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BAM-GGR 008

Guideline for Numerical Safety Analyses in the Context of Type Approval of Packages for the Transport of Radioactive Material

Revision 1

Only the german version is legally binding.

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1 General conditions

1.1 Scope of application

This guideline applies within the area of responsibility of the Bundesanstalt für Materialforschung und -prüfung (BAM) – *Federal Institute for Materials Research and Testing* – in its capacity as competent authority for design type tests in accordance with dangerous goods legislation. It shall be considered when preparing safety certificates for package designs for the transportation of radioactive materials that are based partly or entirely on numerical calculations. In the calculation programs used for this purpose, mechanical and thermal analyses of the behaviour of the package parts under test requirements are mainly carried out using the finite element method (FEM). The guideline also applies analogously to other numerical methods, such as the finite difference method (FDM) or the boundary element method (BEM), as well as the finite volume method (FVM), as used, for example, in many programs for computational fluid dynamics (CFD).

1.2 Purpose

The guideline serves to support quality assurance in preparation, control and assessment of safety cases based on a numerical analysis of problems that are part of the scope of testing and assessment of package designs for the transport of radioactive materials. In particular, it is intended to form the basis for the correct performance of numerical analyses in accordance with the state of the art and to support the verifiability of the numerical safety case. Its application should ensure the traceability of the calculation procedure and the preconditions and assumptions on which the calculations are based.

1.3 Legal basis

The safety requirements for the design of package types for the transport of radioactive materials are based on the recommendations of the International Atomic Energy Agency (IAEA): Regulations for the Safe Transport, Advisory Material und Package Design Safety Report [1, 2, 3]. It defines the test conditions under which safety verifications are to be carried out as part of the dangerous goods procedures for the approval of package types [4].

1.4 Fundamentals for numerical simulations

The fundamentals of the numerical solution methods used for simulations in the field of mechanics and thermics, in particular the FEM and the definition of terms, may be found in [5, 6, 7, 8]. For an explanation and definition of terms with regard to verification and validation (VnV) see the presentation of the concept and the standard according to ASME [9, 10], the standard and the guidelines according to NAFEMS [11, 12] and the relevant technical literature [13].

2 Models for numerical safety analyses

2.1 General information

This section describes the basic principles and components of numerical safety analyses for package designs for the transportation of radioactive materials. Notes on the modelling of individual parts[1] of these packages are given in the appendix. The requirements for numerical safety analyses may be found in Chapter 4.

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[1] In this document, the hierarchy system, sub-system, assembly, sub-assembly and component is used. In this document, a “part” is any element of the hierarchy.

2.2 Components of the model

The chosen form of modelling and the solution parameters required for the numerical solution, e.g., using FEM, shall be described and justified. The following issues shall be addressed:

- geometric comparison with reality (overview sketches including simplifications of part geometries and references to the relevant technical drawings),
- considered dimensions (nominal dimension, nominal dimension including tolerance or actual dimension),
- selected element types,
- discretization of the overall structure and important sub-areas (in different perspectives, if necessary),
- material models and data (see also Section 2.3),
- graphical representation of boundary conditions, contact conditions and constraints between nodes, if possible,
- load assumptions (e.g., selected orientation, load application and heat sources) and
- initial, boundary, transition and contact conditions (including a description of the contact formulations applied and its parameters).

2.3 Material models and material data

The material data used and their dependence on significant parameters shall be specified graphically or in tabular form. The suitability of the material models for the task at hand shall be justified.

Separate experimental tests shall be carried out to determine the material data if there is insufficient reliable data available for modelling safety-relevant parts (e.g., cask bodies, lids, screws, seals, shielding materials) or parts that significantly influence the results of numerical analyses (e.g., impact limiters or other shock-absorbing parts in mechanical analyses). Alternatively, parameter studies or sensitivity analyses may be used to prove that the selected material data lead to results that cover the intended analysis objective; see also Section 3.2.1. However, the selection of external input parameters alone does not necessarily result in a covering (so-called conservative) calculation result, as the use of such input parameters may also change the quality of the calculation result, which shall be ruled out.

2.4 Verification and validation

Numerical simulation plays an important role in safety assessments when evaluating package designs for the transport of radioactive materials. Complex phenomena and processes that are difficult to access experimentally and challenging to measure may be modelled and analysed using state-of-the-art simulation methods. Numerical simulations make it possible to investigate a wide range of issues, particularly in mechanics, thermodynamics and fluid mechanics. The accuracy and reliability of simulation results are crucial for drawing valid conclusions and make well founded decisions. Verification and validation are two fundamental methods used in numerical simulation to ensure this accuracy and reliability.

Although verification and validation are closely related, they differ in their main objectives and scope of application. While verification aims to confirm the correct implementation of the numerical model and ensure consistency with the mathematical description, validation focuses on assessing the accuracy and reliability of the simulation results in comparison with experimental results.

Verification is essentially an internal process without reference to experimental data, which aims to ensure that the model is free of errors and to test its behaviour under idealized conditions[2]. Validation,

[2] As created, e.g., by method of manufactured solutions, see also footnote 5.

on the other hand, requires an external comparison of the model results with experimental data or observations from the real world.

The procedure and results of both verification and validation should be documented in a comprehensible manner; see in particular the standards and guidelines according to NAFEMS [11, 12].

The individual aspects of the verification and validation process are described in Chapter 3.

3 Verification and validation

3.1 Verification

Verification is a crucial step in numerical simulation[3] and refers to the process of checking the implementation of a numerical model to ensure that it is consistent with the underlying mathematical equations and solution methods and uses the correct mathematical concepts and algorithms [10]. This is achieved by comparing the results of the numerical calculation with analytical solutions to verify consistency. The main objective of verification is to detect errors in the implementation, not to evaluate the accuracy of the model regarding its real-world behaviour. The aim is to ensure that the model delivers consistent and physically reasonable results (e.g., energy balances) under idealized conditions. The ASME-Standard [10] is supplemented by the presentation of the ASME verification and validation concept [9]; this document contains detailed verification guidelines for numerical simulation.

The verification process shall be documented in a comprehensible manner, also as part of the application documents, to be able to reuse the verified model later. The documentation should include reasons for the choice of verification methods used and their limitations, as well as a description of the methods and the results achieved [10].

Verification is divided into code verification and calculation verification. Code verification consists of numerical verification of the program code and software quality engineering [10].

If, as in most cases, commercial software whose source code is not accessible to the licensee is used for the submitted calculations, the software manufacturer shall document its quality assurance.

If these numerical calculations are performed using (commercial) programs[4] as part of the application process, these programs are considered by BAM to be verified and quality-assured in terms of their program code, provided that the software manufacturer has certified quality assurance. If the applicant uses open-source program code, the applicant is responsible for quality assurance and its documentation.

3.1.1 Numerical verification

Numerical verification is divided into analytical methods, numerical benchmark solutions, as well as consistency tests. If similar (semi)analytical solutions are known for the numerical problem considered, these should be used for comparison.

Analytical methods are subdivided into analytical solutions and the method of manufactured solutions. They involve comparing solutions calculated by the numerical model with known analytical solutions. This comparison allows implementation errors or algorithmic errors to be identified and corrected. The use of analytical methods is effective for simple and well-defined problems [10].

[3] For verification and validation with a focus on CFD, see also [13].

[4] Examples include ANSYS Mechanical, CALCULIX (under GNU General Public License, GPL), Code_Aster (under GPL), Comsol, LS-DYNA, PAM-CRASH, SIMULIA (previously ABAQUS); ANSYS CFX, ANSYS Fluent and OpenFOAM (under GPL). In principle, the use of open-source codes, such as those under the GPL, is permitted for application procedures, provided that their verification can be demonstrated.

Numerical benchmarks use numerical solutions as a basis for comparison. The reference used should have an assessable accuracy.

The consistency test is the most accessible to the user in practical terms of the previously mentioned subdivisions of numerical verification. The consistency test should include local and global confirmation of the conservation of mass, momentum and energy. Furthermore, the consistency of geometric features may be checked, e.g., special symmetry properties or the conservation of the result when changing the coordinate system.

3.1.2 Convergence analysis

Convergence analysis deals with the study of the convergence of the numerical model. It examines whether the solutions approach a smooth or well-defined solution with increasing spatial or time discretization. Convergence analysis helps to determine the necessary spatial and time discretization to achieve sufficiently accurate results and therefore supports the selection of a suitable numerical solution method [10].

The use of a posteriori error estimation is recommended in practice. This involves calculations with different spatial mesh density (h-adaptivity) or different orders of element scheme (p-adaptivity), among other things [10]. Details can be found in the description of the concept [9].

3.2 Validation

Unlike verification, validation refers to the process of assessing the accuracy and reliability of a numerical model by comparing the simulation results of a specific process or load configuration with experimental data [9].

When validating a numerical calculation, the calculation results are compared with real observations. Initially, the specific application for which the mathematical predictions are to be confirmed is defined.

The validation includes a quantification of the uncertainties[5] of the results, which relates to both the calculation and the experimental data. This so-called uncertainty analysis includes the consideration of measurements, materials, loads and reactions. It may require supplementary experiments and calculations to ensure predictive capability over the defined scope of application.

The supplementary experiments should be planned with the objective in mind to ensure that the numerical model is of sufficient quality for the analysis objective.

Accuracy requirements are defined for the validation process, taking into account the specific application and analysis objectives. If these accuracy requirements are met, the model can be considered validated for the defined application [10].

3.2.1 Parameter studies, sensitivity analyses and validation of model data

Sensitivity analyses[6], e.g. in the form of parameter studies, are used to determine the dependence of the model's output variables on the input variables and, if applicable, the internal parameters, such as settings for contact algorithms, etc. This may be done qualitatively or quantitatively or both qualitatively and quantitatively. The sensitive parameters of the input data should be determined with sufficient accuracy. In addition, positions and measured variables (usually displacement or strain, velocity, acceleration, force and temperature) of the validation experiment can be determined which should be

[5] In particular, the influence of filters used and filter-like effects shall be taken into account in both experimental investigations and simulations, respectively, the filters used shall be coordinated with each other.

[6] In most cases, sensitivity analysis is the only way to verify a claimed covering relationship between selected input data and output variables to be minimized or maximized (and thus the so-called conservativeness of the simulation result) in a nonlinear simulation model.

of particular importance regarding the simulation model. As the validation experiment does not necessarily confirm this postulated relationship between output variables and input variables, this is an iterative process in which the simulation model shall be adjusted accordingly, e.g., by selecting a more suitable material model or a more detailed modelling of connections. This form of pre-test calculations links the verification process to validation [14].

3.2.2 Experiments for validation

The aim of the validation experiments is to obtain the experimental data required for the validation of the verified numerical model. The validation experiment should be designed in such a way that all initial and boundary conditions, material properties and external forces relevant to the analysis objective are considered. These variables should be defined as accurately and completely as possible. Concurrently, applied loads, relevant response variables and changes in boundary conditions should be recorded during the experiment. Also, the uncertainties of the individual measurements should be documented [10].

3.2.3 Other components of validation

Other components of validation include quantifying experimental uncertainties, evaluating accuracy and documentation.

The results of the validation experiments are subject to uncertainties due to measurements, tolerances (e.g., measurements and material properties) and discrepancies in the setup and boundary conditions of the experiment. These uncertainties shall be quantified and documented to properly evaluate the simulation results.

Quantification is followed by an analysis of the agreement between the simulation results and the measurement results, as well as an evaluation of the accuracy of the calculation model in relation to the intended use of the model. The model accuracy is evaluated for each component, sub-assembly, assembly and sub-system for which validation data is available or measurable.

The documentation should show whether and how accurately the model reflects the validation experiments and prove that the model is capable of making predictions for the intended purpose. Documentation of the entire validation process is a mandatory part of the application documents and should be submitted together with the models.

3.3 Verification and validation in the simulation workflow

The integration of verification and validation into the simulation process involves more than just evaluating the simulation results. The results of the verification and validation process may help to improve and optimize the model. Identifying implementation errors and analysing the discrepancies between the simulation results and the experimental data makes it possible to refine the model and increase its predictive capability.

Furthermore, quantifying uncertainty provides insights into the sensitivity of the model to various parameters and assumptions. It allows to identify the critical factors that influence the behaviour of the model and to make targeted improvements to increase the accuracy of the predictions.

The integration of verification and validation into the simulation process enables continuous improvement of simulation models and helps to achieve reliable simulation results that reflect real-world conditions.

In practice, the simulations to be evaluated do not achieve a validated model in the sense of the above-mentioned VnV standards. Instead, the models used for the predictive calculation of the validation experiments are “calibrated” because their discrepancies are partly too large; they are adjusted to the results of the experiments. This is a permissible step for validation, but in the strict sense it entails another independent experiment until sufficient agreement between the model and the experiment is achieved. For reasons of cost and time, validation is often not possible as an iterative process, which is why the discrepancies between the calibrated models and the existing experiments shall be considered when determining the reliability of the simulation results. This results in narrow limits for the usability of calibrated models exclusively for the purpose for which they were validated.

BAM may create its own models for the entire package, shock-absorbing parts and foundations or assemblies of particular relevance as part of its assessment activities. These models are usually calculated using software other than that used by the applicant to assess the suitability of the modelling and software as independently as possible from the applicant's approach.

4 Requirements for numerical safety analyses

4.1 Completeness

The numerical safety analysis is complete if the report to be submitted for documentation and review, as well as the associated documents, include all information essential for reviewing the analysis in a comprehensible form. In particular, the safety analysis shall meet the requirements of the legal basis (see Section 1.3) with respect to the results to be demonstrated. The report shall meet the requirements summarized here and explained in more detail in the following subsections regarding:

- information on the software used (Section 4.2),
- all necessary elements of the numerical safety analysis (Section 2),
- range and presentation of the input data (Section 4.3),
- range and presentation of the results (Section 4.4),
- assessment of the calculation results (Section 4.5),
- references, bibliographical references and source citations (see Bibliography) and
- the clear use of terms in the context of verification and validation.

4.2 Software used

4.2.1 Documentation

The documentation of the program version used shall be named (e.g., literature reference) and made available to BAM upon request.

4.2.2 Program suitability, reliability and quality assurance

Proof of the program's suitability in principle may be provided by referring to publicly available publications. For proof of the applicability and reliability of the program system, see Section 3.1. Generally, a program version that is actively maintained by the software manufacturer should be used.

The software used shall be subject to a continuous control process due to changes in the source code (as a result of improvements or the introduction of new features) and the necessary adaptation to new hardware and operating systems. This is generally done by the commercial providers of the software. If the software provider does not work according to an accredited quality assurance system or if the applicant uses their own or third-party software available in the source code, quality assurance measures shall be carried out and documented, e.g., in accordance with the NAFEMS Guidelines [12]. This applies both to the software used for the actual calculation and to pre- and postprocessing[7]. Quality assurance measures taken by the program provider do not release the user from their duty of care in the sense that, in the event of new program versions or other changes to the software environment, the plausibility of the calculation results shall be reviewed by comparing them with specific previous calculations. Thus, the suitability and accuracy for the specific application shall be checked again in each case.

[7] Software for geometry processing, mesh generation and the evaluation and graphical presentation of calculation results.

4.3 Data range

4.3.1 Input parameters

The input parameters to be documented in numerically based safety analyses shall include all data necessary for independent reproduction of the FE calculation. If a preprocessor is used, the corresponding file for the model in the native format of the preprocessor shall be submitted for review in addition to the input file for the FE calculation program. These files shall be stored by the applicant on a suitable medium and kept as an indispensable part of the submitted documents.

A sufficient description of the structure of the input file shall be included so that the input data may be checked at any time, even independently of the FE calculation program used.

4.3.2 Relevant results

The relevant results form the basis for the final safety assessment of the analysis results. The selection of the relevant physical variables (e.g., specific stress components or equivalent stresses, acceleration histories, part temperatures or temperature histories, etc.) shall be justified.

4.3.3 Other results

The other results (e.g., deformation figures, stress distributions, energy balances, heat flow and temperature fields) of the calculations performed shall be presented to enable simple plausibility checks.

4.4 Presentation of the result data

The scripts used to collect and process the data are part of the submitted documentation and shall be explained if necessary.

4.4.1 Data preparation

The results data shall be presented in such a way that all aspects essential for processing the respective task (documentation, discussion and verifiability of the selected FE model, evaluation and, if necessary, verification and validation of the calculation results) are available in a clear and comprehensible form. The assignment of the input data described in the analysis report to the input file of the calculation program shall be comprehensible and unambiguous.

4.4.2 Graphical representation

The calculation results should preferably be presented in graphical form. Sufficient resolution and legibility shall be ensured.

The detailed results for the particularly critical areas of the structure that are relevant to the design shall be presented based on the global representation of specific temperature, stress, or displacement fields in the overall structure or larger sub-structures. These detailed results (such as local stresses, strains and temperatures) shall be presented as a function of position or as a function of time. When simulating transient processes, such as package drop tests or heating tests, the calculation shall be performed up to a point in time at which the extreme values of the respective safety-related parameters (stresses, deformations, temperatures, etc.) have undoubtedly been reached.

Typical graphical representations include, for example:

- geometric initial configurations,
- structures deformed under load,
- stress or temperature conditions for selected structural areas and
- time-dependent displacement and stress histories.

4.4.3 Tabular representation

The results used for safety assessments shall be clearly presented in tables together with the corresponding permissible limit values.

4.4.4 Presentation of other results

The following should be presented, for example:

- graphical representations of FE mesh in severely deformed areas (e.g., areas in contact, deformation of shock-absorbing parts and penetration of the cask into yielding ground),
- displacement, speed and acceleration time histories of centres of mass or temperature time histories of selected sub-structures (lid, cask, seals, contents, moderator, etc.),
- energy balances (breakdown of partial energies[8] for the overall model or for selected sub-systems) or heat flow fields and, if applicable, heat transfer coefficients calculated by the program and
- Mass-time history or mass increase-time history if mass scaling was used to limit the timestep width.

4.5 Assessment of the calculation results

The results of the calculations shall be evaluated in accordance with the regulations underlying the safety report or, alternatively, recognized assessment concepts. The rules to be observed for the evaluation of the results and for comparison with acceptable material stresses are derived from the specific requirements for stress and temperature assessment in connection with the respective package parts and material. With regard to mechanical evaluation and material properties, reference should be made, for example, to IAEA-TECDOC-717 [15], BAM dangerous goods procedural rule 007 [16] and 012 [17], KTA regulations 3905 [18] and 3201.2 [19] and the FKM guidelines [20, 21].

4.6 Staff qualifications

Correct application of the FE method within the meaning of this guideline requires, in addition to adequate basic technical and scientific qualifications in the fields of IT, numerics and engineering, relevant experience in solving similar technical problems using numerical solution methods. The specifications set out in the NAFEMS Standard [11], “7.2 Competence,” are considered by BAM to be suitable requirements for the qualification to be proven.

4.7 Responsibilities

If the numerical safety analysis was carried out by a third party (provider), the client is obliged to ensure that the third party complies with this guideline. This also includes providing the above-mentioned evidence of the software used and staff qualifications. Furthermore, the client bears technical responsibility for the completeness and accuracy of the numerical safety assessment because, among others, the client significantly influences the analysis effort by specifying requirements when placing the order and is obliged to monitor the work of the external service provider under its own quality management system.

[8] In particular, artificial energies that may arise, for example, as a result of the use of a contact pair of type penalty or finite element approaches with hourglass control. The partial energies shall be represented relative to suitable quantities, e.g., the total energy or external work.

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Appendix Notes on modelling

Motivation

The following sections provide specific information on modelling selected parts of package designs for the transport of radioactive materials. The list is not exhaustive and the modelling described is not necessarily the only one that meets the state of the art. Modelling information specifically for LS-DYNA may also be found, for example, in the recommendations [22].

Energy-absorbing materials

Shock-absorbing parts are mainly made of materials that can absorb most of the kinetic energy in a way that reduces loads on the package parts under test conditions. These materials typically exhibit a “plateau” and or a decrease in a force-permanent deformation–plot, i.e., a softening.

Only non-local material models, those with other suitable approaches (gradient-enhanced model or higher-order continua) [23] or material models with regularization should be used to avoid localization effects resulting from softening, [24].

The purely phenomenological description of a softening behaviour directly via the stress-strain relationship in a classical (elastic-)plastic material model without regularization should be avoided and requires separate analysis of the usability of the result.

If the description of the behaviour of the shock-absorbing part refers directly to part tests and not to a material model whose parameters were identified from the part tests, this shall be taken into account appropriately in the modelling. The use of phenomenological data from the part tests as material data should be avoided.

Puncture bar impact

To model the puncture bar impact, it is necessary to have a sufficiently fine mesh of both the components coming into contact and the areas to be evaluated. The influence of the element edge lengths on the stress to be determined shall be shown in a convergence study, see also, for example, [25].

The friction between the contact surfaces has a significant influence on the calculation results in the case of puncture bar impact, not only quantitatively but also qualitatively. Therefore, the coefficient of friction to be used, which should be as physically accurate as possible, shall be determined by comparing the calculated expansion or barrel shaping of the puncture bar at the contact point with that measured after an adequate drop test. Alternatively, the influence of the friction coefficients within a range covered by the literature on the calculated stresses, especially in the contact area, may be determined within the framework of a sensitivity analysis.

According to IAEA regulations [1], the puncture bar length shall be adjusted to cause maximum damage. An iterative procedure for determining this geometry is described in [26].

Lid system and seals

Examples of modelling parts of the lid system and selected load cases are described in [27]. The assessment criteria for the lids and screws are presented in [17]. The modelling of the lid screws depends on the expected stress.[9] The preload should preferably be applied by preload elements. For example, preloading by fictitious temperatures should be avoided.

The behaviour of seals in the lid system should be modelled using special sealing elements, such as gasket elements in SIMULIA, if statements regarding the lid sealing system are to be made. These

[9] In the case of pure tensile stress, the use of bar elements may be sufficient if the local stresses around the contact surfaces are not taken into account, e.g., by using a spider bolt model for screw connections with nuts. If additional bending stress may occur, this shall be considered.

elements can be used to model the deformation behaviour during assembly, initial compression, subsequent release, and temperature dependence, see also [28]. Modelling with (1D-)spring elements directly coupled to the nodes of volume elements should be avoided.

Attachment points, in particular trunnions

The modelling of load attachment points, load application, assessment of the stress on the load attachment points and its bolts are described in [29]. The assessment criteria may be found in BAM-GGR 012 [17].

Contents

The contents of the package (e.g., basket with fuel rods or canister with highly radioactive waste from reprocessing) may be simplified by a cylindrical surrogate content or shell of equivalent mass if the structural details are not important for the analysis objective. The entire cask or parts of the cask should not be stiffened or reinforced in an impermissible manner. Moreover, the kinematics of the package before and after the impact should not be impermissibly influenced. An impact of the contents on the lid system or other inner cask areas that is relevant for the analysis of mechanical integrity and is usually delayed shall be taken into account and, if necessary, investigated. In doing so, the design-related gaps in the cask cavity, the masses and stiffness properties of the impact partners, and the contact areas shall be appropriately considered.