



Transactions, SMiRT-25 Charlotte, NC, USA, August 4-9, 2019 Division III

QUALITY MANAGEMENT, VERIFICATION, AND VALIDATION OF STRUCTURE MECHANICAL COMPUTER CODES AT GRS

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ABSTRACT

Quality assurance is a key for the development and release of software for safety assessment. Quality standards and management processes are prescribed by international guidelines and national regulations, but the formulation of appropriate quality measures and an appropriate verification and validation scope is strongly influenced by the simulated phenomena. In this contribution, the quality management, measures to ensure fixed quality features and most important the verification and validation of the structure mechanical computer codes PROST, WinLeck and ASTOR developed by GRS are discussed. The scope of the tools and the corresponding test cases are discussed. The paper summarizes criteria for a verification and validation approach as well as practical issues.

INTRODUCTION

Computer software is present in all stages of nuclear technology. Computer codes are used in the design of nuclear components, in the plant control, in the safety assessment as well as in safety research. While the relevance for nuclear safety depends on the actual application field, quality assurance is a key for the development and release of software. Consequently, quality standards and management processes, e.g. for codes used in safety assessments, are prescribed by international guidelines (IAE 2009) and national regulations, e.g. (NRC 1993). In such guidelines, functionality and accuracy are implicitly most prominent within the quality requirements, but usability and maintainability as well as efficiency are also to be considered.

A key step in the quality management is the verification and validation (V&V), which is the check of the software by appropriate test and application cases. While verification is understood as the testing of the accordance with the specification during development, validation is the proof of applicability to the designated field in an independent stage prior to the release for application. The formulation of a sufficient approach for the V&V is a significant part of software development which requires scientific insights to the simulated phenomena, see e.g. (Williams et al. 2017) and (Herb 2018) for recent publications. The paper summarizes the V&V procedures applied for the mentioned GRS codes in comparison to the various requirements provided in (IAEA 2009, NRC 1993).

This paper is organized as follows. In the next section, the general quality management approach is discussed. In the following three sections, the three structure mechanics codes PROST, WinLeck and ASTOR are presented with their approaches for V&V procedures. Because the fields of application of the three codes are notably diverse and the focus is on V&V for code development, the description of the physical details modelled in the codes are omitted in this paper, and references for further information are given.

VERIFICATION AND VALIDATION

The Specific Safety Guide SSG-2 (IAEA 2009) states that the V&V process should consist of two phases: An assessment by the developers and an assessment by an independent person or group (see Figure 1).



Figure 1. Simplified illustration of V&V steps and roles before release.

Regulatory Framework

The need for quality assurance in the development and application of computer codes is emphasised in Requirement 18 of the General Safety Requirements GSR-4 (IAEA, 2016). Regulations are given in the Special Safety Guide SSG-2 (IAEA, 2009). Additional general requirements come from the ISO standard for quality management, ISO-9001 (ISO, 2015). In the US, a specific guide regulates the quality assurance in software development in nuclear safety (NRC, 1993). In other countries, such as Germany, there is no dedicated guideline and hence the higher level regulations apply. GRS in the role of a developer of software for their assessment and simulation in the field of nuclear safety (see e.g. Schaffrath and Wielenberg, 2018) developed an approach considering the regulation of IAEA SSG-2, ISO-9001, and incorporating specific requirements for quality assurance based on expert statements and experience from research projects. It is worth to note that GRS software products include a wide range of phenomena associated with operating nuclear power plants (neutronics, thermal-hydraulics, structure mechanics), but also with geological processes relevant for waste management and deposit. As this framework is wider than the IAEA approach, some procedures turn out to be constructed close to the thermal-hydraulic simulations of nuclear power plants, and it requires an appropriate interpretation for different code scopes.

Verification scope

The aim of the verification is to ensure that the implemented numerical methods and schemes as well as the user options and their restrictions are in line with the requirements on code design (IAEA, 2009). It encompasses the verification of the code design (design concept, basic logic, flow diagrams, numerical methods, algorithms, couplings to other codes, computational environment) as well as the verification of the source code (logic, programming and language standards). As appropriate measures, the use of checklists, reviews, inspections, audits and comparisons with independent calculations are recommended. The management of non-compliances found during design or utilization phase is described as continuous reporting, correction and assessment of effects on already conducted calculations.

Validation test types

The Special Safety Guide SSG-2 specifies four types of validation tests. Basic tests are simple tests which may have analytical solutions or are derived from basic experiments. Separate effect tests study single physical phenomena without interference with other effects. The reference data in the separate effect tests should come from experiments performed at full scale, or appropriate simulations. Integral tests include all processes of importance, while the test itself might be performed at smaller scale or reduced pressure.

Nuclear power plant level tests and operational transients are based on tests on actual nuclear power plants.

The Special Safety Guide SSG-2 distinguishes between system thermohydraulic codes, core physics codes, component-specific and phenomenon-specific codes, computational fluid dynamic codes and coupled codes. The validation test types are oriented more on system thermohydraulic codes, i.e. component-specific and phenomenon specific codes are apparently less in the focus. Therefore, it is necessary to specify and to interpret the guidance, in compliance with ISO quality management standard, for the structure mechanics computer codes.

Practical realization

Test procedures are time consuming if done by hand. Furthermore, short releases and fast patches are quality attributes for its own, thus unnecessary workloads and slowdown effects should be avoided.

The effort of standardized tasks like regression tests can be minimized by a framework for automated testing. While automated testing is standard for software development, the assessment from the user (not developer) point of view is a run of defined test procedures and data sets. The implementation of mostly automated regression testing as proposed by Herb (2018) within the code validation is a promising path for efficient, fast and reliable V&V, but has to be adapted to the individual application scope and typical validation cases of simulation software. The status of realization of such automated regression testing within the structure mechanical codes PROST, WinLeck and ASTOR developed by GRS is described in the following sections of the paper.

PROST - DETERMINISTIC AND PROBABILISTIC FRACTURE MECHANICS ASSESSMENT OF PRESSURIZED COMPONENTS

PROST is mainly a fracture mechanics code for the deterministic and probabilistic assessment of pressurized tubes and vessels. A number of analytical fracture mechanical models are implemented in PROST, allowing the assessment of cracked tubes and other structures under operational and accidental load scenarios. Different damage mechanisms like fatigue and corrosion, which lead to the growth of cracks, are considered. All these methods can be used in a deterministic assessment based on the computation of fracture mechanical parameters, or in a probabilistic assessment based on the computation of leak- and rupture probabilities. Hence, the code has two scopes with different expected outputs: Detailed information of one single (or few) individual simulations, or statistics of specific events of (very) many simulations. This is depictured in Figure 2.

These two application types have impact on the validation procedure. For the deterministic application, analytical fracture mechanical models are crucial. These methods compute the stress intensity factor K, the *J*-integral and the limit load for specific structure geometries, crack configuration and load types. Those quantities, however, are partly not accessible in experimental tests, but in numerical finite element method (FEM). A typical situation is that multiple models are available for the assessment and can be compared with the similar reference data set. The validation of probabilistic applications imposes conceptual challenges, since failure frequencies are difficult to verify by experiments, and even the transfer of computed probability to real plants is challenging (Heckmann et al., 2015). Therefore code-to-code benchmarks play an important role, such as performed in the NURBIM project (Schulz et al., 2004).

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Figure 2. Deterministic and probabilistic PROST application and output evaluation.

In this context an automated workflow for simulation and result documentation with a special format for validation cases has been developed. This format allows to specify one or several PROST data sets, along with replacement options concerning the applied models. The computed values are compared with a reference data set from literature. An automated documentation of the validation test results is generated, which becomes part of the validation report of the code. Two example cases from both types of validation cases are shown in Figure 3.

The left example is taken from the fracture mechanical benchmark BENCH-KJ (test case Task 2 C3, see OECD/NEA, 2017). The J-Integral at the deepest point of a semi-elliptical crack in a straight pipe is estimated with different levels of the SINTAP assessment procedure (SINTAP, 1999). Higher levels are expected to have a higher accuracy and a wider range of applicability, thus levels 0 and 1 are restricted to load factors below 0.5. The reference values are computed with finite elements analysis. A purely informative result is the elastic calculation. The right example is taken from the NURBIM benchmark, see Schulz et al. (2004). As probabilistic applications involve very many individual computations, a test case requiring only moderate numerical effort is selected (the base case of the small pipe geometry). Different sampling techniques are applied and compared to the reference solution obtained during the benchmark. Therefore, the expectations on the accuracy are lower.

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Figure 3. Deterministic validation case (left) and probabilistic case (right).

WINLECK - LEAKAGE RATES

The WinLeck code computes leak area and the flow rate of leaks. The focus is on crack-like leaks in the coolant loops of NPPs, which prediction is important for detectability, as it is required for leak-beforebreak assessment. Thus, WinLeck computes the opening of wall-penetrating cracks under pressure and loads as well as the two-phase flow through narrow slits. For this purpose, several analytical fracture mechanical and unidimensional fluid dynamical models are implemented and can be applied.

In contrast to the system analysis of an entire plant, the simulated system is only one (generally small) location in a single pipe. Thus, with respect to the Special Safety Guide SSG-2 classification, the application scope is even smaller than for a component-specific code, and the requirements have to be interpreted within this frame. With this background, the test scope of the different validation test categories has to be identified, which requires an interpretation of what are separate effects in leak rate computation, and what is an appropriate power plant test. The current realization of the tests and examples are shown in Table 1.

Туре	Realization		Example tests
Basic tests	Numerical results of single models from the literature		KTA (2014)
Separate effect tests	Leak area	Empty tubes in test facilities	German et al. (1982)
	Flow resistance	Leak tests with cold water	John et al. (1988)
	Flow rate	Flow through artificial slits	John et al. (1988)
Integral tests	Combination of separate effects		John et al. (1988)
NPP level Tests	Real leak opened under load with plant-specific fluid conditions		Grebner (1995)

The philosophy of WinLeck is to provide easy access and combination of multiple models by their implementation in the code. For the validation of these models, the WinLeck code was used to process more than 800 experimentally measured data points from various resources (see Heckmann et al., 2018).

However, the assessment of such a large number of different tests is complex and requires a good understanding of model applicability as well as uncertainty coming up from the test conditions. Such a task is apparently suitable for an individual research project, but not for a stable regression testing program. Therefore, the validation matrix for WinLeck consists of a reduced number of well understood test series. One example of such a test series is shown in Figure 4.



Figure 4. Separate effect test for flow rate with measured leak rates from John et al., 1988

The separate effect tests in the figure are based on a leak flow series described by John et al., 1988: It is an artificial slit with measured flow resistance, hence the leak geometry and its flow resistance are known and the predictions of the flow rates based on calculations with ten different models or implementations are compared. This test series comprises accurate models as well as simplified estimation schemes which are only good in certain regimes (e.g. 'm. Be.' for large subcooling $T - T_{sat}$) and approaches with expected trend (e.g. 'Bern.' is overestimating and 'mverl' is underestimating). Such a data series of an experiment can be generated and visualized with an input file within the validation procedure.

ASTOR – INTEGRITY ASSESSMENT OF PRESSURIZED COMPONENTS DURING SEVERE ACCIDENTS

ASTOR is a Java-based structure mechanics tool currently under development at GRS providing several established and self-developed analytical models for failure assessment of pressure barrier components, including RPV, during severe accident scenarios. In the in-vessel phase of a severe accident, parts of the pressure barrier (reactor circuit) are getting heated by hot gases with temperatures up to 1500 °C from the core melt or zirconium oxidation processes, deposited radionuclides or the corium itself. If manual depressurization of the reactor circuit, e.g. as an accident management measure, proves to be unsuccessful, the components will experience a combined high temperature/high stress loading. The first failing component, the exact location and the failure mode then determine the further course of the accident and the risk of containment-bypasses, e.g. by consequential steam generator tube failure, high pressure melt ejection or containment damages from consequential hot-leg burst. Also, small early leaks, e.g. through failed instrumentation tubes, sealings or deformed flanges, can significantly influence the plant status concerning thermohydraulic processes and release of aerosols. In this load regime, particular aspects like material plasticisation, short-term creep and geometry changes have to be considered. Thus, ASTOR is a phenomenon-specific best-estimate structure mechanics tool, which might be used either standalone or in post-processing of thermohydraulic analysis, to restart calculations with modified assumptions concerning leaks or breaks in the pressure boundary. It is also prepared to be used in uncertainty analyses, e.g. with the GRS code SUSA (Kloos 2016). Since ASTOR is currently in an earlier development phase than PROST and WinLeck, the focus in the following paragraphs is laid on general quality requirements fixed within the code design and chosen features to meet these. Planned verification and validation procedures are presented as well.

Regarding *functionality*, the tool should cover all components of the pressure barrier suspected to fail and their associated failure modes, since the weakest link in the chain determines the initial failure position. A further requirement is the mitigation of conflicts of objectives for different application cases (e.g. between applicability, accuracy, detail level of input data, efficiency, ...). To meet these requirements, ASTOR is designed as collection of various analytical models with overlapping applicability and different advantages and disadvantages. The Larson-Miller-Approach (Larson and Miller 1952), e.g., has a low complexity, but shows shortcomings in the handling of geometric and material nonlinearities, while the GRS-developed model FAST covers those non-linearities at the cost of a more sophisticated material data input. Input data sets are standardized as far as possible so that the active model can be easily switched. To fill gaps that are not covered by analytical models or are too complex for analytical analysis, the tool provides a coupling to the multiple-purpose FEM structure mechanics code Code_Aster (EDF R&D 2019) within the Salome MECA platform (OPEN CASCADE SAS 2019). In this case, prepared scripts and parametrized models are completed with input data at runtime, the calculation is started, and results are evaluated automatically.

The *usability* of the tool should be simple, intuitive and robust, since parts of the target-group are experts from other disciplines not familiar with the details of structural analysis, who may use the tool in conjunction with other software. Simplicity has furthermore a general positive effect on efficiency and robustness of the code utilization. To meet this requirement, a series of design patterns are realized. A self-explanatory graphical user interface, showing only valid input data combinations, assists during input. Following the rule of least surprise, the behaviour of the GUI uses standard concepts like grouping of elements within a frame known from operating system environments. Input masks and data dependencies follow a strict left-to-right and top-to-bottom scheme. Where possible, appropriate default values and settings are suggested. As an alternative to user input, load transients, geometry and material data can be chosen from predefined data sets stored in a global library file, making ASTOR an expert system. Post-processing includes a graphical visualisation of the results using the external Java library JFreeChart (Object Refinery Limited 2019). Robustness is furthermore supported by model-specific checking routines returning information, warning and error messages as well as a series of runtime exceptions, e.g. for missing files.

A central objective for the *maintainability* of the source code is the preparation for an easy future enhancement with additional models. Maintainability further goes along with general positive effects on code quality and readability. Therefore, the internal structure of the code is divided into frontend, solver and data library. Redundant code is further eliminated by using the object-oriented capabilities of Java. New models can be built based on templates that already provide a time-integration scheme and auxiliary routines using the concept of inheritance. Wrapper classes are written to enrich often used data-structures, e.g. multidimensional arrays, with application-specific capabilities, such as structure mechanical interand extrapolation functions or GUI elements. Those basic data structures (level 0) can be aggregated to higher level structures, such as load transient, geometry data, material data or result set (level 1), component analysis (level 2), set of component analyses (level 3) or file (level 4) and stored using a xml-based format. In this way, different filetypes are built for different purposes (Figure 5). The input file contains several component analyses representing either different components of one accident scenario or variants of one calculation. The library file contains predefined data sets for loading, geometry and material data and is read at the start of the program. The output file is similar to the input file, but marked as read only, so that the results are stored together with the original input. Finally, the regression testing

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file contains a set of test cases. In Test mode, the solver compares the just generated results to a predefined result from an earlier calculation or an external source, which is used for V&V.



Figure 5. Design of ASTOR concerning the modular data structure

Verification procedures in ASTOR are organized into three categories: white-box testing, unit-tests and combined integral-/functional tests. Since the tool has only limited size and a 'flat' but modularized internal structure, the scope of verification testing can be considerably reduced in comparison to larger codes. User interface, file management and downward compatibility to older files are tested by saving and subsequent loading of prepared files that cover all storable items. For the test of the data library calculation and interpolation routines, a special GUI area can be used which provides a generic direct access to the data. Auxiliary routines within the solver are tested by using the possibility to easily declare internal values as an additional result. The integration- and functional tests cover a large spectrum of functionality, including all validation cases and applications of the interfaces to other codes. They are collected in a library that can be used for automatic regression testing (Figure 5).

For *validation*, a broad basis of sources are taken into account due to the limited number of available (large-scale) experiments in this field (e.g. Maile et al. 1990) and real accidents like TMI 2 (1979) or Fukushima Dai-ichi, Unit 1 (2011). These encompass scaled experiments, experiments on small samples, method comparisons (Arndt et al. 2017), plausibility checking and hand calculations of simple cases. Furthermore comparative analyses results from international benchmarks (OECD/NEA 2019) are considered. Validation testing procedures encompasses basic test (material models), single effect tests (thermal and mechanical effects) and integral tests (whole calculations).

SUMMARY AND CONCLUSION

This paper discusses the verification and validation approaches as well as general measures to ensure quality for the structure mechanical computer codes PROST, WinLeck and ASTOR developed by GRS. The V&V framework is imposed by an IAEA guide as well as an ISO standard, and the specific field of application requires an interpretation and specification of the quality assurance procedure. With the PROST code failure of cracked pipes can be predicted with consideration of ageing mechanisms. Typical simulation results are fracture mechanical parameters and failure frequencies, which are partly inaccessible for experimental tests. The WinLeck code computes the flow rate out of leaks, thus the scope is smaller than in a component-specific code. Concerning quality management the functional requirements and the V&V procedure of the ASTOR code have been described with consideration that the data from large-scale experiments and real severe accidents are very limited. In this context a procedure based on automated frameworks has been established to reduce the manpower in regression tests.

ACKNOWLEDGMENT

This work was performed in the framework of the German Reactor Safety Research and was funded by the German Federal Ministry of Economic Affairs and Energy (BMWi, project no. RS1551 and RS1555).

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