



ONR GUIDE			
Validation of Computer Codes and Calculation Methods			
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1. INTRODUCTION

- 1 ONR has established its Safety Assessment Principles (SAPs) ^[1] which apply to the assessment by ONR specialist inspectors (assessors) of safety cases for nuclear facilities that may be submitted by licensees, or other duty-holders – e.g. a requesting party in Generic Design Assessment (GDA). This technical assessment guide (TAG) is one of the guides developed by ONR to further assist ONR's inspectors in their assessment work in support of making regulatory judgements and decisions.

2. PURPOSE AND SCOPE

- 2 This TAG provides advice to ONR assessors on the interpretation of the SAPs covering the validation of computer codes and other calculation methods used to perform plant analysis in support of the safety cases. The guide also explains what the ONR assessor should expect to see in a validation report produced by a licensee in support of a code or calculation method used for analysis within a nuclear safety case.
- 3 This TAG is intended to apply primarily to the assessment of the validation of physics, thermal and structural analysis computer codes and calculation methods used within the design basis safety studies. Any validation submission for beyond design basis calculation methods should conform in a general way to the guidance given in this TAG. The principles outlined here are also generally applicable to transient, radiological and other analyses forming part of fault analysis and also in other areas of the safety case underpinned by analysis and/or data, e.g. engineering substantiation. Advice to inspectors assessing nuclear installations chemistry, C&I and other studies is provided in the relevant specific TAGs.
- 4 With respect to Computational Fluid Dynamics (CFD) analysis methods, which have special application, Appendix 1 provides guidance on the main issues which should be covered in CFD reports, and their significance.
- 5 Appendix 2 provides base information on the Code Scaling, Applicability, and Uncertainty evaluation (CSAU) methodology [10], which was developed by the US NRC and is considered relevant good practice for validation of computer calculations in the safety analysis area.
- 6 Practical guidance for the validation of Finite Element Analyses in the structural integrity area is presented in Appendix 3.
- 7 This TAG is not directly applicable to the assessment of the validity of software used for control and protection of operational nuclear plant and processes. These are covered in ONR's NS-TAST-GD-046 Computer Based Safety Systems, which provides references to the applicable standards, e.g. IEC 60880:2006 Nuclear power plants - Instrumentation and control systems important to safety - Software aspects for computer-based systems performing category A functions.
- 8 This TAG contains guidance to advise and inform ONR inspectors in the exercise of their professional regulatory judgement. Comments on this guide, and suggestions for future revisions, should be emailed to the HOW-2 team.

3. RELATIONSHIP TO LICENCE AND OTHER RELEVANT LEGISLATION

- 9 Licence Condition 14 - Safety documentation requires the implementation of adequate arrangements for the production of safety cases. Computer code analysis

of plant design and operation forms an important part of a modern safety case. The computer codes should be validated prior to their use in the production of safety cases.

- 10 Licence Condition 19 - Installation of new plant requires “adequate documentation to justify the safety of the proposed construction or installation”. In order to be adequate – i.e. suitable and sufficient - the documentation (safety case) should be based on safety analyses carried out by appropriately validated computer codes.
- 11 Licence Condition 22 –Modification or experiment on existing plant requires the implementation of adequate arrangements for the modification or experiment on existing plants. Computer code analysis of plant modifications forms an important part of the supporting safety cases. The computer codes should be validated prior to their use in the production of safety cases.
- 12 Licence Condition 23 – Operating Rules requires the production of an adequate safety case which identifies the necessary operating rules and operating conditions. The adequacy of these rules and conditions are often demonstrated by computer codes analyses of design basis faults.

4. RELATIONSHIP TO SAPS, WENRA REFERENCE LEVELS AND IAEA SAFETY STANDARDS ADDRESSED

- 13 ONR SAPs are benchmarked against the WENRA reference levels for nuclear installation safety and against the applicable IAEA safety standards. Computer codes validation is addressed in SAPs AV.1 to AV.8, ECE.15, etc. This guide provides additional information on the subject, assuming that the inspector is already familiar with the SAPs.

5. ADVICE TO INSPECTORS

5.1 DEFINITIONS

- 14 Many of the terms used in this TAG are already defined in the SAPs at a general level. This section provides more detailed interpretations relevant to the TAG specifics.
- 15 **Validation** is the process of testing and evaluation of the whole computer code or calculation method after the completion of its development and prior to its application to ensure compliance with the requirements of the intended application. Validation provides the evidence that the computer code or calculation method is fit for purpose by comparison of their results with data from experiments or other trusted sources.
- 16 **Verification** is the process of ensuring that the model specification has been complied with and that controlling physical equations have been correctly translated into the computer code or, in the case of hand calculations, correctly incorporated into the calculation procedures.
- 17 **Quality Assurance** is the process of reviewing, inspection, testing, checking, auditing or otherwise determining and documenting whether or not items, processes, services or documents which support the computer code or calculation method conform to specified requirements.

Note: Software Verification & Quality Management is not subject to this TAG. Useful information on this subject is provided in (Refs. 2 – 6).

- 18 The safe state of a nuclear facility is provided by the following **Fundamental Safety Functions**:
- a. Control over criticality and heat generation;
 - b. Cooling of safety critical components;
 - c. Containment of the radioactive materials.
- 19 **Safety Parameters** are plant parameters which indicate the state of the facility in terms of safety (core power, peak clad temperature, containment pressure, etc.). A safe state is established when the safety parameters are within their safety limits.
- 20 **Fault studies** predict the safety parameters behaviour during postulated events to check whether the facility will remain in a safe state during the event (or not). The prediction is based on computer simulation of the relevant equipment and processes.
- 21 **Safety margin** is the difference between: the worst value predicted for a safety parameter occurring during the postulated event, and the relevant safety limit.
- 22 **Fault studies computer code** is a computer code which applies specific physical correlations and mathematical methods to model (partly or completely) a facility and simulate its behaviour during postulated fault transients. The input data for such codes is usually separated in two groups: (1) parameters of the facility structures, systems and components (SSC) and (2) assumptions for the sequence of events (systems operation/failures, operator actions, etc.). The results provide predictions of the facility safety parameters and allow for evaluation of the safety margin available in each case.
- 23 The **Conservative codes**/approach to fault studies aims to calculate a system response using limiting values of model parameters bounding the uncertainty arising from measurement errors, knowledge insufficiency and modelling simplifications by modification of the known physical correlations, measured data and accident conditions in a way that tends to reduce the estimated safety margins. The purpose is to provide a robust demonstration that adequate safety margins are preserved with a high level of confidence. For example, SAP FA.7 recommends: "Analysis of design basis fault sequences should use appropriate tools and techniques, and be performed on a conservative basis to demonstrate that consequences are ALARP".
- 24 The main advantage of the conservative approach is its capability to construct an integral model of a complicated system while keeping the cost of model development and running at a reasonably low level.
- 25 The main disadvantage of this approach is that excessive pessimisms could lead to grossly unrealistic results and prevent a balanced assessment of risk. The inspector must clarify the grounds for selection of the conservative values and assumptions applied in each case.
- 26 The **Best Estimate codes/approach** applies the available realistic information about plant parameters, behaviours and phenomena so as to provide an unbiased estimate of the system response. It is used primarily in Probabilistic Safety Assessment (PSA) for evaluation of DBA Initiating Fault Frequencies (IFFs), and for Severe Accident Analysis (SAA).
- 27 The main advantage of this approach is the production of a realistic view of the accident development. From the licensee's perspective, the combination of a realistic model with a statistical treatment of uncertainties can provide a larger demonstrated

safety margin than using a set of pessimistic data. This method is internationally referred to as “Best Estimate Plus Uncertainty” (BEPU).

- 28 The main disadvantage of this approach is related to the risk of arriving to unreasonably optimistic results due to inadequate treatment of uncertainty. It is worth noting that uncertainty quantification demands significant resources.
- 29 The inspector should compare the treatment of uncertainty against established good practices e.g. the CSAU method recommended in a US NRC guide (Ref. 10).

5.1 GRADED APPROACH

- 30 The graded approach to assessment of computer calculations is applied in line with the ONR principle of proportionality, i.e. application of effort and expenditure of resources in proportion to the safety significance of the subject.
- 31 The assessor should be aware of where the calculation fits in the overall estimate of risk presented in the safety case and should have an understanding for the level of results confidence and uncertainty qualification of any calculated results. For example, SAPs (Figure 1) illustrate the inter-relationship between the three types of fault analysis, DBA, PSA and SAA, and how, in combination, they address the range of potential initiating events with nuclear safety significance off the site.
- 32 Where a **deterministic safety case** is made, analysis will demonstrate to a high level of confidence that safety measures are effective for events initiated within the domain of operating conditions permitted by the plant operating rules (see TAG 35 [14]). The analysis should ideally quote and substantiate confidence levels for its calculations. Where this is not practicable, the safety case should provide enough information to allow a judgement to be made that the results are suitably conservative.
- 33 However, it may not be reasonable to consider an event where all extreme conditions occur simultaneously. For example, fault sequences occurring in extreme conditions can reasonably be limited to events with a predicted frequency (probability) in the region of 1.E-7 per year. For events of such low probability it is reasonable to account for only the most significant uncertain parameters. The required level of validation rigor should be proportionate to the risk significance of the analysis.
- 34 In the case of frequent events (which are anticipated within the life of the facility or within the life of a fleet of similar facilities) it may be appropriate to apply statistical techniques to demonstrate that the protection provided by the plant design meets the selected acceptance criteria.
- 35 Some fault sequences which fall outside the design basis still require analysis to demonstrate that the available safety measures are reasonably practical. Such analysis will normally consider the likely plant response and therefore the use of best-estimate approach may be suitable.
- 36 The inspector should consider the level of statistical rigor appropriate to the study of each particular fault and compare that presented against established practice. The cost of data needed to substantiate analysis methods should also be considered in the formulating of regulatory expectations.

5.2 VALIDATION REPORT - GENERAL EXPECTATIONS

- 37 ONR expects a licensee to present a validation report for each of the computer codes/calculation methods used in a safety case. The ONR assessor needs to be satisfied with this report in a number of areas as explained below.
- 38 The validation report should identify the shortcomings in the computer code method of solution, the uncertainties of the associated physical models and the inaccuracy in the experimental data used in the validation work. This information should be used to define the sensitivity analyses to be performed as part of the safety case. The object of such analyses is to confirm and demonstrate that “cliff-edge effects” do not exist. The sensitivity analyses should cover the uncertainties/approximations in the mathematical models, input data and boundary conditions of the analysis.
- 39 A validation report which complies with the established good practices is expected to cover the following areas:
1. limits of application;
 2. details of models used;
 3. details of numerical methods;
 4. correlations used;
 5. treatment of uncertainty:
 - a) comparisons with experimental data; b) comparisons with plant data;
 - c) comparisons with analytical solutions; d) comparisons with other calculation methods; e) bias calculations; f) review of new data;
 6. uncertainty of best estimate calculations;
 7. user's proficiency
 8. quality assurance;
- 40 Each of these items is discussed in more detail in the following sub-sections.

5.2.1 LIMITS OF APPLICATION

- 41 The validation report should define the limits for application of the calculation method and indicate the dominant processes which are expected to occur in any situation to which it is applicable. The limits of applicability are often based on an identifiable change in the dominant processes which are predicted to take place. Calculation methods are often developed to cover a limited range of plant states (e.g. flow regimes). Consequently, different calculation methods may be used for modelling different phases of the analysed fault.
- 42 The inspector should make sure that the validation report defines the processes which the calculation method is designed to model and identifies the changes in those processes which make the method no longer applicable outside the identified limits.

5.2.2 DETAILS OF PHYSICAL MODELS USED

- 43 The derivation of the equations used to model the various processes and the simplifying assumptions made should be fully described. Modelling a fault progression requires the development of mathematical equations to describe the processes which are believed to occur. In general, a number of simplifications are made to enable a tractable formulation. For example, complex three-dimensional

geometries may be reduced to one- or two-dimensional approximations in order to simplify the modelling. This is particularly true in modelling turbulence and neutron transport. The validation report should enable the assessor to follow the derivation of the controlling equations and should justify any simplifying assumptions.

5.2.3 NUMERICAL METHODS

- 44 In many cases the physical complexity of the process being modelled means that an analytical model of the entire domain cannot be derived. Solution of the controlling equations requires numerical approximation techniques, such as finite differences and finite elements methods. The validation report should justify the solution methods used and should demonstrate the accuracy of the numerical approximation. Numerical problems that can occur with such techniques should be listed along with an explanation as to why they will not invalidate the calculations for the safety case.
- 45 The codes should apply internal procedures to check that the numerical schemes employed provide compliance with the basic conservation laws throughout the calculation. There should be a demonstration, by successive refinement, that the nodalisation used is fine enough to provide a converged solution. Where such approach is not practicable, the report should provide substantiation against integral experiments and explain why any lack of convergence does not invalidate the results.
- 46 Deterministic methods may be inherently more accurate for the range of conditions upon which the physics is based but validation outside of this domain is questionable. Monte Carlo methods may be subject to good validation in their domain but still fail to converge under certain scenarios, which should be a focus for additional validation effort. Multi-physics assessment is subject to the use of several methods and, just as importantly, several interfaces between physical domains. For this reason, only limited credit may be claimed in safety analysis for the use of multi-physics analysis (e.g. hydrodynamic codes), and there should be an expectation of diverse and sound safety arguments in addition to code results.

5.2.4 CORRELATIONS USED

- 47 Sometimes the physical complexity of the process being modelled means that the full set of governing equations is not tractable or that it is not practicable to derive them from first principles. In these cases, empirical correlations may be used to represent the essential parts of the physical process and so enable the problem to be 'closed'.
- 48 The validation report should present the important empirical correlations along with their ranges of applicability. This should be supported by a description of the technical basis and justification for the use of each correlation in the range of interest to the safety case. The report should also explain what steps have been taken to prevent the correlation being used outside that range.

5.2.5 TREATMENT OF UNCERTAINTY

- 49 The simplified check-list presented below is neither mandatory nor exhaustive. Still the inspector should check for:
- Identification of the input parameters with highest impact on the analysis results (operational experience, experiments, previous calculations, expert judgment,).
 - Establishment of the expected uncertainty intervals of the most important input parameters (e.g. based on measurement precision).

- Sensitivity calculations with input variations within the uncertainty intervals to establish the confidence bands for the key safety parameter(s).
- Comparison of the confidence bands for the key safety parameter(s) against the identified safety margins.
- Consistency of the calculated results with the conclusions of the validation report.

Comparison with experimental data

- 50 One way of testing the combined effect of the various elements of the mathematical modelling is to compare the calculated predictions against experimental results. Two types of experiments are used: 'separate effects' tests are designed to examine at the most a few phenomena, while 'integral' tests are designed to enable most of the phenomena of interest to the nuclear installation to occur in an interactive way. Commissioning test results could also be a useful source for code validation and may be necessary to demonstrate compliance with SAP AV.1.
- 51 Integral tests are usually limited to fairly small scales by considerations of cost and complexity. Data from both types of experiments should be used to validate the predictive capabilities of the computer code/computation method.
- 52 Assessors need to be particularly aware of the potential selective use of "comfortable" experiments in the validation report and should seek justification for the exclusion of other experiments which seem relevant.
- 53 When analysing separate effects tests, the correlations that are being tested should be identified and reference to the claimed accuracy of prediction should be made. A distinction should be drawn between any data base that was used to develop the correlations and that which is being used for the validation exercise. Wherever possible, comparisons should be made with integral experiments at a range of scales to explore the ability of the calculation method to extrapolate from small scale tests to the conditions of the nuclear installation in relation to such integral experiments.
- 54 Many calculation methods are 'tuned' to a greater or lesser degree to results from a specific experimental facility. Tuning is the process of recalculating the same test case with adjustments, for example, in input parameters, user options or nodalisation until the best possible agreement is obtained. A calculation method that has been gradually tuned to a succession of slightly differing test cases may show excellent agreement with results from a particular facility. However, its actual predictive capabilities can only be established by calculations for a range of different facilities.
- 55 Code results are sure to fit with the experiments used as a basis for code tuning. Hence such experiments should be excluded from the set used for code validation.
- 56 If additional experimental data is required as part of a study, the inspector should consider whether it is appropriate to carry out 'pre-test', 'blind' or 'double-blind' calculations. The delivery of formal definitions of these terms is beyond the scope of this TAG, but brief clarifications are provided below to guide the inspector's work:
- A 'pre-test' calculation is carried out prior to the test being done and has to assume appropriate initial and boundary conditions.
 - A 'blind' calculation is usually carried out after the test and will employ initial and boundary data from the actual test.
 - A 'double-blind' calculation is a more restricted blind calculation on a facility for which the user has no prior modelling experience.

Comparison with plant data

- 57 Tests carried out in full sized plant during commissioning or start-up procedures, as well as operational transients or accidents, can be a useful source of data and should, where practical, be included in the validation report. In general plants are now well instrumented and licensees should be encouraged to retain and analyse data from plant transients.

Comparison with analytical solutions

- 58 Certain well defined problems may have established analytical or numerical solutions. Also asymptotic analytic solutions may be available for limiting cases. In the areas of structural mechanics and neutron physics for instance, numerical 'benchmark' problems already have a long tradition. The use of numerical benchmark problems will provide information on the mathematical solution ability of the calculation method rather than on the physical modelling and their value may be limited. Nonetheless it is important to ensure that numerical solution errors are small compared with modelling errors and benchmark problems may be a way of establishing bounds on these errors, albeit for limited types of problems. A numerical benchmark problem requires:
- a) the model equations to represent a well-posed mathematical problem with an unique solution;
 - b) every term in the equations to be defined and written down explicitly;
 - c) the initial and boundary conditions to be defined explicitly.

Comparison with other calculation methods

- 59 In addition to comparing the calculations with experiments, useful information can be obtained by comparing one calculation method against another. The comparison calculation method should have been developed independently of that used in the safety case and should be sufficiently different from it in either numerical methods or physical modelling to make the comparison worthwhile. Clearly, comparison with a calculation method which is a derivative of or very similar to that used in the safety case would not necessarily yield useful results.
- 60 The calculation method used for comparison will also need a statement about its validation, and the inspector should consider whether it has been subject to appropriate testing and practical application.

Uncertainty of best estimate calculations

- 61 A best-estimate calculation employs modelling that attempts to describe realistically the physical processes occurring in the plant. The modelling should provide a realistic calculation of any particular phenomenon to a degree of accuracy compatible with the current state of knowledge of that phenomenon.
- 62 Deriving the overall uncertainty for a best-estimate calculation method may be a difficult undertaking. Uncertainties are not restricted to the combined effect of uncertainty in input data. This can also come from applying models derived from small scale experiments to the full-sized plant (scaling uncertainties), as well as from the uncertainties associated with the initial and boundary conditions. The overall calculation uncertainty estimation should take all such factors into account.
- 63 The methodology used to combine the various sources of calculation uncertainty should be described and justified. The bias of any such judgements should be clearly

stated. Justification should be provided for the assumed uncertainty distribution of each parameter which is judged to be of relevance to the overall uncertainty.

Inherent calculations bias

- 64 Uncertainties in the representation of important physical processes may be such that models of these processes have biases built in the calculation procedure. Any bias in the calculation needs to be quantified based on experimental data and allowed for in the final evaluation of the available safety margin.

5.2.6 QUALITY ASSURANCE

- 65 Additional to the justification of the modelling process, there is a need to establish that the computer code correctly represents the physical model by ensuring that a systematic approach has been adopted for designing, coding, testing and documenting the computer program. In this respect the American Nuclear Society has produced a useful guide against which the degree of assured quality can be judged, namely, ANSI/ANS-10.4-2008 [2].
- 66 A computer code should be validated and verified for the particular engineering application, hardware and software configuration used in the safety analysis. The validation report should present details of the hardware on which the code was run and version numbers for the supporting software such as compiler, linker, loader and library routines. Evidence that the hardware and software have been suitably qualified should be provided. The process of change from one software platform to another should be supported by an appropriate set of regression tests.
- 67 User manuals should be suitable for their purpose and of an appropriate standard: IEC Standard 26512-2011 [3] provides guidance on the content of software and user documentation against which the report can be assessed.
- 68 Evidence that the software has been produced and maintained to the required standard for the application should be sought. For example, conformance with ISO 9000 series [4, 5 & 6] will indicate that good programming practices have been used.
- 69 The validation report should demonstrate that the sections of code used in the generation of the results have been adequately tested by sample problems and benchmark calculations (Reference [5] provides guidance on this subject).
- 70 Evidence should be supplied that adequate procedures are in place to control the production and maintenance of the computer code used in the safety case. In particular, there should be auditable controls over how source code can be amended and new versions issued. Collectively these procedures are known as Configuration Management. Compliance with relevant company, national and international standards, codes of practice or guidelines should be demonstrated.
- 71 The preparation of input data for the calculations should also follow rigid validation procedures and should be auditable so as to assure their quality. Each item of data should have a clearly defined origin within the plant documentation or else its source should be identified and justified. Details and justification should be given of data embedded in the code. Since it is often impossible to check manually the integrity of all input data, there should be suitable measures within the computer code to identify input data errors and erroneous results.

5.2.7 REVIEW OF NEW DATA

72 Computer codes validation should be regarded as on-going process and not as a once-and-for-all act. As new experimental results and/or plant data become available, the computer code developers should demonstrate that the calculated results are in good agreement with the new data. The licensees on the other hand are expected to demonstrate that their safety case is valid by application of codes which represent the new data correctly.

5.2.8 USER'S PROFICIENCY

73 The validation report should contain sufficient information to enable ONR to make a judgement on the proficiency of the code/method user(s).

74 User effect has been examined in References 7 and 8 which point out that the analyst must have a good knowledge of:

- a) the nuclear installation systems;
- b) the phenomena addressed, applicability of the models and their limitations;
- c) the meaning and significance of the input and output variables;

75 Given the complexity of the issues, the codes should not be treated as "black boxes". For example, the time step convergence should be checked through sensitivity studies. If numeric instabilities cannot be avoided, the validation report will need to provide special justification for any reliance being placed on the results.

76 'Blind' or 'double-blind' calculations of test problems provide a particularly important source of information for the validity of a computer code and whenever possible the validation report should include such calculations.

77 Where international bodies such as the CSNI offer relevant international benchmark exercises, the inspector should consider raising a research project to facilitate ONR's participation in these activities.

78 It is also important that the licensee's organisation is set up to support the proficiency of users. There should be adequate procedures for reviewing calculations methods and data used by suitably qualified experts. The licensee is expected to establish suitable peer review groups with relevant experience in interpreting experimental and plant data. These groups should endorse the codes, their application to the problem in hand and the competence of the users. This means that there is an adequate resource for reviewing calculation methods and data used by keeping abreast of expert opinion, relevant scientific and engineering knowledge and understanding, plant data and experimental data. For a code which has been widely applied and accepted in a series of safety cases, confidence in the user is also increased by comparison of new results with past analyses to confirm that variations in conditions have the physically expected effect, or remain in accordance with previous experience.

79 Some confidence can be gained if the calculation method has been approved for use in safety case calculations by relevant committees. Methods developed within the UK nuclear industry will generally have been subjected to detailed examination by expert committees and a particular version is usually approved for use in specified applications. An endorsement of a calculation method for safety case calculations by the licensee's own safety assessors would add further weight to the validation report provided the usage is within the conditions of the endorsement.

6. REFERENCES

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7. GLOSSARY AND ABBREVIATIONS

BEPU	Best Estimate Plus Uncertainty
CFD	Computational Fluid Dynamics
CSAU	Code Scaling, Applicability, and Uncertainty Evaluation
CSNI	Committee on the Safety of Nuclear Installations
DBA	Design Base Analysis
GDA	Generic Design Assessment
IAEA	International Atomic Energy Agency
LWR	Light Water Reactor
MC/QE	Models and Correlations Quality Evaluation
NPP	Nuclear Power Plant
NRC	Nuclear Regulatory Commission
ONR	Office for Nuclear Regulation
TAG	Technical Assessment Guide
PIRT	Phenomena Identification and Ranking Table
PSA	Probabilistic Safety Assessment
SAA	Severe Accidents Analysis
SAPs	Safety Assessment Principles
SOAR	State-of-the-Art Report
SSC	Structures, Systems and Components of a nuclear facility (installation)
WENRA	West European Nuclear Regulators' Association

APPENDICES

APPENDIX 1: GUIDANCE FOR THE ASSESSMENT OF COMPUTATIONAL FLUID DYNAMICS (CFD) SIMULATIONS IN SAFETY CASES.

A1.1 CFD is a powerful, rapidly evolving, simulation tool used for the prediction and analysis of fluid flows. The reliance which can be placed on results of CFD simulations depends on a number of issues, such as the modelling of physical processes, numerical sub-models employed, user expertise, etc. The main objective of this Appendix is therefore to provide guidance to assessors of safety cases on the main issues which should be covered in CFD studies, and their significance. Notably this Appendix aims to provide guidance on the main sources of uncertainties related to the use of CFD and on the methodology used for their quantification. The CFD validation experience accumulated by the petro-chemical industry could also be worth considering when searching for examples of good practice.

Sources of Uncertainty in CFD Simulations

- A1.2 Initial and Boundary Conditions: Inlet flow parameters often have high uncertainty. Initial and boundary condition may result from a system code calculation which gives only 1D area averaged flow parameters whereas, CFD requires 2D inlet profiles. This can be overcome if the system boundary is selected at a point with reasonably well developed flow; for which the turbulent energy and scale profile is known. In any event, assumptions should be justified and appropriate sensitivity studies performed.
- A1.3 Physical properties of the materials: the assessor should verify that the source data library and the associated uncertainties are justified, together with its range of applicability and the interpolation methods used,
- A1.4 Uncertainties related to the parameters of physical models: wall functions will almost always be used to resolve economically the region of local equilibrium of turbulence energy. These are sources of uncertainty in the same way that all closure models for free-stream turbulence. Some good work on appropriate relations for mixed convection was done at Manchester University [9]. The assessor should find grounds for confidence that the assumptions are appropriate to the conditions analysed.
- A1.5 Numerical uncertainties: ONR should resist accepting analysis without adequate quantification of numerical error. Expect to see a demonstration of the effect of the size of mesh and time step and pay particular attention to cell Peclet number. CFD methods can be coded with their own estimate of numerical error. This can be used to confirm an appropriate solution, or for automatic mesh refinement. Such approach should be encouraged. In general, linear discretisation in spatial or temporal domains should be treated with particular caution.
- A1.6 Uncertainties due to scaling: The local geometry and the values of some non-dimensional numbers can be out of the range of the model employed. For example, care should be taken to ensure that buoyancy is adequately represented if the Raleigh Number requires this. The assessor should also ensure that experiments used to qualify the model are performed at appropriate values of the governing non-dimensional groups. Moreover, the assessor should verify that any simplification of the local geometry – (i.e. not modelling the presence of nozzles) is justified, since it may have a large impact on the calculation results.

- A1.7 Uncertainties arising from physical instabilities and/or chaotic behaviours in Navier-Stokes equations can be computed with small changes in the input data. In cases where this may be relevant (such as regions of boundary-layer separation), the use of steady-state solutions should be discouraged and/or the use of stochastic uncertainty sampling encouraged. Notably, it is judged that the use of 59 samples is sufficient to comply with the 95/95 criterion.
- A1.8 Closure models: the closure models used, should be based on experimental data representative of the processes and parameters analysed.
- A1.9 User proficiency: The assessor has to keep in mind that CFD-generated results rely strongly on the competence and expertise of the user. It is generally accepted within the CFD community that the user is one of the prime causes of uncertainty in results of CFD simulations. To construct a CFD model of a particular flow the user must have a good appreciation of the physical phenomena which are significant. The reason is that at the outset the user must specify, for instance, whether the flow is laminar or turbulent, steady or unsteady, whether the Boussinesq approximation for buoyancy effects is applicable or not, what are appropriate and sufficient boundary conditions, etc. Hence training in fluid mechanics is essential for a competent user.
- A1.10 User competence is thus a major issue in CFD applications. The licensee should therefore be recommended that submissions which include results of CFD simulations should provide evidence that the analysis has been carried out by competent users.
- A1.11 Guidance on CFD simulation in the context on Thermal Hydraulic safety can be found in OECD CFD Best Practice Guidelines (BPGs) (NEA/CSNI/R(2014)) [11].

Uncertainty Quantification

- A1.12 The two main types of methods for Uncertainties Quantification of system codes (methods based on the propagation of input parameters uncertainty and methods based on the extrapolation of accuracy) may be extended to CFD with some adaptation that should be accurately justified.
- A1.13 An example for determination of results uncertainty by the propagation of input parameters uncertainty is found in the PREMIUM benchmark on the quantification of the uncertainty of the physics models in system thermal-hydraulic codes (www.oecd-nea.org/nsd/docs/indexcsni.html) [12].
- A1.14 An example of uncertainty quantification by extrapolation of accuracy can be found in EVALUATION OF RICHARDSON EXTRAPOLATION IN COMPUTATIONAL FLUID DYNAMICS, Numerical Heat Transfer, Part B, 41: 139± 164, 2002.
- A1.15 The assessor needs to be aware that the uncertainty due to numeric error is of primary importance compared to other sources of uncertainty; even if methods for numerical error evaluation are applied, they may fail or be difficult to use in practical applications.

APPENDIX 2: SCALING OF PARAMETERS BETWEEN REACTORS, EXPERIMENTAL FACILITIES AND COMPUTER CODES

A2.1 Integral and separate effects testing of analysis models should be carried out under conditions as representative as possible of the plant to be studied. Since integral experiments are often not carried out at full scale, account needs to be taken of the effect of changes in scale. The main objective is to preserve kinematic and dynamic similarities between the test facility and the plant.

A2.2 Two useful sources of information on the subject are recommended:

- NUREG/CR-5249 EGG-2552 R4 Quantifying Reactor Safety Margins Application of Code Scaling, Applicability, and Uncertainty Evaluation Methodology to a Large-Break, Loss-of-Coolant Accident US NRC, December 1989^[10]
- The OECD/NEA/CSNI State-of-the-Art Report (SOAR) on Scaling, 2016^[13]

Scaling fundamentals

A2.3 In general, the dynamics of a system depends on the balance of forces and inertia and this can be preserved by preserving the ratio of forces represented in relevant non-dimensional groups. For example, the extent of turbulence within a flow can be represented by preserving the balance of viscous and inertial forces expressed in the Reynolds Number.

A2.4 Scaling correlations can usually be derived from the dominant physics in each phase of the transient and similar values of key parameters used in the test rig to those anticipated in the reactor. It is difficult to reach sufficient level of resemblance between the behaviours of the reference system and the experimental model for all phenomena in a given transient as the dominant phenomena will change from one phase of the transient to another and with this, the scaling groups also will also change.

A2.5 Scaling distortion is generally attributed to three groups of factors:

- a) assumptions and simplifications in scaling methods
- b) limitations in constructing and operating test facilities
- c) issues the computer codes scaling capability

A2.6 The analyst needs to preserve the important local phenomena and reduce scaling distortions as much as possible. The important phenomena and processes can be identified from the phenomena identification and ranking table (PIRT) developed in a suitable expert workshop. For example, CSNI has published PIRT for a number of fault analyses in Light Water Reactors (LWR).

CSAU – An established methodology for quantification of uncertainty

A2.7 Ref. 10 is an US NRC guide (NUREG) for application of the CSAU methodology in the analysis of Large Break Loss of Coolant Accident for Pressurized Water Reactors.

A2.8 NRC claims that CSAU is a systematic approach that can be used to identify and quantify overall nuclear reactor uncertainties.

A2.9 The methodology consists of 3 key elements:

- a. Requirements and Capabilities, in which the scenario modelling requirements are identified and compared to computer code capabilities to determine the code applicability to the particular scenario and to identify potential limitations.
- b. Assessment and Ranking of Parameters, in which the code capabilities to calculate processes important to the scenario are assessed against experimental data to determine the code accuracy, scale-up capability, and ranges of parameter variations needed for sensitivity studies.
- c. Sensitivity and Uncertainty Analysis, in which the effects of individual contributors to the total uncertainty are obtained and the propagation of uncertainty through the transient is properly accounted.

Checklist for successful application of CSAU

Modelling Requirements and Code Capabilities

- 1) The nuclear power plant and its operating state are specified.
- 2) The fault progression scenario is defined and logically subdivided into physically descriptive phases. A PIRT process that identifies and ranks the important processes and phenomena related to the plant and scenario is completed:
 - The most cost-efficient, yet sufficient, analysis reduces all candidate phenomena to a manageable set by identifying and ranking the phenomena with respect to their influence on the safety parameters that are tested against the acceptance criteria.
 - Each phase of the scenario (and the relevant system components) is separately investigated.
 - The processes and phenomena associated with each component are examined. Cause and effect are differentiated.
 - After the processes and phenomena have been identified, they are ranked with respect to their effect on the safety criteria for the analysed transient. PIRT is established to guide the subsequent uncertainty quantification.
- 3) A computer code is specified. The code is a frozen version of a mature computer code.
- 4) The code documentation, that includes a Models and Correlations Quality Evaluation (MC/QE) report, defines its modelling capabilities, simulation quality, and proper use.
- 5) The code is demonstrated to contain the physical models essential for simulating those components and phenomena identified and ranked in the PIRT.
- 6) The assessments have been accomplished at various scales, and it is demonstrated that the code models and correlations are capable of simulating the phenomena at various scales.

- 7) For those models and correlations that are less certain because of basic and/or scale-related limitations, the deficiencies are identified for later quantification of their uncertainty.

Assessment and Ranking of Phenomena and their representative Parameters

- 8) An assessment matrix is developed which includes separate effects and integral effects tests. The test condition ranges are sufficient to span the nuclear power plant conditions. Test results from facilities of different scales are included for evaluating scale effects.
- 9) The facility nodalisation is defined and it is demonstrated that the nodalisation scheme:
 - a. Can be used to simulate the various phenomena and processes in the separate effect tests;
 - b. Can similarly be used for systems simulations of the integral-effect tests;
 - c. Provides representative plant simulations or a separate bias can be quantified to account for any deficiencies;
- 10) A judgment of code accuracy is made, using:
 - a. Comparisons between code and experimental data with the NPP nodalisation scheme;
 - b. Combinations of individual contributor uncertainties determined with NPP calculations or bounding assumptions.
- 11) The effects of scale on the uncertainty can be quantified or bounded for each important contributor in terms of bias and distribution, or a separate bounding bias can be formulated.

Sensitivity and Uncertainty Analysis

- 12) The effects of uncertainties in the NPP initial operating state and the code capabilities to duplicate that state are quantified.
- 13) NPP calculations are performed, defining the sensitivity of safety-related variables to plant and model uncertainties.
- 14) The individual uncertainties in terms of the primary safety criteria (resulting from code limitations, scale, NPP input, etc.) are combined.
- 15) Individual contributors that are not quantifiable in terms of bias and distribution because of economics or insufficient data are conservatively bounded and used as separate biases.
- 16) A statement of the total uncertainty of the code in calculating the primary safety criteria is made, using a justified combination process.

APPENDIX 3: GUIDANCE FOR THE ASSESSMENT OF COMPLEX FINITE ELEMENT STRUCTURAL SIMULATIONS IN SAFETY CASES

A3.1 Computer simulations have been used extensively for structural assessments in the nuclear industry, to support licensee's safety cases for initial design, plant life extension or justification for modifications. Finite element analysis (FEA) simulations may be routine and straightforward requiring little detailed assessment by ONR. Conversely they may involve complex interactions of subsystems or components and exploration of the system's performance over a wide range of environmental and operating conditions. Simulation of these complex problems can involve considerable uncertainties which need to be reflected in the safety case and may require more detailed assessment by ONR.

A3.2 When assessing complex FEA structural simulations, the inspector needs to be aware of the geometric complexities and tolerances, material properties, aging effects, operating environment, and component interactions. The inspector needs to examine all operating, abnormal, fault and extreme conditions to understand changes in safety margin, reliability, aging effect and the need for increased maintenance and inspection. However, the inspector should bear in mind that the ultimate goal is to assess that the safety margin, with the consideration of the associated uncertainties, is still sufficient for the plant to operate within the safety envelope.

A3.3 In order to assess the uncertainties in the safety margin, the inspector should start with assessing the rigor of the validation of the FEA model.

Validation of the FEA model

A3.4 Ideally the FEA model would be validated by direct experimental testing. However, it is not always practicable or financially viable to commission testing to validate a structural simulation; in this case, validation via extrapolation is normally conducted.

A3.5 In the case of validation of an FEA model by experimental testing, the inspector needs to consider firstly, whether the proposed experimental facility captures key phenomena being investigated; secondly, that experiment is scaled to provide a direct link between the scaled facility and prototype plant; thirdly, that adequate high-quality measurements are available to ensure that experimental data uncertainties are quantifiable and acceptably low; and lastly, the extrapolation from the test conditions to the plant conditions is justified.

A3.6 Experimental validation matrices may include data from experimental facilities at different scales, so that scaling effects can be evaluated to identify any scaling distortions and provide confidence in scaling assessments performed as part of the validation process. Ideally, extrapolation requires that two or more different scale experiments, the associated simulations be conducted and the validity of the simulations be demonstrated. These simulations should be shown to resemble the system being assessed; the similarity being a significant factor when the work is reviewed.

A3.7 Although the licensee is normally interested in the global effect of the system under certain conditions, one should not lose sight of some local effects that could also play a significant part in the safety requirement. Therefore, validation of the simulation of local interactions, e.g. a detailed 3D sub-model to calculate the contact pressure or local deflection, is similarly important in assessing the credibility of the analysis that supports the safety case.

A3.8 Having established the validity of the various scale simulations of the same system, the last but most important step for the licensee is to justify the validity of the extrapolation. The licensee should lay out these arguments in a clear and concise manner in their safety case.

A3.9 In situations where experimental validation is limited, the inspector may need to exercise considerable judgement on the level of validation that has been achieved. They will need to consider whether this is adequate for the safety case taking into account the complexity of the analysis and the uncertainties that have been allowed for in the case.

Uncertainty in the safety margin

A3.10 The licensee needs to provide a statement on the uncertainty with the nuclear safety requirements used as the basis for determining the acceptability of the proposed claims. This is accomplished when the effect of important individual contributions to uncertainty in the primary safety criteria are determined. These individual contributions are then combined to give the desired uncertainty statement. The statement of total uncertainty for the analysis should be given as an error band or a statement of probability for the limiting value of the primary safety criteria.

A3.10 The ultimate objective of the inspector for the assessment of the structural simulation in the safety case is to evaluate the various aspects of the uncertainties and assess the veracity of the total uncertainty statement.

A3.12 The inspector needs to be aware that the uncertainties in the structural simulations come from:

- Operating state, i.e. initial conditions including design and manufacturing tolerances, uncertainties in the operating conditions etc.
- Modelling methodology, e.g. 2D or 3D simplifications and assumptions
- Contact behaviour, e.g. friction coefficient
- Boundary conditions
- Material aging effect
- Spatial discretisation, i.e. mesh density
- Temporal discretisation, i.e. time steps

A.3.13 If the total uncertainty error band of the safety margin is so large that the minimum safety margin is insufficient for the safety criteria, the safety case needs to justify whether the probability of the minimum margin could satisfy the operating requirement. A safety case made on this basis is likely to result in increased inspection frequency or more stringent monitoring conditions.

General Questions on an Organisation's Simulation Capabilities

A3.14 The inspector should consider assessing the organisation's simulation capabilities prior to any new use of simulations, any new class of simulations, or prior to any simulations for high-consequence regulatory decisions. Assessment can focus on some or all of the following:

A3.14.1 What is the intended use of the simulations?

- What decision must be made and what strategy should be used in the simulation to adequately inform the decision? This decision is usually in conjunction with testing.
- What environments and scenarios of the system need to be assessed?
- What are the important system response quantities that are relevant to the nuclear safety requirement, upon which decisions will be made?

A3.14.2 What is the geometric, or representational, fidelity in the simulation model and is it adequate for making the intended decisions?

A3.14.3 What are the most important physics and material models and what can be said about the applicability and accuracy (including measurement uncertainties) of these models for the intended use?

A3.14.4 What evidence exists that codes are solving the equations correctly and what is the numerical accuracy of simulation results?

A3.14.5 What is the relevant experimental database against which model accuracy is assessed?

A3.14.6 What is the extent of model extrapolation outside of the validation database?

A3.14.7 What are the most important sources of error, uncertainty, and variability in the formulation of the simulation model and how do they impact simulation results?

A3.14.8 What is the maturity of the organisation in performing the proposed simulations?

- Do the analysts have expertise and experience in performing similar simulations?
- Is the infrastructure adequate, i.e., computers, memory, storage, codes, etc.?

A3.15 Many organisations equate the credibility of simulation results with the experience and judgment of their senior analysts. Without diminishing the value of senior analysts, an evidence-based approach to simulation credibility will reduce both the technical risk of producing incorrect simulation results and management's risk in the use of simulation results in a decision-making context.