appendix), with the steps associated with the description of the *scope of utilisation*(*) and with identification of the principal physical phenomena, with *validation*(*) and with quantification of the *uncertainties*(*) and with transposition are to be sent to ASN.

The *verification*(*) step (see chapter 3.2) is not generally the subject of a technical examination and the associated elements do not therefore need to be transmitted.

7.2. Case of SCT qualification for modification of the scope or range of utilisation or for a new study method

In the event of modification of the intended scope or *utilisation range*(*), or of implementation of a new *study method*(*), it is necessary to ensure that these changes do not compromise the elements of the *qualification*(*) file, in particular with regard to the identification of the principal physical phenomena and, as applicable, the adequacy of the *validation*(*) base. If this is not the case, it is necessary to extend the *validation*(*) base and define the *field of validity*(*) resulting from the transposition step, following the approach described in chapters 3 and 4.

The description of the modification of the scope or *utilisation range*(*) and the justification of the *validity range*(*) of the SCT are elements to be transmitted to ASN.

7.3. Case of a new SCT version

A new version of an SCT is the result of one or more changes corresponding to the following actions:

- corrective maintenance (correction of an error in the source code);
- adaptive maintenance (adaptation to a change in the IT environment);
- progressive maintenance or development (modification of algorithms, of *calculation schemes*(*), of physical models, introduction of new functions such as new solvers or new physical models, etc.).

The impact of changes on SCT *qualification*(*) is analysed in accordance with an approach that takes account of their importance. As applicable, this analysis may be based on either an argument, or on a *non-regression*(*) analysis of the *verification*(*) and *validation*(*) carried out using a base representative of test cases (base to be defined on a case by case basis). Certain changes, in particular those linked to the physical models and affecting the response of the SCT, may require a recalculation of or addition to the *validation cases*(*).

The description of these changes and their impacts on the *validation*(*) and transposition steps are to be transmitted to ASN.



GLOSSARY

Adjustment

Process consisting in adjusting the parameters of the *scientific computing tool*(*) model, so as to minimise the difference between the calculated values and the reference values.

Validation cases

Any data set considered to be pertinent and selected for carrying out separate effects or integral validation of an SCT (experimental test, operating experience feedback, *simulation*(*) using a *reference scientific computing tool*(*), *analytical solution*(*), etc.).

SCT chaining/coupling

An SCT may comprise several SCTs interconnected by interface tools allowing “*chaining*(*)” (when the results of a first SCT act as input data for a second) or *coupling*(*) (*chaining*(*) with feedback or when the SCTs perform their respective *simulations*(*) in parallel, for example with sharing of the intermediate results).

Scope of utilisation

All the situations or scenarios studied in the safety case and that are to be substantiated using this SCT.

Nuclear safety case (definition of the order in reference [3])

Art. 1.3

“All the elements contained or used in the preliminary safety report and the safety reports mentioned in articles 8, 20, 37 and 43 of the decree of 2nd November 2007 and contributing to the demonstration mentioned in the second paragraph of article L. 593-7 of the Environment Code, which prove that the risks of an accident - radiological or otherwise - and the scale of their consequences are – on the basis of current knowledge, practices and the vulnerability of the facility’s environment – as low as possible in acceptable economic conditions.”

Art. 3.8:

“I/ The nuclear safety case is based on:

- *up-to-date and referenced data; it notably takes account of the available information mentioned in article 2.7.2;*
- *appropriate, clearly explained and validated methods, integrating hypotheses and rules adapted to the uncertainties and limits of knowledge of the phenomena involved;*
- *calculation and modelling tools qualified for the fields in which they are used.*

II/ The licensee specifies and justifies its criteria for validating the methods, for qualifying the calculation and modelling tools and for assessing the results of the studies carried out to demonstrate nuclear safety.”

Validation range

Variation range for the characteristic geometrical or physical variables (pressure, temperature, flowrate, power, etc.) for which the SCT results are considered to be satisfactory.

Validity range

The validity range is the result of the possible adaptation of the *validation range*(*) following transposition, for the intended application.



Utilisation range

Variation range for the characteristic geometrical or physical variables (pressure, temperature, flowrate, power, etc.) for the scenarios of the intended *scope of utilisation*(*).

Comparative evaluation

Study comparing the results from one SCT with those from another SCT or with reference calculation results.

Normal operation (definition of the order in reference [3])

Art. 1.3

“*Operation of the facility, which includes all routine states and operations in the facility, including scheduled maintenance or outage situations, whether or not radioactive materials are present. Normal operation also includes all situations defined as such in the demonstration mentioned in the second paragraph of article L. 593-7 of the Environment Code.*”

Variables of interest

The variables of interest are those for which the values make it possible, either directly or indirectly, to determine compliance with the technical acceptance criteria related to the behaviour of the fuel and applicable to the study in question.

Uncertainty

Range of variation in the result of a measurement or calculation which characterises the possible values and probably contains the real value of the target response concerned.

Study method

Approach defining certain hypotheses (initial conditions, limit conditions, etc.), the consideration of *uncertainties*(*), penalties, *calculation schemes*(*) and the calculation sequences necessary for the safety assessment, consistently with the rules of the *nuclear safety case*(*).

Non-regression

Lack of significant deterioration of the calculation results for *variables of interest*(*) by an SCT.

Scientific computing tool (SCT)

SCTs are software performing *numerical simulation*(*) of physical phenomena. They consist of one or more solvers and may comprise pre- and post-processors

- the solvers are designed by means of several successive steps:
 - o formulation of physical modelling hypotheses, generally leading to a system of equations;
 - o definition of algorithms for numerical resolution of these equations;
 - o implementation of these algorithms;
- the pre-processors can be used to introduce the calculation data (mesh, physical characteristics, etc.);
- the post-processors are used to exploit the calculation results, more specifically in graphic form.

Reference scientific computing tool

Scientific computing tool for which the predictive performance is considered to be superior to that expected of the scientific computing tool to be validated.

For example, in neutronics, “Monte-Carlo” or deterministic type SCTs with a very high number of energy groups and spatial meshes may, in certain cases, can be considered to be a reference SCTs.



Influential parameters

Geometrical or physical input parameters for the study in question or the *validation cases*(*) which, owing to their contribution to the principal physical phenomena, have an impact on the *variables of interest*(*).

Qualification

Recognition by the licensee that an SCT is able to provide results that are usable for a *nuclear safety case*(*).

Calculation scheme

Set of modelling choices made for performance of a numerical *simulation*(*). It more specifically defines the choice of physical models, the correlations, the discretisation both spatial (meshing) and temporal (time pitch), the calculation options and, more generally, all the choices which determine performance of the calculation.

Simulation (numerical)

Action which implements one or more SCTs, with calculation schemes and input data, to produce numerical results describing the evolution of a physical situation.

Analytical solution

Solution of a theoretical problem which can be expressed in the form of mathematical expressions.

Nuclear safety

Definition of article L591.1 of the Environment Code: *Nuclear safety is the range of technical provisions and organisational measures concerning the design, construction, operation, shutdown and decommissioning of basic nuclear installations as well as the transport of radioactive substances, designed to prevent accidents or mitigate their effects.*

Validation

Validation consists in ensuring that an SCT can satisfactorily simulate the physical phenomena within the *validation range*(*).

Verification

Verification consists in ensuring that the SCT functions as required (correct computing and numerical performance, correct numerical results).



APPENDIX

Description of the scientific computing tool

The SCT description must, generally speaking, explain its operation, the models and numerical methods used in the intended scope of utilisation of the *scientific computing tool*(*).

The document describing the *scientific computing tool*(*) should include:

- a precise and complete identification of the version of the *scientific computing tool*(*) and, as applicable, the versions of any calculation tools it comprises (case of *couplings*(*) and pre- or post-processing utilities). For example, for a neutronics calculation tool: version of the SCT, of the library of procedures and of the library of nuclear data (cross-sections, etc.);
- identification of the IT platforms on which the SCT has been ported and verified;
- the description of upgrades with respect to the previous qualified version (if there is one);
- the description of the models, in the broadest sense, chosen to simulate the physical phenomena identified in the utilisation range of the *scientific computing tool*(*): resolved equations, closure laws, numerical models, spatial representation mode (0D, 1D, 2D, 3D), *calculation schemes*(*) and spatial and temporal convergence criteria, libraries of materials properties, etc.;
- the summary functional description of the tool: the general diagram of the IT architecture, the list of the main modules of the computing tool and their key functions, the presentation of the chaining of these modules and the numerical diagrams implemented; the description of the numerical diagrams and the equations they resolve more specifically makes it possible to assess the overall consistency.

In the case of SCT *chaining*(*), the above elements will be supplied for each link in the chain and the chaining mechanism will be described; the same will apply for the case of *coupling*(*) of coupled SCTs, for which a general *coupling*(*) flowchart and elements substantiating control of the convergence of *coupling*(*) (spatial convergence, temporal convergence, but also *coupling*(*) iterations) will also be presented.

THE ASN GUIDES COLLECTION

- N°1 Disposal of radioactive waste in deep geological formations
- N°2 Transport of radioactive materials in airports
- N°3 Recommendations for the preparation of annual public information reports concerning BNIs
- N°4 Self-assessment of risks for external-beam radiotherapy patients
- N°5 Management of security and quality in radiotherapy care
- N°6 Final shutdown, decommissioning and delicensing of BNIs in France
- N°7 Civil transport of radioactive packages or substances on the public highway (*3 volumes: shipments, packages requiring and not requiring approval*)
- N°8 Conformity assessment of nuclear pressure equipment
- N°9 Determining the perimeters of a basic nuclear installation (BNI)
- N°10 Local involvement of CLIs in the 3rd ten-year inspections of the 900 MWe reactors
- N°11 Notification and codification of criteria related to significant radiation protection events (*excluding BNIs and radioactive material transport operations*)
- N°12 Notification and codification of criteria related to significant safety, radiation protection or environmental events applicable to BNIs
- N°13 Protection of BNIs against external flooding
- N°14 Remediation of structures in BNIs in France
- N°15 Control of activities in the vicinity of BNIs
- N°16 Significant patient radiation protection event in radiotherapy: notification and classification on the ASN-SFRO scale
- N°17 Contents of radioactive substance transport incident and accident management plans
- N°18 Disposal of effluents and waste contaminated by radionuclides, produced in facilities licensed under the Public Health Code
- N°19 Application of the order of 12/12/2005 relating to nuclear pressure equipment
- N°20 Drafting of the medical physics organisation plan (POPM)
- N°21 Processing non-compliance with a specified requirement for an EIP
PWR - Radiological accident risks
- N°22 Safety requirements and recommendations for PWR design
- N°23 Definition and modification of the waste zoning plan for BNIs
- N°24 Management of soils polluted by BNI activities
- N°25 Drafting of an ASN statutory resolution or guide: procedures for consultation with stakeholders and the public
- N°27 Stowage of radioactive packages, materials or objects for transportation
- N°28 Qualification of scientific computing tools used in the nuclear safety case
- N°31 Notification of radioactive substances transport events (*on the public highway, by sea or by air*)
- N°32 In-vivo nuclear medicine facilities - Minimum technical rules for design, operation and maintenance



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