Nuclear Science
NEA/NSC/R(2019)7
March 2023
www.oecd-nea.org

Existing Practices for Multi-physics Validation

Report on Sub-Task 3, Task Force 2

OECD
BETTER POLICIES FOR BETTER LIVES

NEA
NUCLEAR ENERGY AGENCY

Nuclear Energy Agency

NEA/NSC/R(2019)7

Unclassified English text only

2 March 2023

NUCLEAR ENERGY AGENCY
NUCLEAR SCIENCE COMMITTEE

Cancels & replaces the same document of 4 October 2022

Existing Practices for Multi-physics Validation

Report on Sub-Task 3, Task Force 2

This document is available in PDF format only.

JT03513412

ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

The OECD is a unique forum where the governments of 38 democracies work together to address the economic, social and environmental challenges of globalisation. The OECD is also at the forefront of efforts to understand and to help governments respond to new developments and concerns, such as corporate governance, the information economy and the challenges of an ageing population. The Organisation provides a setting where governments can compare policy experiences, seek answers to common problems, identify good practice and work to co-ordinate domestic and international policies.

The OECD member countries are: Australia, Austria, Belgium, Canada, Chile, Colombia, Costa Rica, the Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Israel, Italy, Japan, Korea, Latvia, Lithuania, Luxembourg, Mexico, the Netherlands, New Zealand, Norway, Poland, Portugal, the Slovak Republic, Slovenia, Spain, Sweden, Switzerland, Türkiye, the United Kingdom and the United States. The European Commission takes part in the work of the OECD.

OECD Publishing disseminates widely the results of the Organisation's statistics gathering and research on economic, social and environmental issues, as well as the conventions, guidelines and standards agreed by its members.

NUCLEAR ENERGY AGENCY

The OECD Nuclear Energy Agency (NEA) was established on 1 February 1958. Current NEA membership consists of 34 countries: Argentina, Australia, Austria, Belgium, Bulgaria, Canada, the Czech Republic, Denmark, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Japan, Korea, Luxembourg, Mexico, the Netherlands, Norway, Poland, Portugal, Romania, Russia (suspended), the Slovak Republic, Slovenia, Spain, Sweden, Switzerland, Türkiye, the United Kingdom and the United States. The European Commission and the International Atomic Energy Agency also take part in the work of the Agency.

The mission of the NEA is:

– to assist its member countries in maintaining and further developing, through international co-operation, the scientific, technological and legal bases required for a safe, environmentally sound and economical use of nuclear energy for peaceful purposes;

– to provide authoritative assessments and to forge common understandings on key issues as input to government decisions on nuclear energy policy and to broader OECD analyses in areas such as energy and the sustainable development of low-carbon economies.

Specific areas of competence of the NEA include the safety and regulation of nuclear activities, radioactive waste management and decommissioning, radiological protection, nuclear science, economic and technical analyses of the nuclear fuel cycle, nuclear law and liability, and public information. The NEA Data Bank provides nuclear data and computer program services for participating countries.

Foreword

The modelling and simulation of nuclear systems allow scientists and engineers to probe aspects of the operation of these systems beyond what has been precisely measured. This has numerous applications, including interpolation between known operational scenarios and extrapolation into the unknown, providing information to underpin safety, optimise performance and design new facilities and experiments. As computational resources have increased in the past decades and with higher-fidelity modelling approaches, leveraging novel simulation methods has become critical to the nuclear industry. However, the potential value of all simulation is tightly bound to the body of evidence, which supports the accuracy of the methods in the application domains.

The Organisation for Economic Co-operation and Development (OECD) Nuclear Energy Agency (NEA) Expert Group on Multi-physics Experimental Data, Benchmarks and Validation (EGMPEBV) was created in 2014, under the aegis of the Nuclear Science Committee (NSC), to address the needs of member countries in certifying and utilising benchmarks for the validation of novel multi-physics codes. These benchmarks and the guidance on their use will help experts validate their codes, enabling their use in the wider nuclear community. Under the second task force created in the EGMPEBV, experts compared their approaches and their relative strengths and limitations, including a critical review of the current state-of-the-art in verifying, validating and performing uncertainty quantification with coupled multi-physics simulation.

This report provides a self-contained review of the current approaches for single and multi-physics validation, including both coupled and uncoupled uncertainty quantification and propagation. Through a detailed inter-comparison study, this report compiles the common elements that are required for best practices.

Acknowledgements

The Nuclear Energy Agency (NEA) expresses its sincere gratitude to Dr Maria Avramova (North Carolina State University, United States), who co-ordinated the efforts of the Expert Group on Multi-Physics Experiments, Benchmarks and Validation on existing practices for multi-physics validation, and for preparing this report.

The NEA acknowledges the work of A. Boldyrev (Russian Federation), D. Cuervo (Spain), M. DeHart (United States), J. Hou (United States), E. Ivanov (France), K. Ivanov (United States), E. Moiseenko (Russian Federation), N. Mosunova (Russian Federation), A. Petruzzi (Italy), U. Rohatgi (United States), S. Shevchenko (Russian Federation) and K. Velkov (Germany), who contributed to the report, and to J. Dyrda (NEA), J.P. Hudelot (France), and T. Valentine (United States), who reviewed the content.

Table of contents

Tables

Figures

List of abbreviations

1D	One-dimensional
2D	Two-dimensional
3D	Three-dimensional
APEX	Advanced plant EXperiment
ASAP	Adjoint sensitivity analysis procedure
ASTRUM	Automated statistical treatment of uncertainty method
ATWS	Anticipated transient without scram
BCL	Battelle Columbus Laboratory
BE	Best estimate
BEMUSE	Best-estimate methods – Uncertainty and sensitivity evaluation
BEPU	Best Estimate Plus Uncertainty
BFBT	Full-size Fine-Mesh Bundle Tests
BIC	Boundary and initial conditions
BOC	Beginning of cycle
BOL	Beginning of life
BT	Bayesian Theorem
BWR	Boiling water reactor
CANDU	CANada deuterium uranium
CASL	Consortium for advanced simulations of Light Water Reactors
CASUALIDAD	Code with the capability of Adjoint Sensitivity and Uncertainty AnaLysis by Internal Data ADjustment and assimilation
CAP	Nuclear Containment Analyses Package
CEA	Alternative Energies and Atomic Energy Commission (Commissariat à l'énergie atomique et aux énergies alternatives, France)
CCTF	Cylindrical core test facility
CCVM	CSNI code validation matrix
CDF	Cumulative distribution function
CFD	Computation fluid dynamics
CFR	Code of federal regulations
CHF	Critical heat flux

CIAU	Code with capability of IAU
CIAU-TN	Code with capability of IAU for coupled thermal-hydraulic/neutronics calculation
CSAU	Code scaling, applicability and uncertainty
CSNI	Committee on the Safety of Nuclear Installations (NEA)
CT	Computer tomography
CTF	Core test facility
CWO	Core-wide oxidation
DAA	Data adjustment/assimilation
DAKOTA	Design Analysis Kit for Optimisation and Tera-scale Applications
DNB	Departure from nucleate boiling
DNBR	Departure from nucleate boiling ratio
ECC	Emergency core cooling
ECCS	Emergency core cooling system
EG	Expert group
EGMPEBV	Expert Group on Multi-physics Experimental Data, Benchmarks and Validation (NEA)
EGUAM	Expert Group on Uncertainty Analysis in Modelling (NEA)
EM	Evaluation model
EMDAP	Evaluation model development and assessment
ENDF	Evaluated Nuclear Data File library (United States)
EOC	End of cycle
EOL	End of life
ESBWR	Economic simplified boiling water reactor
FGR	Fission gas release
FOM	Figure of merit
FP	Fuel performance
FSAP	Forward sensitivity analysis procedure
FSA	Fractional scaling analyses
FSAR	Final safety analysis report
FFTBM	Fast Fourier transform-based method
GASAP	Global adjoint sensitivity analysis procedure
GRS	Gesellschaft für Anlagen- und Reaktorsicherheit gGmbH (Germany)
GUI	Graphical user interface
H2TS	Hierarchical two-tiered scaling

HFP	Hot full power
HZP	Hot zero power
HPI	High-pressure injection
IBRAE RAN	Nuclear Safety Institute of the Russian Academy of Sciences
ICSBEP	International Criticality Safety Benchmark Evaluation Project (NEA)
IFPE	International Fuel Performance Experiments (NEA)
IRPhE	International Reactor Physics Experiment Evaluation (NEA)
IAU	Internal assessment of uncertainty
IE	Improved estimate
IET	Integral effect test
IMTHUA	Integrated methodology for thermal-hydraulics uncertainty analysis
INL	Idaho National Laboratory (United States)
IRWST	In-containment refuelling water storage tank
ISP	International standard problem
ITC	Isothermal temperature coefficient
ITF	Integral test facility
JEFF	Joint Evaluated Fission and Fusion library (Europe)
KS	Kolmogorov/Smirnov
LBLOCA	Large break loss-of-coolant accident
LMO	Local maximum oxidation
LOCA	Loss-of-coolant accident
LOFT	Loss-of-fluid test
LSTF	(Japanese) Large Scale Test Facility
LWR	Light water reactor
MOX	Mixed-oxide
MP	Multi-physics
MSLB	Main steam line break
M&S	Modelling and simulation
NA-SA	Nucleoeléctrica Argentina
NDC	Nuclear Development Committee (NEA)
NEA	Nuclear Energy Agency
NF	Nuclear facility
NJOY	Nuclear Data Processing Code
NRS	Nuclear and radiation safety

NSC	Nuclear Science Committee (NEA)
NUPEC	NUclear Power Engineering Corporation
OECD	Organisation for Economic Co-operation and Development
P_N	Spherical harmonics method
PCI	Pellet-clad interaction
pcm	Per cent mille
PCMI	Pellet-clad mechanical interaction
PCT	Peak cladding temperature
PDF	Probability density function
PHWR	Pressurised heavy water reactor
PIE	Propagation of input errors
PIRT	Phenomena identification and ranking table
PKL	Primarkreislauf − large-scale test facility
PML	Principle of the maximum likelihood
ppm	Parts per million
PP	Properties and phenomena
PREMIUM	Post-BEMUSE reflood Model Input Uncertainty Methods
PSBT	PWR sub-channel and bundle tests
PTS	Pressurised thermal shock
PVM	Parallel virtual machine
PWR	Pressurised water reactor
QoI	Quantities of interest
QPIRT	Quantified Phenomena Identification and Ranking Table
R&D	Research and development
REA	Rod ejection accident
RIA	Reactivity initiated accident
rms	Root mean square
ROM	Reduced order modelling
RP	Reactor physics
SAPIUM	Systematic APproach for Input Uncertainty quantification Methodology
SBLOCA	Small break loss-of-coolant accident
SCC	Stress corrosion cracking
SCCRED	Standardised and Consolidated Calculated and Reference Experimental Database
SCTF	Slab core test facility

SCWR	Super critical water reactor
SEC	Scientific and Engineering Centre
SET	Separate effect test
SETF	Separate effect test facility
SETS	Stability enhancing two-step
SFR	Sodium fast reactor
S_N	Discrete ordinates method
SMR	Small modular reactor
SRV	Safety relief valves
SS	Steady-state
ST	Sub-task
SPACE	Safety and Performance Analysis Code
SUSA	Software for Uncertainty and Sensitivity Analysis
S&U	Sensitivity and uncertainty
TF	Task force
TH	Thermal-hydraulics
TIETHYS	The International Experimental Thermal HYdraulics Systems database (NEA)
TMI-1	Three Mile Island Unit 1 (United States)
TREND	Treatment and Representation of Evaluated Nuclear Data
SEC NRS	Scientific and Engineering Centre for Nuclear and Radiation Safety of the Russian regulatory authority (Rostechnadzor)
TREAT	Transient Reactor Test Facility (Idaho National Laboratory, United States)
TT	Turbine trip
UMS	Uncertainty method study
UAM	Uncertainty analysis in modelling
UMAE	Uncertainty methodology based on accuracy extrapolation
UPI	Upper plenum injection
UPTF	Upper Plenum Test Facility (Germany)
US DOE	United States Department of Energy
US NRC	United States Nuclear Regulatory Commission
UQ	Uncertainty quantification
VVER	Water-water energetic reactor (Russia)
V&V	Verification and validation
VUQ	Validation and uncertainty quantification

WGAMA	Working Group on Accident Management and Analysis (NEA)
WPRS	Working Party on Scientific Issues of Reactor Systems (NEA)
XSUSA	Cross-section uncertainty and sensitivity analysis

Executive summary

The Nuclear Energy Agency (NEA) Expert Group on Multi-physics Experimental Data, Benchmarks and Validation (EGMPEBV) was created in 2014 under the auspices of the NEA Nuclear Science Committee (NSC) to establish the processes for the certification of experimental data and development of benchmark models for validation of Multi-Physics (MP) Modelling and Simulation (M&S) computational systems. The aim of the group is to provide member countries with guidelines and recommendations for validating and improving their novel multi-physics simulations and access to key experimental data.

The organisation of the EGMPEBV relies on three task forces (TFs), focused on: 1) experimental data qualification and benchmark evaluation; 2) methods and standards; and 3) specific applications.

Task Force 2 was designed to develop validation methods and guidelines and uncertainty qualification for the multi-physics, multi-scale codes in the context of emerging demands such as longer fuel cycles and power uprate.

Task 3 of Task Force 2 was designed to develop guidelines for current (traditional) multi-physics validation and uncertainty quantification. The present report summarises the current practice in the validation process, discusses uncertainty analyses and current methodologies used to extrapolate beyond the validation domain.

Code developers, research organisations and professional societies have developed various practices for validation of M&S tools and data. The approaches may vary depending on the limitations of the M&S tools and data as well as the intended application of such M&S tools. This report summarises some of the primary practices, including recommendations and guidelines that have been developed within NEA member countries.

1. Introduction and definition of terms

1.1 Background

The Expert Group on Multi-physics Experimental Data, Benchmarks and Validation (EGMPEBV) was formed under the auspices of the Nuclear Energy Agency (NEA) Nuclear Science Committee (NSC) in 2014 [1]. The expert group (EG) has the task of establishing the processes for the certification of experimental data and development of benchmark models for validation of Multi-Physics (MP) Modelling and Simulation (M&S) computational systems. In addition, this EG will seek to establish appropriate processes and procedures for the use of data and benchmark models for validation of M&S tools and data. In detail, the objectives of the EG are to provide member countries with:

- the guidance and processes for certifying experimental data for its use as a benchmark or for its use in general testing of modelling and simulation tools;
- access to certified experimental data from the contributions of individual member countries;
- guidance and recommendations for developing benchmark models from certified experimental datasets;
- access to standardised benchmark models with detailed uncertainty evaluations and uncertainty methodology guidelines;
- recommendations and guidelines for the range of applicability of the certified experimental datasets;
- guidelines and consensus recommendations for validating MP simulations;
- a limited number of demonstrations of the validation recommendations.

The EGMPEBV is currently organised into three task forces:

- Task Force 1 on Experimental Data Qualification and Benchmark Evaluation: The TF-1 team has the aim first to identify the main challenges for validating MP M&S tools and then to develop and implement processes for evaluating and producing experimental datasets that could be used for validating novel MP M&S tools.
- Task Force 2 on Validation Guidelines and Needs: The TF-2 team has been formed to identify needs and to develop best practices for development of methodologies for validation.
- Task Force 3 on Example Application of Validation Experiments: The TF-3 team has the objective to organise MP M&S benchmarks involving validation experiments.

In order to achieve the above objectives and given the multidisciplinary nature of the activities, the three TF teams will liaise closely with other relevant NEA working parties and expert groups, including those operating under the guidance of the Nuclear

Development Committee (NDC) and the Committee on the Safety of Nuclear Installations (CSNI), to ensure that the respective programmes are complementary, to provide advice and support where required and undertake common work where appropriate. Several different expert groups of the NEA have established rigorous processes for the accumulation and preservation of existing and new experimental data for single physics phenomena. Under the auspices of:

- Nuclear Science Committee (NSC):
  - the International Criticality Safety Benchmark Evaluation Project (ICSBEP);
  - the International Reactor Physics Experiment Evaluation (IRPhE) Project;
  - the International Fuel Performance Experiments (IFPE) database;
- Committee on the Safety of Nuclear Installations (CSNI):
  - the CSNI Code Validation Matrix (CCVM) of Separate Effect Test Facilities (SETFs);
  - the CSNI Code Validation Matrix (CCVM) of Integral Test Facility (ITF).

Several processes have been developed by which experimental data is "qualified" for use in benchmarks and several benchmark models are developed for the validation of modelling of single physics or limited multi-physics phenomena.

Additionally, the Expert Group on Uncertainty Analysis in Modelling (EGUAM) within the Working Party on Scientific Issues of Reactor Systems (WPRS) has been leading an international effort to establish the processes for performing coupled neutronics and thermal-hydraulics simulations for a variety of reactor types but with a focus on light water reactors (LWRs). The efforts of these working groups will form the basis for the processes and priorities of the EGMPEBV to reduce duplication and take advantage of the knowledge built by these groups over the years.

The EGMPEBV effort will strive to leverage the efforts of the NSC and the CSNI into a demonstrated methodology for qualifying experimental data, creating "benchmarks" and establishing validation guidelines for MP M&S tools.

The principal objectives of Task Force 2 initiative are:

- development of consensus guidelines for validation of multi-physics M&S tools and data;
- development of guidelines for performing uncertainty qualification and evaluating ranges of applicability for predicting M&S performance outside of the validation domain;
- identifying the needs for specific experiments with the intended purpose of validating multi-physics M&S tools and data.

The present report summarises the status of the existing practices for multi-physics validation. Code developers, research organisations and professional societies have developed various practices for validation of M&S tools and data. The approaches may vary depending on the limitations of the M&S tools and data as well as the intended application of such M&S tools. The report is developed that summarises some of the primary practices, including recommendations and guidelines that have been developed within the member countries of the NEA.

1.2 Objective of the present report

This report identifies several commonly used assessment frameworks and summarises the general approach, the strengths, the weaknesses and ease of use of these frameworks. The report includes an overview of the phenomena identification and ranking table (PIRT) process along with the key issues that must be considered when identifying relevant physical phenomena and the coupling among the phenomena such as thermal-hydraulics and neutronics. The report includes a summary of the principal issues to consider when coupling physical phenomena that have varying degrees of fidelity in the temporal, spatial and/or energy domains. Likewise, the report summarises current approaches for estimating total uncertainty at various levels of the validation hierarchy and the cautions and challenges in such estimates. The report also provides recommendations as to the treatment of experimental uncertainty and the inference of measured data with respect to simulated responses of interest. A critical topic in estimating the total uncertainty at the application conditions of interest is how to estimate the model form uncertainty using validation metrics. Finally, the report includes a summary of the primary recommendations for the use of multi-physics modelling and simulation tools extrapolated beyond the validation domain.

1.3 Structure of the report

The report is organised in six chapters including the introduction and definition of terms, validation of single physics, validation of multi-physics, uncertainty quantification approaches, summary of validation and uncertainty quantification (VUQ) state of practice and conclusions.

Examples and current approaches for validation of single physics calculations are provided in Chapter 2 while examples and current approaches for validation of multi-physics simulations are given in Chapter 3. Uncertainty quantification frameworks for single and multi-physics simulations are described in Chapter 4. A summary of VUQ practices is provided in Chapter 5 and conclusions are given in Chapter 6.

1.4 Definitions

First, some definitions will be introduced such as single physics, pre-traditional and traditional multi-physics models, integral effects, separate effects and plant measurable parameters. In addition, the definition of validation and uncertainty quantification as well as discussion of traditional versus validation experiments will be provided.

Single physics modelling and simulation focus on single physics phenomena and consider the interactions with other physics phenomena via boundary conditions.

Multi-physics modelling and simulation describes non-linear multi-physics phenomena by on-line treatment of feedback effects of different physics.

While integral effects describe the behaviour of a reactor system at nominal, off-nominal or accident conditions, the separate effects describe the behaviour of single component or characteristics of one phenomenon.

Plant measurable parameters are integral parameters or local distributions, which can be directly or indirectly measured during the plant operation and/or transient conditions. The obtained measured values must be supplemented with corresponding experimental/measurement uncertainties.

There are many interactions between different physics phenomena at different scale in different components of nuclear power plants. Especially important are the multi-physics interactions in reactor cores. In the past, these different interactions were treated either as boundary conditions (i.e. each physics calculation was performed independently, and the impact of other physics phenomena was taken into account through boundary conditions) or using very simplistic models for some of the physics phenomena. Examples for the latter are the point kinetics model implemented in the system thermal-hydraulic models or one-dimensional thermal-hydraulic models implemented in neutronics core design codes. These simulation models are defined as pre-traditional multi-physics tools.

The traditional multi-physics tools include mostly neutronics/thermal-hydraulics coupling into reactor core on assembly/channel basis. The coupling of reactor core to the system and coupling of the system to containment also belongs to traditional multi-physics simulations.

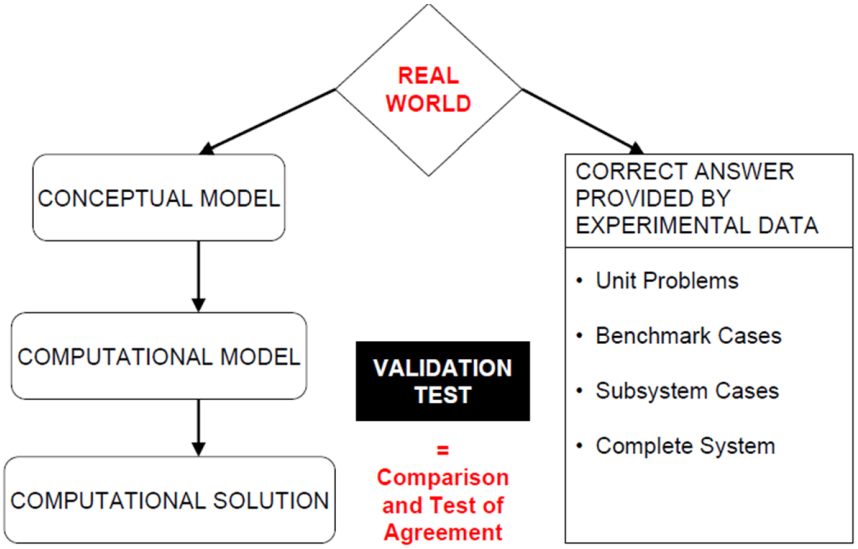
The novel multi-physics tools, which include high-fidelity coupling on pin/sub-pin (pin-resolved)/sub-channel level of several physics' phenomena in the reactor core such as neutronics (reactor physics), thermal-hydraulics, fuel performance, structural mechanics, chemistry, etc.

Verification and validation (V&V) and uncertainty quantification (UQ) are used as a measure of performance of the reactor physics system. In the literature and among different reactor vendors and regulatory agencies there are different terminologies of V&V and UQ. The most common are the following definitions:

- verification is a process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model;
- validation is a process of determining that a model is an adequate representation of the real world from the perspective of the intended uses of the model;
- qualification is a process of determining the degree to which a model represents a domain of real-world solutions;
- uncertainty quantification is a determination of the degree of accuracy of the model representation for intended applications.

As discussed in [2], the process of determining the degree to which a computational model provides an accurate representation of the real world from the perspective of the intended uses of the code is generally referred to as validation. This is depicted in the schematic shown in Figure 1.1, which shows that the validation is performed in many phases.

Figure 1.1. Phases of validation process



Source: Oberkampf and Trucano, 2004.

Although one of the goals of the various modelling and simulation projects is to reduce reliance on expensive experimental validation, the complexity of these new computational tools presents an even greater validation challenge. The amount of data needed to validate a single figure of merit (FOM) resolved over a fine mesh is orders of magnitude greater than that used for an integral code experiment. When dealing with multiple physics and scales, not only does the volume of data increase geometrically but one must account for the coupling terms as well. Additional challenges arise from the fact that some of the key parameters are not directly measurable but must be derived from other measurable quantities, injecting even more uncertainty into the result. Furthermore, results of such complex simulations are more sensitive to user effects due to many options, which are difficult to isolate and quantify.

Thus, the difficulty of validating high-fidelity, multi-physics codes has rendered traditional methods used for single physics and integral codes entirely inadequate. New experimental and analytical techniques must be devised, tested and compared. In addition, new types of experiments are needed as validation experiments [2]. The objective of a validation experiment is to determine the predictive accuracy of a model (or group of models), which is different from objectives of the so-called traditional experiments. The traditional experiments are usually categorised as:

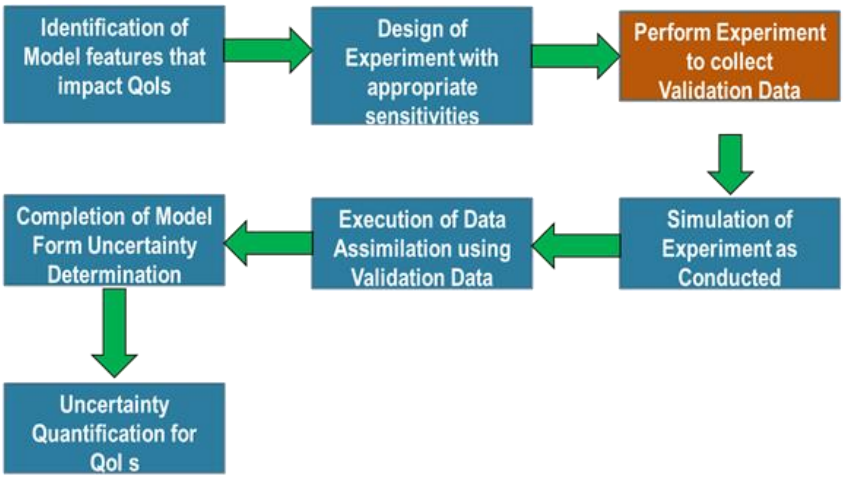
- scientific discovery experiments (with objective to improve fundamental understanding of physics (a process or phenomena) – for example departure from nucleate boiling);
- calibration experiments (with objective of constructing and improving a model for a well-understood process i.e. determining parameters in existing mathematical models – for example experiment for bubbly flows);
- system performance experiments (with objective to determine reliability, performance and/or safety of components or systems i.e. assessing subsystem or complete system performance – for example loss-of-coolant experiment).

According to [3], a model validation experiment is an experiment that is designed and executed to quantitatively estimate a mathematical model's ability to simulate a well-characterised experiment. The customer of a model validation experiment is usually a model developer or computational analyst. The six characteristics of a validation experiment are defined as follows [3]:

- a validation experiment should be jointly designed and executed by experimentalists and computation specialists (close working relationship during the whole process);
- a validation experiment should be designed to capture the relevant physics, all initial and boundary conditions, and all auxiliary data needed for a simulation (computational simulation input data should be measured in the experiment and key modelling assumptions understood as well as characteristics and imperfections of the experimental facility should be measured and included in the simulation);
- a validation experiment should use any possible synergisms between experiment and computational approaches (offset strengths and weaknesses of computation and experiment);
- independence between computational and experimental results should be maintained where possible (the flavour of a blind comparison should be maintained if possible and all input data needed for the simulation should be measured and provided);
- a hierarchy of experimental measurements should be made, which presents an increasing range of computational difficulty (the data should include functionals, local variables, derivatives of local variables and computational solution data should be processed in a manner similar to the experimental measurement data);
- a validation experiment must carefully employ experimental uncertainty analysis procedures to delineate and quantify random and correlated bias errors (experimentalist should provide uncertainty estimates on system response data and input quantities needed by the code, use traditional or statistical design of experiments methods to estimate random and correlated bias errors in measurements, and if possible, conduct experiments using different diagnostic techniques or different experimental facilities).

The design and utilisation of validation experiments, as proposed by Professor Dr Paul Turinsky from North Carolina State University (NCSU), are illustrated in Figure 1.2.

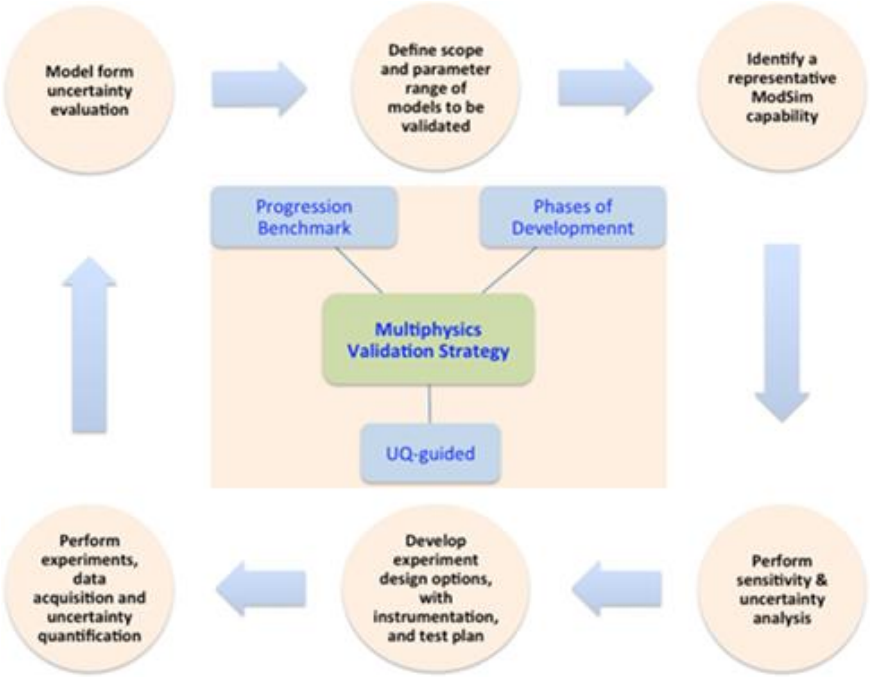
Figure 1.2. Design and utilisation of validation experiments



Source: NCSU, 2019.

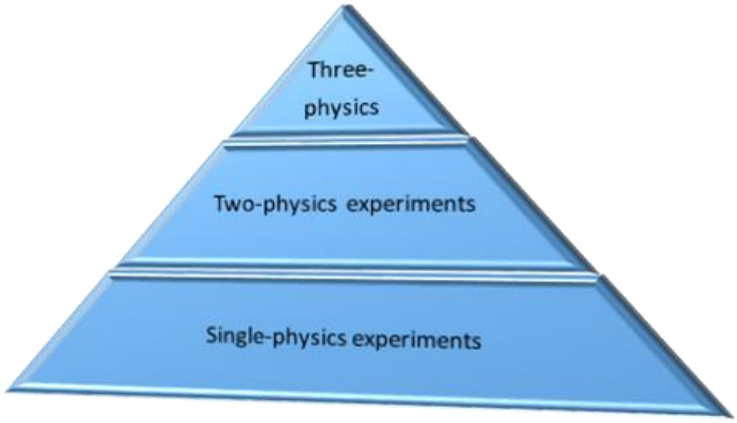
During the past several years, methodological guidelines and procedures for designing and conducting a validation experiment have been developed [2]. These guidelines have been utilised by Professor Dr Nam Dinh from NCSU to develop a concept for multi-physics model validation as shown in Figure 1.3. The validation experiments provide a rigorous foundation for validation of multi-physics simulations. Schematics of the validation experiment hierarchy for a multi-physics model benchmark is depicted in Figure 1.4.

Figure 1.3. Concept for multi-physics model validation



Source: NCSU, 2019.

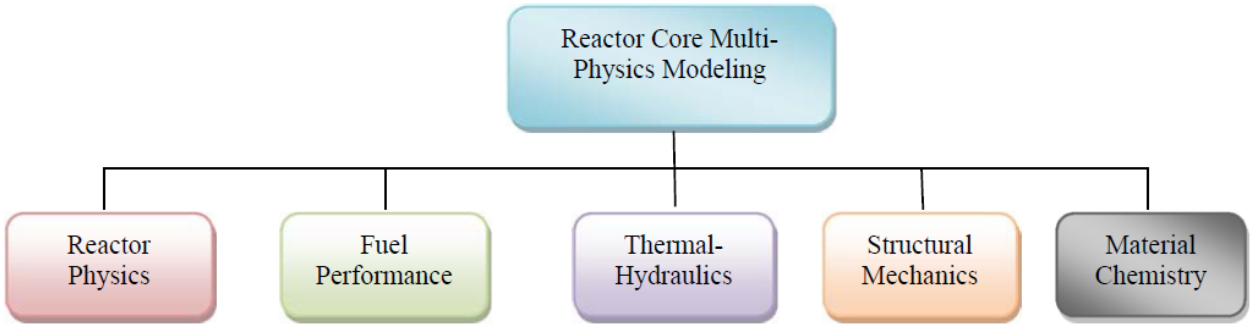
Figure 1.4. Multi-physics validation experiment hierarchy



Source: NCSU, 2019.

The multi-physics coupling mechanisms and feedback effects in a reactor core are shown in Figure 1.5. These interactions occur at different time scales, which we can separate as short (seconds and minutes) and long (months and years) time phenomena. The utilised approach is to design separate series of progressive validation experiments (to assess the impact of individual physics on multi-physics simulations) for both short and long multi-physics time phenomena in a reactor core.

Figure 1.5. Multi-physics coupling mechanisms and feedback effects in a reactor core



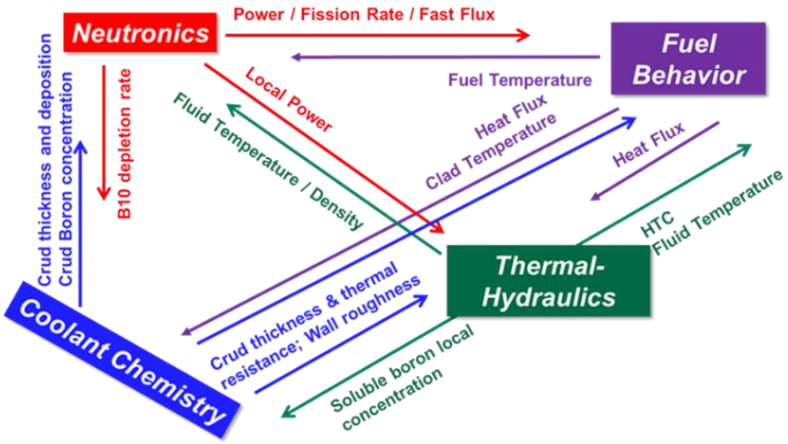
Source: CEA, 2019.

The currently developed reactor modelling and simulation capabilities that couple multiple physics phenomena have the following validation challenges:

- consistent multi-physics validation path from single- to two-, and to n-physics validation;
- complexity and high fidelity of these new computational tools;
- using new types of experiments − validation experiments.

Usually in LWR core simulations the modelling of structural mechanics could be neglected thus reducing the multi-physics coupling mechanisms to four physics as shown in Figure 1.6.

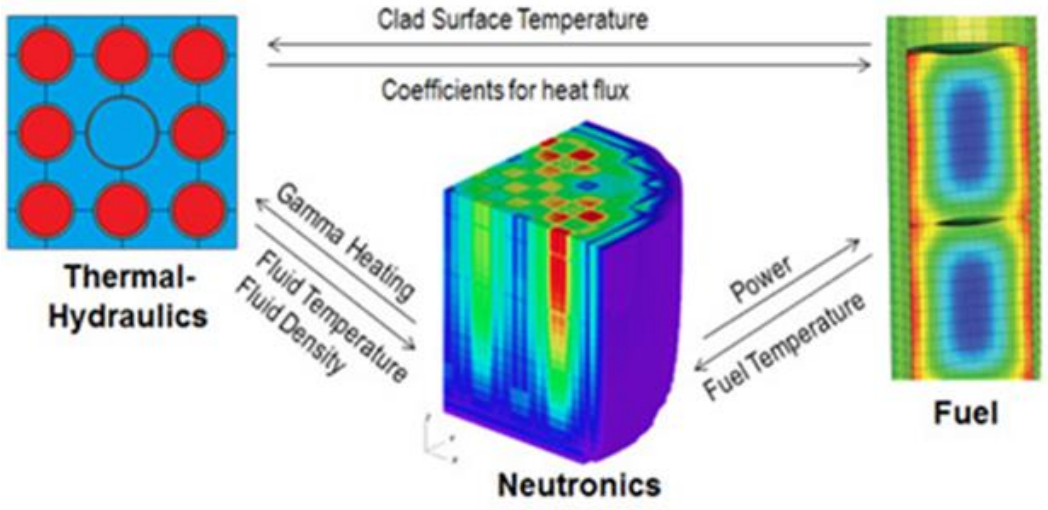
Figure 1.6. Multi-physics coupling mechanisms in LWR core



Source: NCSU, 2019.

The short-time transient phenomena in a LWR core is of high importance and is related to industry safety concerns such as design basis and anticipated transients without scram. The multi-physics coupling in this case includes coupling of neutronics reactor physics (RP), thermal-hydraulics (TH), and fuel physics fuel performance (FP) as shown in Figure 1.7.

Figure 1.7. Multi-physics coupling mechanisms for short-time transient phenomena in LWR core

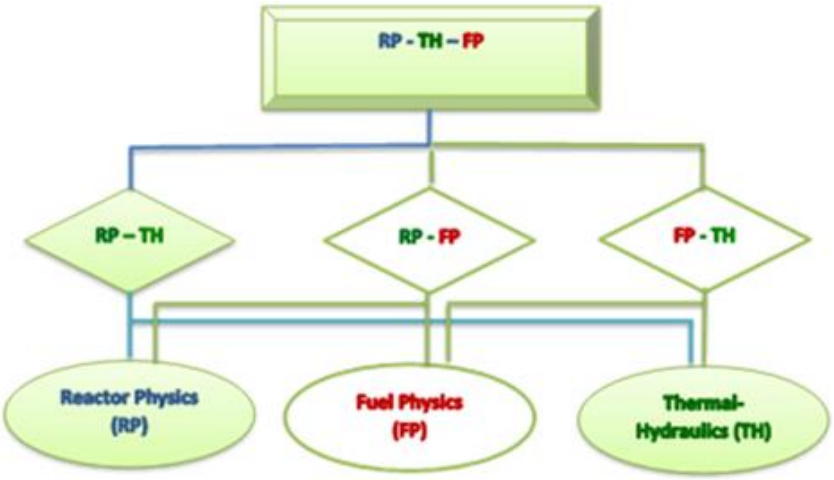


Source: CASL, 2018.

In this report, the validation of traditional multi-physics tools is discussed with focus on the above-mentioned three-physics coupling between RP, TH and FP. The first step in multi-physics validation is the validation of different single physics models involved in the coupling for the specific application of interest. The second step is to validate different two-physics coupling mechanisms (RP-TH, RP-FP, TH-FP) using experimental data. The third and final step is to validate the full multi-physics coupling (RP-TH-FP). This approach includes progression of exercises (based on experiments and measurements) as shown in Figure 1.8. In real life, usually not all needed experimental data is available, especially

when based on traditional experiments that have been used to validate the pre-traditional and traditional multi-physics tools. For example, assuming that the experimental data, which addresses "light green" physics areas in Figure 1.8, is available while the data for white areas is not. The light green areas will cover just part of the multi-physics validation pyramid but will follow a logical path (blue line) to decompose the impact of each single physics effect and consistently include coupling with other physics as described below.

Figure 1.8. Multi-physics validation hierarchy



Source: NCSU, 2019.

2. Validation of single physics

Examples and current approaches for validation of single physics calculations are provided in this chapter.

2.1 Core reactor physics

The current core reactor physics calculations process is a two-step process – first single assembly lattice physics calculations are performed for preparation of a parametrised few-group nodal parameter library, which is used by the core nodal simulators for core-wide calculations.

Examples and validation matrices for both steps are presented below. In general, the verification and validation (V&V) approach for light water reactor (LWR) physics software includes the following components [4]:

- verification:
  - self-consistency tests (convergence in space, time, energy);
  - comparisons to numerical benchmark solutions;
  - comparisons to higher-order methods;
  - comparisons to other code results.
- validation:
  - comparisons to critical measurements;
  - comparisons to isotopic measurements;
  - comparisons to power reactor physics tests;
  - comparisons to power reactor core-follow measurements;
  - comparisons to power reactor transient measurements.

Different data libraries and software systems within the framework of typical reactor physics calculation schemes are verified and validated. The fundamental data libraries Evaluated Nuclear Data Files (ENDF) are among the most difficult things to verify. Inter-comparisons are performed between different data libraries like ENDF and Joint Evaluated Fission and Fusion (JEFF) libraries. Nuclear Data Processing Code (NJOY) is usually used to process the data in multi-group format. The lattice physics codes are usually verified by using single assembly and mini-core (colour-set) numerical benchmarks and Monte Carlo reference solutions. The isotopic predictions of lattice codes are validated using measurements. Some "interpretation" is required to make these measurements lattice "benchmarks". Isotopic validation is useful but limited in terms of sensitivity to reactivity.

The lattice physics codes are usually validated using critical experiments. Hundreds of those are available [5] but some of the best (for LWRs) are proprietary. About 100 per cent mille (pcm) (one sigma) spread is routinely obtained in the comparisons with measured

data. Some critical experiments can also be run directly with nodal codes. For the nodal core simulators, the best verification model is a comparison with full-core lattice model since the cross-sections for the nodal core model are generated by the lattice model. Usually acceptable results in such comparisons are if k_{eff} is within 50 pcm, nodal powers root mean square (rms) are less than 1%, and pin-wise rms are less than 2%. For nodal simulators validation using measured data at beginning of cycle (BOC) hot zero power (HZP) conditions is very important.

Note that the core thermal-hydraulic models are usually validated using measured loop test data like pressure drop across the core and for different axial layers between the spacer grids. The coupled nodal/thermal-hydraulic core steady-state models are validated by using data from core measurements. The transient coupled core simulators are verified using numerical benchmarks (kinetics – without feedback and dynamics with feedback) in which the cross-section libraries are provided. The validation sometimes also requires coupling to the vessel and system thermal-hydraulic models for simulation of different transients for which measured data exist.

Development and qualification of new reactor physics code systems as well as merging the existing tools in unified systems capable of analysing different reactor types is a lengthy process. The term of qualification stands for V&V, which includes [6]:

- comparisons to high-order methods, such as Monte Carlo methodologies;
- comparisons to critical experiments;
- comparisons to plant measurement (this the heaviest part and the most important).

The number of critical experiments and spent fuel analyses is limited. Mostly, these experiments are at exposure zero and the existent fuel samples available for spent fuel validation do not cover the particular interests of modern assembly designs (burn-up steps up to 70 GWD/MTU or more, various void levels, 0 up to 80% void, different enrichments and gadolinium content). Gamma scans pin by pin are even more uncommon than the critical experiments, and the errors in the history of the samples can be significant. Some of the experiments are proprietary. The reactivity changes with exposure cannot be assessed by measurements unless a three-dimensional (3D) core simulator is used, which is an indirect way to prove the quality of the spent fuel analysis. Therefore, "numerical experiments" as performed by Monte Carlo criticality, Monte Carlo based depletion and coupled Monte Carlo/thermal-hydraulic calculations are provided to bridge gaps where measurements are lacking, to make comparisons for specific fuel assemblies.

The following integral experiments are required for reactor physics software qualification:

- mock-up experiment;
- chemical assays on irradiated fuels;
- reactivity versus burn-up;
- fundamental experiments.

Interest in high-quality integral benchmark data is increasing as efforts to quantify and reduce calculation uncertainties accelerate to meet the demands of next generation reactor and advanced fuel cycle concepts. The International Reactor Physics Experiment Evaluation Project (IRPhEP) and the International Criticality Safety Benchmark Evaluation Project (ICSBEP) continue to expand their efforts and broaden their scope to identify, evaluate, and provide integral benchmark data for method and data validation [7,8].

Benchmark model specifications provided by these two projects are used heavily by the international reactor physics, nuclear data and criticality safety communities.

The plant operating data used for qualification of reactor physics software consist of start-up and cycle follow-up measurements:

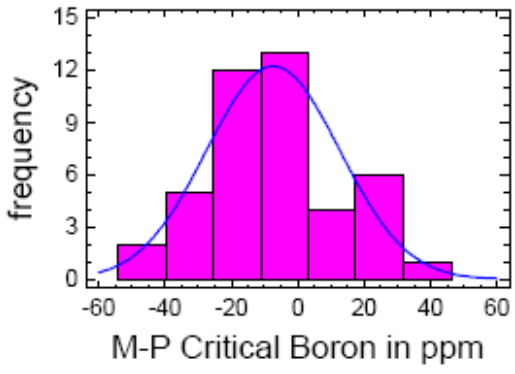
- critical eigenvalue:
  - hot, operating conditions;
  - cold shut-down/start-up critical configurations.
- in-core instrumentation comparison;
- gamma scans (power, exposure, and fission gas);
- post-irradiation examination radiochemical analysis.

The United States Nuclear Regulatory Commission (US NRC) requires in reactor physics software licensing submittals to have comparisons with plant measurements. The US NRC will not issue a licence without plant data. The qualification of the nuclear core design system serves two purposes:

- to demonstrate the capability of the system to perform accurate nuclear design calculations;
- to provide a basis for licensing the methodology with the US NRC.

Qualification calculations are always performed for parameters that are measured at plant start-up. For a pressurised water reactor (PWR), these parameters usually include: BOC HZP critical boron, BOC HZP isothermal temperature coefficient (ITC) and BOC HZP rod worth. Reactor physics calculations are usually performed for all these parameters for all cycles in the qualification plant database where existing measurement data were available. Figure 2.1 shows a sample histogram of the differences between measured data and calculation critical boron results. These results show very good performance, with an average difference very close to zero and a standard deviation on the order of 20 parts per million (ppm).

Figure 2.1. Histogram of HZP BOC measured – predicted differences for critical Boron



Source: Mayhue et al., 2008.

One example of reactor physics validation are the results of recent validation studies for the WIMS/PANTHER code package for PWR reactors [9]. A wide range of reactor cores

have been analysed by this route, ranging in size in both axial and radial directions. The fuel types vary in both fuel geometry and fuel composition. A range of comparisons of predictions with measurements has been carried out and the resulting agreement is reported in the paper. These measurements included the following:

- measurement at HZP:
  - critical boron concentrations at various rod bank configurations;
  - bank worth of various rod bank configurations;
  - isothermal temperature coefficients;
  - Boron worth.
- measurements at power:
  - Doppler coefficients;
  - flux maps at various power levels.

The summary of the statistical analysis of the validation results over 90 cycles is given in Table 2.1:

Table 2.1. HZP validation results

HZP BOC Parameters	Units	Predicted – measured		Sample size
		Mean	1s	
Critical boron concentrations				
ARO	[ppm]	1	26	96
All rodded configurations	[ppm]	-13	19	231
Rod bank worth	Δ_r [%]	0.4	5.4	295
MTC	[pcm/C]	-2.7	1.3	90
Boron worth	Δ_r [%]	-2.7	5.5	92

Where Δ_r denotes a (PANTHER/Measured – 1) difference.

Source: Hutton et al., 2000.

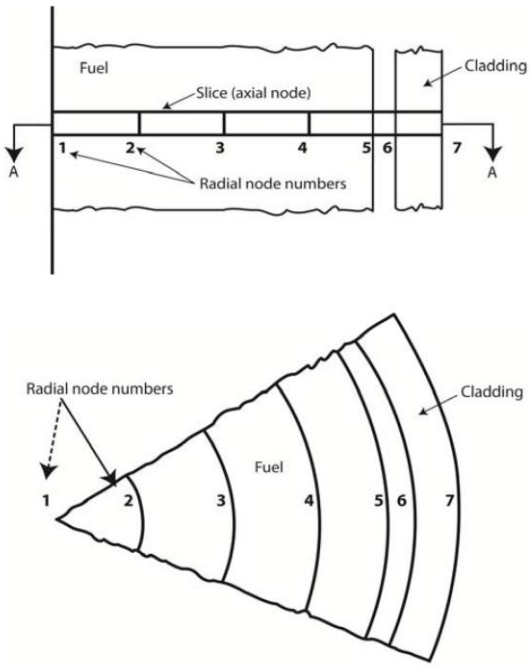
2.2 Fuel performance

Fuel performance codes are usually developed to solve equations embodying the phenomena as thermal performance, structural mechanics, actinide behaviour and fission product behaviour, etc. It is common that traditional fuel performance codes employ the so-called 1.5D representation of the fuel rod geometry, that is, the fuel rod simulations are performed on an axisymmetric, axially-stacked, one-dimensional radial model. Examples of fuel performance codes using such a simplified geometrical representation include FRAPTRAN [10,17,24], SCANAIR [11], TRANSURANUS [12] and SFPR [13].

Take the FRAPTRAN and its steady-state companion code FRAPCON [15,22,23] for example, the finite differencing approach is utilised to calculate the fuel performance related parameters at each of the user specified slices of the fuel rod, as seen in Figure 2.2 [15], each representing one axial node at a specific elevation defined by the user.

Each axial fuel node is radially subdivided into a set of concentric rings or annuli, providing nodes with constant volume, thickness, or other properties, such as power or fuel burn-up [15]. When variables at any given axial node are calculated, they are linked to those at other axial nodes via shared properties, such as 1D temperature linked via coolant heat transfer.

Figure 2.2. Radial discretisation for the finite differencing method used in FRAPCON/FRAPTRAN models



Source: Geelhood et al., 2011.

The FRAPTRAN code is developed to model the phenomena that influence the performance of fuel rods in general and the temperature, embrittlement and stress of the cladding. The code has a heat conduction model to calculate the transfer of heat from the fuel to the cladding and a cooling model to calculate the transfer of heat from the cladding to the coolant. The code has an oxidation model to calculate the extent of cladding embrittlement and the amount of heat generated by cladding oxidation. A mechanical response model is included to calculate the stress applied to the cladding by the mechanical interaction of the fuel and cladding, by the pressure of the gases inside the rod, and by the pressure of the external coolant.

The SCANAIR code [11] consists of three main modules dealing with thermal dynamics, structural mechanics and gas behaviour. These modules are closely coupled in the following way: during each time step, a first convergence is reached between thermal and thermal-hydraulics solutions. Then, using the calculated temperatures, a second iteration occurs between the gas behaviour module and the mechanical solutions. Upon achieving the convergence of this second resolution, temperatures are re-calculated and so on until full convergence of the different modules.

The SFPR code [13] was developed for mechanistic multi-scale modelling of single fuel rod behaviour under various regimes of LWR operation (normal and off-normal, including severe accidents). The code simulates evolution of fuel defect structure (microscale,

~10^{-5} m), pellet-cladding stress strain state (mesoscale, ~10^{-2} m), heat conduction and changes in rod geometry (macro-scale ~1 m). It provides self-consistent description of the following processes: release of gaseous fission products from UO_2 or mixed-oxide (MOX) fuels; fuel pellet swelling; mechanical and physico-chemical "pellet-cladding" interactions; mechanical properties degradation of cladding material due to oxidation/hydrogenation.

The SFPR has a modular structure and includes three main modules: structural mechanics, thermal conduction and fuel behaviour modules. The last module was developed on the base of stand-alone fuel performance code MFPR [14]. The MFPR code self-consistently describes: fission products generation and intragranular transport accompanying by formation of secondary phases – precipitates at the grain boundaries; evolution of fuel micro-structure (point defects, such as vacancies and interstitials, and extended defects, such as gas bubbles, sintering pores and dislocations), which strongly influences the intra- and intergranular diffusion transport of fission product atoms in irradiated fuel; evolution of the intergranular porosity resulting in the fuel swelling; radial diffusion of oxygen in temperature gradient in a fuel pellet resulting in significant changes in local oxygen potential and, consequently, in thermos-physical properties of fuel; fission product transport through intergranular to open porosity and fuel-cladding gap; partial fission product condensation in the gap and formation of solid fission product layer ("Joint Oxide Gain" or JOG structure).

The microscopic parameters characterising the crystal defect structure naturally arise, however, being physically grounded; these can be fixed from the analysis of available experimental data (and/or from atomic scale simulation: DFT, classical MD, KMC) and then used without any artificial tuning in further calculations. This is the main goal of the mechanistic approach realised in the MFPR code. For improvement and validation of the 1D thermo-mechanical models the capabilities of the 3D finite element method (FEM) were used.

During last five years, on the basis of approaches and methods realised in the SFPR code, the mechanistic multi-scale BERKUT code has been developed that describes the fuel rod behaviour in the fast reactors.

The validation of fuel performance codes is primarily performed by comparing the code predicted parameters with that obtained in the experiments. For example, an integral assessment has been performed to quantify the predictive capabilities of FRAPTRAN using a set of experimental data from reactivity initiated accident (RIA) and loss-of-coolant accident (LOCA) operating conditions [16,23].

The validation metrics for the RIA accident assessment are the following:

- residual cladding hoop strain;
- cladding failure (and enthalpy at failure);
- fission gas release.

The list below gives the validation metrics for LOCA accident assessment:

- cladding ballooning, failure, and pressure;
- residual hoop strain;
- high-temperature oxidation predictions.

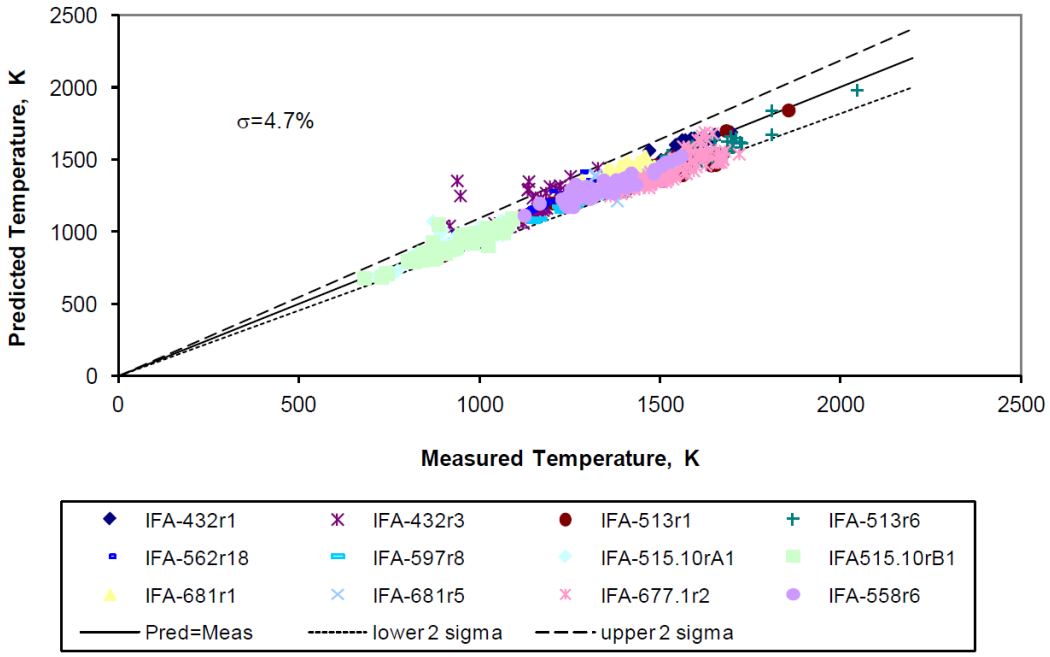
The integral validation assessment of steady-state and cycle depletion fuel performance calculations is usually done by comparing the code predictions for fuel temperatures,

fission gas release (FGR), rod internal void volume, fuel swelling, cladding creep/growth, cladding corrosion, and hoop strain to data from integral irradiation experiments and post-irradiation examination programmes [25]. The cases used for code assessment are usually selected based on the following criteria: well-characterised design and operational data were provided, and the reported results spanned ranges of interest for both design and operating parameters. For LWRs, the fuel rod cases are selected to represent both boiling water reactor (BWR) and PWR fuel types, with pellet-to-cladding gap sizes within, above, and below the normal range for power reactor rods. The fill gas is pure helium in most cases, but cases are included for which helium-xenon fill gas mixtures were used to assess the gap conductance model. The linear heat generation rates at beginning of life (BOL) range up to 60 kW/m (18 kW/ft), and during end of life (EOL) power ramps, they range up to 47 kW/m (14 kW/ft). The rod-average fuel burn-ups range up to 62 GWd/MTU. The EOL FGR ranges from less than 1 percent to greater than 50% of the produced quantity.

The integral validation assessment of transient fuel performance calculations is usually done to evaluate the predictions of the thermal and mechanical behaviour of LWR fuel rods during reactor power and coolant transients such as reactivity accidents, BWR power oscillations without scram, and LOCAs at burn-up levels up to 62 gigawatt-days per metric ton of uranium (GWd/MTU). The assessment is performed by comparing the fuel performance code calculations to data from selected integral irradiation experiments and post-irradiation examination programmes [25]. The cases used for code assessment are selected on the criteria of having well-characterised design and operational data and spanning the ranges of interest for both design and operating conditions. Two principal sets of data were used: 1) data from recent RIA test programmes and 2) data from LOCA test programmes.

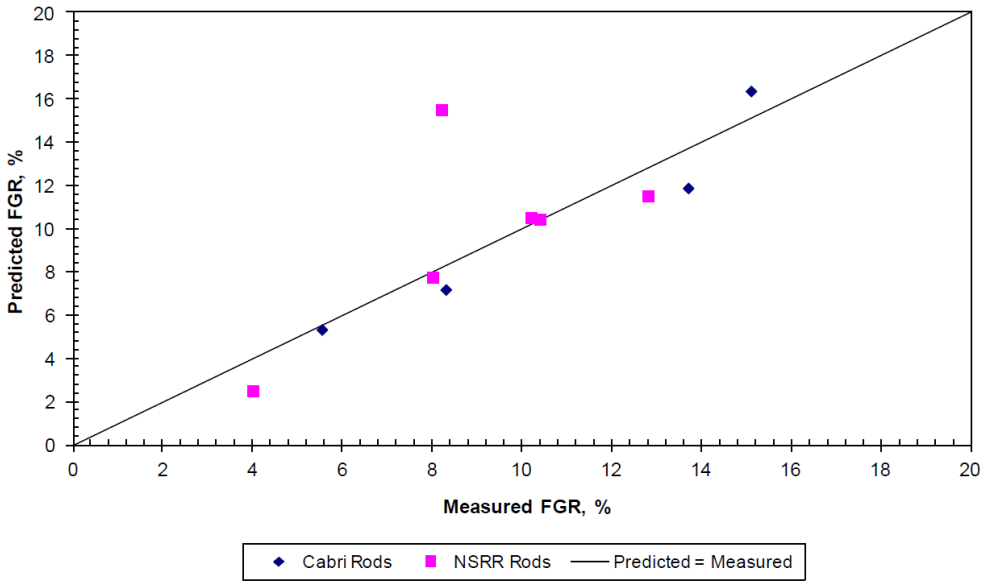
Most reactor system and core thermal-hydraulics codes, as well as some reactor physics core simulators have their have their own simplified fuel rod and heat transfer models with conduction solutions [26]. These models are validated using the same approaches described above for the fuel performance codes.

Figure 2.3. Measured and predicted by FRAPCON centreline temperature for the UO_2 assessment cases throughout life



Source: Geelhood and Luscher, 2014.

Figure 2.4. FRAPTRAN-1.5 predictions of RIA FGR for CABRI and NSRR UO_2 rods



Source: Geelhood and Luscher, 2014.

2.3 Core thermal-hydraulics

Modelling of nuclear reactor core thermal-hydraulics is performed using different fidelity methods including system, sub-channel, porous media and Computational Fluid Dynamics (CFD) codes. The V&V of the thermal-hydraulic feedback core model is an extensive programme [27], which includes numerical and experimental benchmarks for a variety of LWR steady-state and transient simulations. The V&V work is meant to demonstrate that the code behaves as expected and produces physically correct and accurate results for these intended applications. Therefore, the intended modelling applications drive the V&V work [28]. Each application has a set of physical phenomena upon which it will be dependent. The core thermal-hydraulics code must be capable of accurately modelling each of these physical phenomena. Usually, a series of tables are prepared that summarise the list of intended applications, the important physical phenomena in these applications, the models that were implemented into the code to capture these important physical phenomena, and the selected experimental tests that are used to show how accurately these models capture the phenomena. There are two columns for tests; one provides a link to validation tests and the other provides links to verification tests. A separate table is provided for each intended application of the code. A LWR core thermal-hydraulics code is usually developed for the following modelling applications: normal PWR and BWR operating behaviours, Departure from Nucleate Boiling (DNB) analysis of PWRs and Critical Heat Flux (CHF) analysis of BWRs, RIA analysis in PWRs and BWRs, etc. In summary, the V&V work seeks to provide a certain level of certainty and confidence in the predictive capabilities of the code for the scenarios it was designed to model: rod bundle geometries with operating conditions that are representative of prototypical PWRs and BWRs in both normal and accident conditions. This is done by modelling a variety of experiments that simulate these scenarios and then presenting a qualitative and quantitative analysis of the results that demonstrates the accuracy to which the core thermal-hydraulic code can capture specific quantities of interest.

For example, the PWR verification matrix for the modernised version of COBRA-TF – CTF (which is considered to replace current core thermal-hydraulic models in vendor's core analysis code systems because of its advanced two-phase three-field modelling) includes [27]:

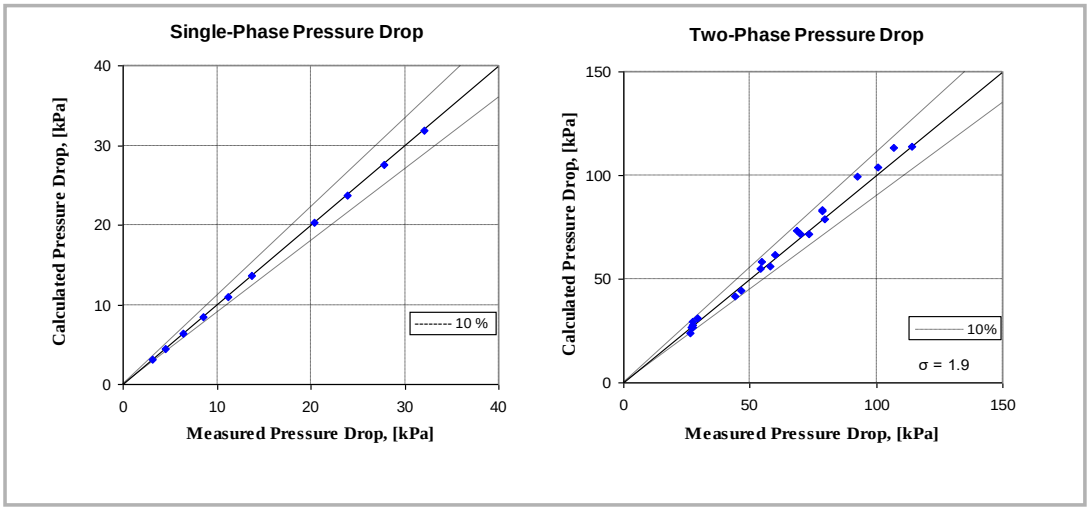
- PWR sample case;
- PWR core calculations:
  - steady state – fuel assembly (FA)-by-FA level;
  - steady state − cell-by-cell level;
  - flow reduction transient − FA-by-FA level;
  - flow reduction transient − cell-by-cell level;
  - power rise transient −FA-by-FA level;
  - power rise transient − cell-by-cell level;
  - pressure reduction transient − FA-by-FA level;
  - pressure reduction transient − cell-by-cell level;
  - main steam line break transient.

The core test facility (CTF) calculations are compared with the results from other codes.

The validation matrix of CTF consists of tests selected to validate the CTF modelling of the following physics phenomena [28]: heat transfer, pressure loss, single phase turbulent mixing, void content, two-phase turbulent mixing and void drift, dry-out, solid structure models and natural circulation.

The CTF BWR validation matrix includes different tests such as Bennett tube test, GE 3x3 experiment, PELCO-S 4x4 test and NEA/NRC Full-size Fine-Mesh Bundle Tests (BFBT), based on the NUclear Power Engineering Corporation (NUPEC) BWR bundle data benchmark [29]. The comparisons of CTF predictions of BWR 8x8 bundle pressure drop with measured values from the NEA/NRC BFBT benchmark are shown in Figure 2.5.

Figure 2.5. Comparisons of the overall bundle pressure drop CTF predictions vs. measurements



Source: PSU, 2018.

When core thermal-hydraulics codes are developed, experimental test must be used to develop and calibrate the models in the closure laws for the fluid equations. The facilities try to reproduce the phenomena that can be observed in the fuel assembly. These facilities reproduce totally or partially an assembly in the reactor of interest and the problem is represented at full scale. To analyse specific phenomenon encountered in the reactor core, the test conditions are set in such a way that this phenomenon is predominant at those conditions.

Validation of core thermal-hydraulics codes has been performed traditionally through in-house experiments carried out by fuel vendors interested in demonstrating cooling capacities of the fuel and safety margins to the nuclear regulatory body. An example of this is the GE 3x3 test developed by General Electric to assess model for inter-sub-channel mixing at single and two-phase conditions [30].

Some of the most known experiments for validation, not only for core thermal-hydraulics codes but also for CFD codes applied to fuel assembly analysis, were those performed with data made available from the NUPEC database obtained in Japan. This corporation performed between years 1987 and 1995 a series of void measurement tests using full-size mock-up tests for both BWRs and PWRs. The void distribution was visualised at the mesh size smaller than the sub-channel under actual plant conditions using state-of-the-art computer tomography (CT) technology. NUPEC also performed steady-state and transient critical power test series based on the equivalent full-size mock-ups. The first set of

experiments released included BWR experiments and became the NEA/NRC BWR BFBT benchmark. This corporation also decided to release the data obtained for PWR analysis to carry out the NEA/NRC PWR Sub-channel and Bundle Tests (PSBT) benchmark [31].

2.4 System thermal-hydraulics

Reactor system and containment coupled codes

In traditional nuclear reactors the sole role of containment was to be the last barrier to release of radioactive emissions. There are many safety systems in the containment that prevent increase in the containment pressure and challenge integrity of the containment in case of LOCAs. The reactor system is also isolated from the containment. Because of special components and phenomena, the containment was modelled with special codes such as CONTAIN, GOTHIC, SPACE, MAP, LOTIC, etc. [32-35]. Most of these are based on a lumped parameter formulation with very large volumes. In addition, containment plays a special role for safety under severe accident conditions when molten fuel flows to containment, and very different phenomena occurs.

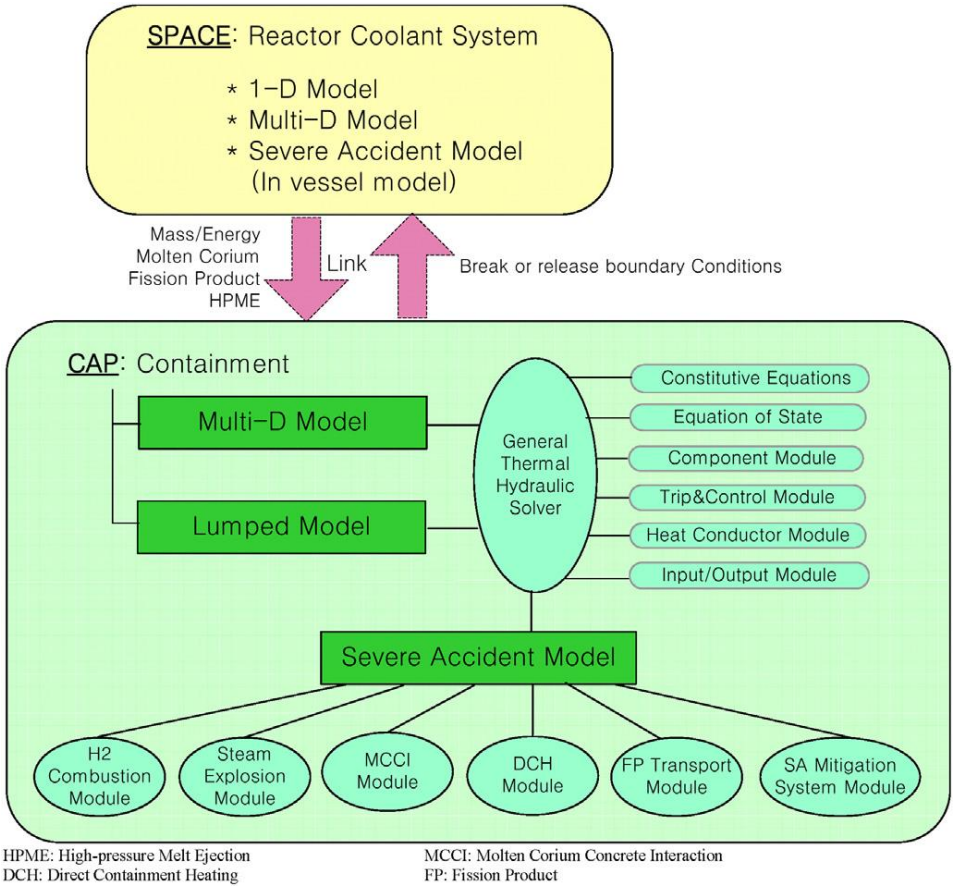
The reactor system codes such as TRAC, RELAP5 were coupled at the time of LOCA where the containment pressure provided boundary conditions to the system codes and the system codes provided mass and energy flow to containment as boundary conditions for containment codes. The system codes were essentially decoupled to containment as the break flow is initially choked and as the primary side depressurises the flow becomes unchoked. The break flow at a later stage will be controlled by the containment pressure. However, the containment volume is very large and the pressure increase is small, so the break essentially sees a fixed containment pressure as a boundary condition. The coupling between system codes and containment codes is accomplished through an executive programme, parallel virtual machine (PVM).

GOTHIC is a containment modelling code. It receives coolant inflow conditions from a separate reactor system code. The coupling approach is explicit. The LOCA code is run for full transient and coolant flow and enthalpy is then provided as a boundary condition to GOTHIC. However, GOTHIC has a simple reactor version model and the larger of the two for coolant flow is used for conservative analyses.

New advanced codes are being developed where the reactor system and containment are tightly coupled with safety for reactor system coupled to containment. This situation is valid for AP1000 and economic simplified boiling water reactor (ESBWR) and for small modular reactors (SMRs) such as the NuScale design. As containment participates in emergency core cooling (ECC) injection and condenses the flow from the reactor system, the system codes have been expanded to include models for containment. In this case the coupling is implicit. There are cases where two codes are still being coupled, the coupling is tight with synchronous coupling and information may be transferred at every time step.

The Korean nuclear industry has developed a system of two codes to simulate reactor and containment performance under accident conditions [36]. The reactor system is modelled with Safety and Performance Analysis Code (SPACE), and the containment is modelled with Nuclear Containment Analyses Package (CAP). CAP can model both design basis accidents and severe accidents. It requires boundary conditions for mass and energy from coolant, molten corium, fission products and high-pressure melt injection. The concept is illustrated in Figure 2.6.

Figure 2.6. Concept of coupled SPACE and CAP coder system



Source: Hong et al., 2015.

In Russia within the "Development of virtual-digital nuclear power plant with VVER reactor" Project, the system thermos-hydraulic code HYDRA-IBRAE/H_2O has been developed by the Nuclear Safety Institute of the Russian Academy of Sciences (IBRAE RAN) to model both reactor systems and containment. The code allows modelling of nuclear power plant behaviour under normal operation, during the transients and accidents. The code includes sub-channel module SCORE to calculate the processes in the core.

Validation against experimental data is essential in the process of system code development and improvement. The models implemented and used in a code are generally developed based on experimental tests performed in specific facilities. It is possible to distinguish among:

- Basic facilities: in these facilities the fundamental phenomena are reproduced; the results are used to improve the equations of the single model or to derive empirically the relation between the relevant parameters; such facilities are designed with the goal to reproduce the specific phenomenon to be investigated.
- Separate effect facilities: in these facilities some relevant zones of the nuclear power plant are reproduced by a suitable scaling law to investigate the local occurrence of a phenomenon; the results of the experiments performed in these facilities are used to create and to validate the (several) models to be included in a code.

- Integral tests facilities: these facilities are simulators of reference nuclear power plants. All the relevant parts and systems of a nuclear power plant are reproduced by a suitable scaling law. The whole plant is reproduced and the global plant responses are obtained as results. The results are used to realise and improve the models and to check the code capabilities.

It should also be noted that the data from nuclear power plants can be used, if available. However, in a nuclear power plant the data obtained are those recorded by the system of control of the plant while, typically, the facilities are equipped with many sensors and many detailed data are generated making the instrumentation of the facilities more suitable for code validation. Huge effort was done by the NEA/CSNI from 1991 to 1997 in the construction of the Separate Effects Test Facility Code Validation Matrix (SETF-CCVM, published 1994) for thermal-hydraulic system codes [37]. Integral Test Facility (ITF) matrices for validation of realistic thermal-hydraulic system computer codes were also established by CSNI focused mainly in PWRs, and BWRs. The ITF-CCVM [38] validation matrix was issued in 1987 and updated in 1996. By the validation matrices, the best sets of openly available experimental data for code validation, assessment and improvement were collected in a systematic way. Quantitative code assessment with respect to the quantification of uncertainties in the modelling of individual phenomena by the codes is also an outcome of the matrix development. In addition, the construction of such matrices was an attempt to record information of the experimental work which has been generated around the world over the last years in the LWR-safety thermal-hydraulics field. 187 facilities covering 67 relevant phenomena for LOCA and non-LOCA transient applications of PWRs and BWRs within a large range of useful parameters were identified and about 2 094 tests were included in the SETF-CCVM matrix. Most of these phenomena are also relevant to advanced water-cooled reactors. The major elements of the SETF-CCVM have been already integrated into the validation matrices of the major best-estimate thermal-hydraulic system codes, e.g. RELAP5, CATHARE, TRACE and ATHLET.

A total number of 177 PWR and BWR integral tests have been selected as potential sources for thermal-hydraulic code validation in the ITF-CCVM report. Counterpart tests, similar tests and NEA International Standard Problem (ISP) tests were also introduced in the report. Counterpart tests and similar tests in differently scaled facilities are considered highly important for code validation and therefore they were included in the tables of ITF selected experiments. Moreover, over the last thirty years, the CSNI has promoted more than 50 ISPs [39]. The main objectives of the ISPs are: to contribute to a better understanding of postulated events, to compare and evaluate the capability of codes (mainly best-estimate codes), to suggest improvements to the code developers, to improve the ability of code users and to address the so-called scaling effect. ISPs were performed in different fields as in-vessel thermal-hydraulic behaviour, fuel behaviour under accident conditions, fission product release and transport, core/concrete interactions, hydrogen distribution and mixing and containment thermal-hydraulic behaviour. ISP experiments were carefully controlled, documented and evaluated.

The scaling issue

A nuclear power plant is characterised by high power (up to thousands of MW), high pressure (tens of MPa) and large geometry (hundreds of m^3), thus it is well understandable the impossibility to perform experiments preserving all these three quantities. The term scaling is in general understood in a broad sense covering all differences existing between a real full-size plant and a corresponding experimental facility. An experimental facility may be characterised by geometrical dimension and shape, arrangements and availability

of components, or by the mode of operation (e.g. nuclear vs. electrical heating). All these differences have the potential to distort an experimental observation precluding its direct application for the design or operation of the reference plant. Distortion can be defined as a partial or total suppression of physical phenomena caused by only changing the size (geometric dimension) or the shape (arrangement of components) of the facility [41].

The scaling analysis is therefore the necessary link between the experiments performed in ITF and SETF and their utilisation in the code validation process. Three main objectives can be associated to the scaling analysis:

- the design of a test facility;
- the code validation, i.e. the demonstration that the code accuracy is scale independent;
- the extrapolation of experimental data (obtained in an ITF) to predict the nuclear power plant behaviour.

For test facility design, three types of scaling principles can be adopted:

- Time reducing scaling: rigorous reduction of any linear dimension of the test rig would result in a direct proportional reduction in time scaling. This is of advantage only for cases where body forces due to gravitational acceleration are negligible compared to the local pressure differentials.
- Time preserving scale: based on a scale reduction of the volume of the loop system combined with a direct proportional (power to volume scaling) scaling of energy sources and sinks (keeping constant the core power to system volume ratio).
- Idealised time preserving modelling procedures: based on the equivalency of the mathematical representation of the full-size plant and of the test rig. It is deduced from a separated treatment of the conservation equations for all involved volume modes and flow paths assuming homogeneous fluid.

ITFs are normally designed to preserve geometrical similarity with the reference reactor system. Generally, all main components (e.g. rector pressure vessel, down-comer, rod bundle, loop piping, etc.) and the engineered safety system (HPIS, LPIS, accumulators, auxiliary feed water, etc.) are represented. ITF are used to investigate, by direct simulation, the behaviour of a nuclear power plant in case of off-normal or accident conditions. The geometrical similarity of the hardware of the loop systems has been abandoned in favour of a preservation of geometric elevations, which are decisive parameters for gravity dominated scenarios (e.g. in case of natural circulation processes). Thus, the reduction of the primary system volume is largely achieved by an equivalent reduction in vertical flow cross-sections. Due to the impossibility to perform relevant experiment at full scale (i.e. in a nuclear power plant), the use of ITF or SETF is unavoidable.

To address the scaling issue, different approaches have been proposed and are available from literature. However, a comprehensive solution has not yet been achieved and moreover, it is evident that the attempt to scale up all thermal-hydraulic phenomena that occur during an assigned transient, results in a myriad of factors which have counteracting effect [42]. For instance, consider a two-phase flow condition in a vessel of a facility when a small break loss-of-coolant accident (SBLOCA) scenario is postulated. The two-phase critical flow is affected by phenomena like the vapour pull through and the subcooled vapour formation by the sharp edge cavitations, the heat losses, the fluid temperature stratification, etc. All these phenomena cannot be scaled up and are characterised by

parameters that appear neither in any balance equations nor in any scalable mechanistic models. This is a typical situation in which a scaling criterion is not applicable. Nevertheless, the influence of those phenomena is time-restricted in relation to the entire transient and thus they can be considered as local phenomena. Therefore, a way to solve the scaling problem is to consider only those phenomena and parameters that have a real impact on the whole problem under investigation. Focusing on a single phenomenon which occurs during a limited time (compared with the entire duration of the problem) should be avoided because it is governed by factors that are not scalable. Therefore, a hierarchy in the definition of the scaling factors is necessary and a global strategy is needed [42] to demonstrate that those phenomena are effectively local and cannot affect the overall behaviour of the main thermal-hydraulic parameters selected to describe the transient.

One possible strategy to address the scaling issue is embedded into the Uncertainty Methodology based on Accuracy Extrapolation (UMAE) methodology where the scaling analysis plays a relevant role, firstly during the code assessment process (as the code development and improvement is based on experimental data obtained in scaled test facilities) and secondly during the demonstration of the qualification of a nuclear power plant nodalisation (that is a necessary step to perform a reliable nuclear power plant calculation). Following the UMAE methodology, the strategy to adopt for solving the scaling problem consists of:

- qualifying the code against experimental data measured in facilities (ITF and SETF);
- demonstrating that the code accuracy (i.e. discrepancy between measured and calculated trends) only depends upon boundary and initial conditions (BIC) values (within the assigned variation ranges) and is not affected by the scale of the concerned ITF;
- applying such code to predict the same relevant phenomena that are expected to be found in a similar experiment (or transient) performed at a different scale;
- performing nuclear power plant Kv-scaled calculation and explaining the discrepancies (if any) between nuclear power plant Kv-scaled calculation and measured trends in ITF considering only BIC values and hardware differences (i.e. distortions).

3. Validation of multi-physics codes − Examples and current approaches

The description of the state of current practices for verification and validation (V&V) of multi-physics calculations for specific applications focuses on V&V of current traditional multi-physics methods and tools. It includes a discussion on the current V&V approaches with examples. Multi-physics validation is a complex problem and cannot be even feasible for some applications. Experimental installations for this type of validation are very limited or even unavailable. Consequently, data is obtained from nuclear power plant measurements. In this case is difficult to define the data requirements for adequate V&V of the codes for the phenomena of interest.

In multi-physics systems, each physics has its own length and time scales. The closure laws, in addition, can create new length and time scales. Transients require that all the physical length and time scales (including closure laws) are resolved by the mesh and time step.

Multi-physics simulator validation has been performed traditionally using international multi-physics benchmarks whose measured data have been supplied by nuclear power plants. These are complex benchmarks, which use different phases, exercises and scenarios to validate different models and the coupling between them. The available measured data is utilised in combination with detailed code-to-code comparisons. The cross-section libraries are generated usually by the benchmark teams, which removes the uncertainties introduced by using different cross-section generation and modelling procedures. This approach allowed development of a more in-depth knowledge of the capabilities of the current generation of neutronics/thermal-hydraulics simulators. Traditional multi-physics benchmark problems scope helps to define requirements for the definitions of future international exercises.

3.1 Multi-physics validation hierarchy and multi-level validation methodology

The qualification procedure of coupled multi-physics code systems is based on the qualification framework (verification & validation) of separate physics models/codes and includes in addition verification and validation of the coupling methodologies of the different physics models. The extended verification procedure involves testing the functionality, the data exchange between different physics models, and their coupling, which is designed to model combined effects determined by the interaction of models. The extended validation procedure compares the predictions from coupled multi-physics code systems to available measured data and reference results. It is important to emphasise that such validation should be based on a multi-level approach like the one utilised in validating coupled neutronics/thermal-hydraulics codes in international standard problems.

- use of the validation hierarchy (see for example the “pyramid” representation in Figure 1.8);
- coupling of physical phenomena (ad-hoc vs. first principles);
- coupling phenomena with varying degrees of fidelity: temporal, spatial, and energy;
- integration of the levels of the validation hierarchy with uncertainty propagation.

3.2 Coupled thermal-hydraulics system/neutron kinetics codes

The development of multi-physics multi-scale coupled methodologies for light water reactor (LWR) analysis requires comprehensive validation and verification procedures, which include well-established benchmarks developed in international co-operation. The Nuclear Energy Agency (NEA) has provided such framework, and over the years many LWR benchmarks have been developed and successfully conducted. The first set of NEA benchmarks that permits testing of the neutronics/thermal-hydraulics coupling and verifying the capability of the coupled codes to analyse complex transients with coupled core/plant interactions have been summarised in [43]. Such benchmarks are the NEA/United States Nuclear Regulatory Commission (US NRC) pressurised water reactor (PWR) Main Steam Line Break (MSLB) benchmark, the NEA/NRC boiling water reactor (BWR) Turbine Trip (TT) Benchmark and the NEA/US Department of Energy (DOE)/Commissariat à l'énergie atomique et aux énergies alternatives (CEA) VVER-1000 Coolant Transient (V1000CT) benchmark. These benchmarks provide a validation basis for the current generation of coupled neutronics/thermal-hydraulics best-estimate codes.

To meet the objectives of the validation of "best-estimate" coupled codes, a multi-level methodology has been introduced to evaluate systematically the transients. Since these benchmarks are based on both code-to-code and code-to-data comparisons, further guidance for presenting and evaluating results has been developed. The presented four benchmarks are developed in an international co-operation to provide a validation basis for the new generation of best-estimate codes. Based on the previous experience, several benchmark exercises were defined for each benchmark consisting of different steady states and transient cases, which allow for a consistent and comprehensive validation process. The introduction of extreme transient scenarios contributes to the study of different numerical and computational aspects of coupled simulations. The participants use a cross-section library, generated by the benchmark team, which removes the uncertainties introduced with using different cross-section generation and modelling procedures. The defined benchmark cross-section modelling approach is a direct interpolation in multidimensional tables with complete representation of the instantaneous cross-section cross-term dependencies. In this way the benchmarks provide the opportunity to study the impact of different thermal-hydraulics and neutronics models as well as the coupling between them on code predictions and to identify the key parameters for modelling important transients for different types of power reactors. This allowed the evaluation of these key parameters, through the performance of sensitivity studies, which led the participants to develop a more in-depth knowledge of the capabilities of the current generation best-estimate thermal-hydraulic system codes.

The results of the NEA light water reactor (LWR) benchmark activities are discussed on the example of Exercise 3 (coupled neutronics/thermal-hydraulic system modelling) for the NEA/NRC BWR TT benchmark. Turbine trip transients in a BWR are pressurisation events in which the coupling between core spatially-dependent neutronics phenomena and system dynamics plays an important role. The data made available from actual experiments carried out at the Peach Bottom 2 plant make the present benchmark particularly valuable. Exercise 3 consists of the base test case (the so-called best-estimate case) and hypothetical cases (the so-called extreme scenarios). The purpose of Exercise 3 Best Estimate Case is to provide comprehensive assessment of all the participating coupled codes in analysing complex transients. To validate such assessments, available measured plant data are utilised for this case during the comparative analyses presented in this report. In addition to the base case, the analysis of the extreme scenarios provides a further understanding of modelling

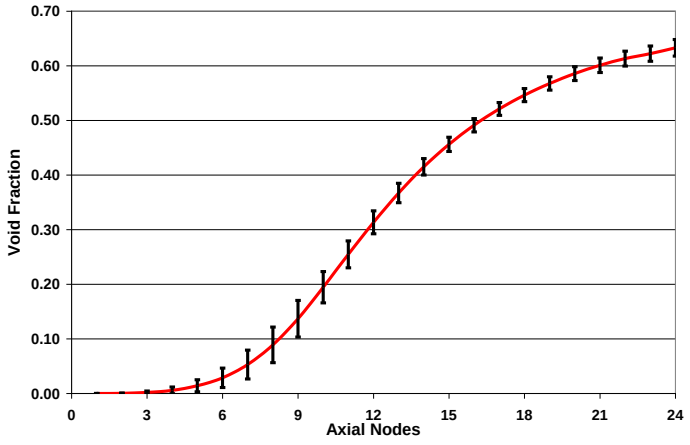
limitations of coupled codes and the interplays between different feedback mechanisms as well as testing the coupled code capabilities in extreme situations. The following four extreme scenarios are analysed by the participants during this exercise:

- Extreme Scenario 1: Turbine trip (TT) with steam bypass relief system failure;
- Extreme Scenario 2: TT without reactor scram;
- Extreme Scenario 3: TT with steam bypass relief system failure without reactor scram;
- Extreme Scenario 4: TT with steam bypass system failure, without scram and without safety relief valves (SRV) opening.

Extreme Scenario 1 (TT without bypass system relief opening) and Extreme Scenario 2 (TT without scram) can be considered as single failures and therefore provide information from the perspective of the safety of the plant. Extreme Scenario 3 (combination of 1 and 2), which considers the coincidence of two independent failures, and Extreme Scenario 4 (in addition to 3 no opening of safety relief valves), which considers the coincidence of three independent failures are extremely unlikely from a safety perspective, while they help with the understanding of the short-time dynamics of the reactor system. In the base case, SRVs are not opened during the transient, although this happens in the extreme scenarios 1, 2 and 3. In hypothetical cases, the dynamical response of the system due to the interaction of the flow in the steam line with the dynamics of SRVs happens to be more challenging for the coupled codes. Hence, Extreme Scenario 4 serves as clear comparison of physical models of the participants' codes. It should be noted that no comparison with measured data is possible for the extreme cases since they are hypothetical scenarios. Therefore, submitted extreme scenario results are compared with an "average" of the results of the benchmark participants.

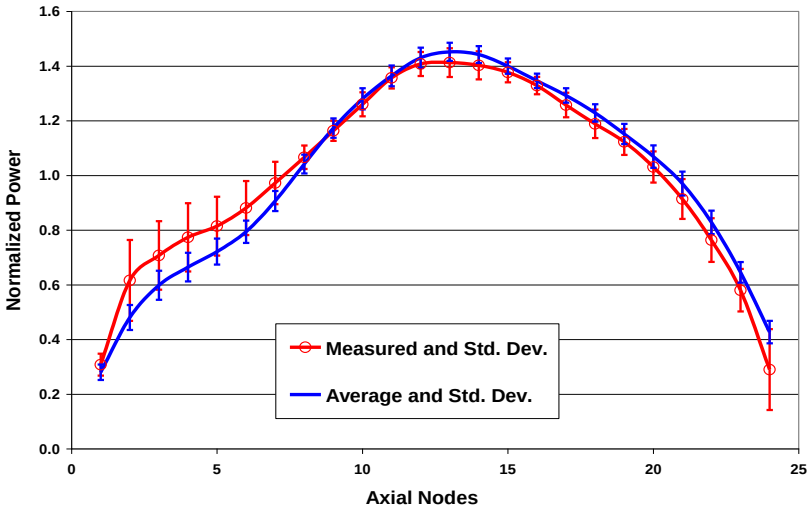
The averaged spatial and time-history distributions over results from 15 participants (using different coupled code systems) are presented in Figure 3.1 through Figure 3.4 and discussed to outline common modelling tendencies. The most challenging part of the BWR steady-state analysis is the prediction of the void fraction distribution. It can be seen from Figure 3.1 that the standard deviation increases in the lower (bottom) part of the core which indicates differences in the void modelling in terms of subcooled boiling and vapour slip. Subsequently these deviations are also reflected in the comparison of the axial power profile predictions due to the void feedback mechanism (see Figure 3.2).

Figure 3.1. Steady-state core average axial void fraction (mean and std. deviation)



Source: PSU, 2018.

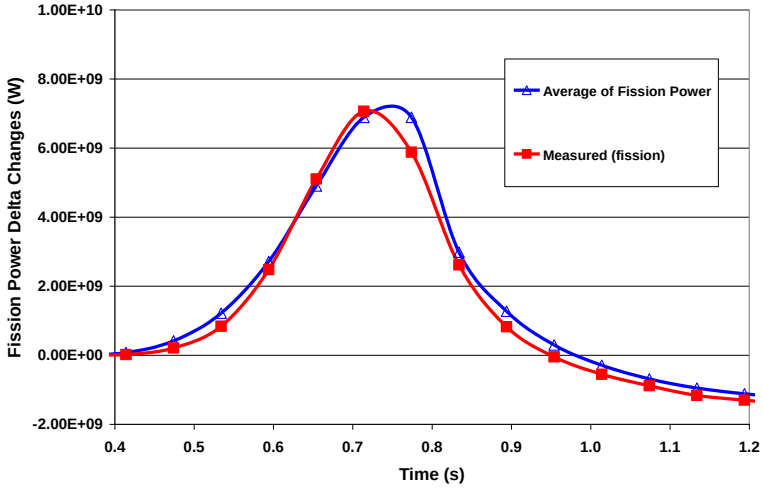
Figure 3.2. Steady-state core average normalised axial power distribution (measured vs. mean and standard deviations)



Source: PSU, 2018.

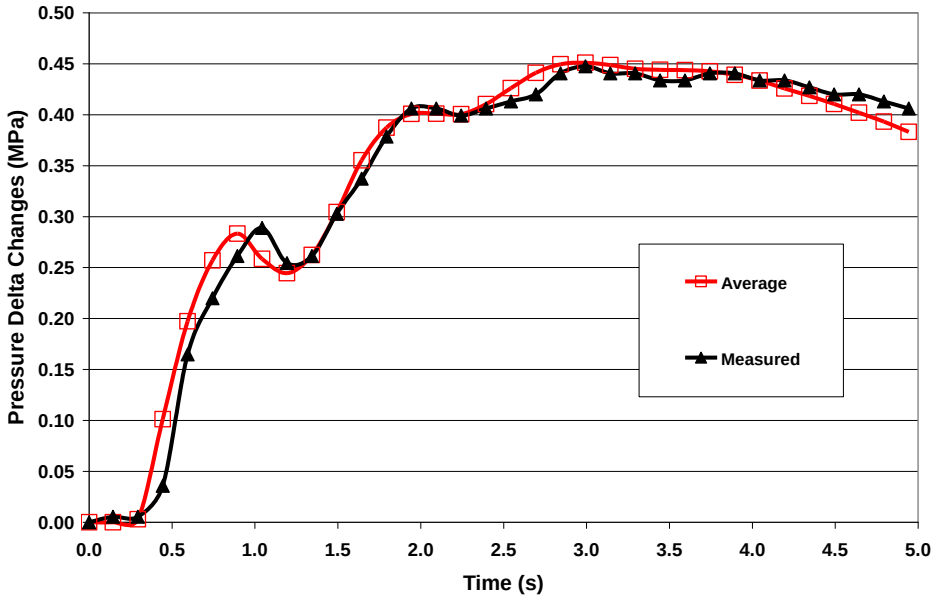
When analysing the power history results in Figure 3.3, it has to be taken into account that in the TT2 test, the thermal-hydraulic feedback alone limited the power peak and initiated the power reduction. The void feedback plays the major role while the Doppler feedback plays a subordinate role. The reactor scram then inserted additional negative reactivity and completed the power reduction and eventual core shut-down. The accurate prediction of void feedback during the transient depends on the modelling of the pressure wave propagation into the vessel. The indication the modelling degree of success is the prediction of dome pressure time history (see Figure 3.4). The participants' results were in good agreement with measured data for the parameters dome pressure, time history and power history. These results increased the trustworthiness of the coupled code capabilities.

Figure 3.3. Best-estimate case − Transient fission power comparison (average vs. measured – zoom)



Source: PSU, 2018.

Figure 3.4. Best-estimate case – Transient dome pressure (average vs. measured)



Source: PSU, 2018.

It is expected that the application of coupled multi-physics codes for safety analyses will grow continuously. In fact, they are the only means to perform best-estimate calculations for accident conditions with a tight coupling of neutronics and thermal-hydraulics effects. Developing multi-level benchmarks, which utilise the available experimental data (such as the described in this paper NEA/NRC BWR TT Benchmark) for consistent validation and verification of coupled multi-physics codes in international co-operation, is important.

The NEA LWR benchmark activities have also stimulated follow-up developments and benchmarks to test new developments [44]. The models utilised have been improved when moving from one benchmark to the next and this created a need to validate these refined models using high-quality experimental data. This new set of NEA benchmarks have been initiated by the Expert Group on Uncertainty Analysis in Modelling (EGUAM), under the Nuclear Science Committee (NSC), to address the current trends in the development of LWR multi-physics and multi-scale modelling and simulation as well as some of the issues identified in the first set of NEA benchmarks. These new benchmarks include the following common features:

- utilisation of high-quality experimental data;
- refined local scale modelling in addition to global predictions;
- more detailed comparisons and analysis;
- including uncertainty and sensitivity analysis of modelling.

The major task of the EGUAM is to address verification, validation and uncertainty analysis of multi-scale and multi-physics modelling and simulation. EGUAM has created a roadmap along with a schedule and organisation for the development and validation of methods and codes required for uncertainty analysis, including the benchmarks adequate to meet those goals.

Reference [45] discusses each of these new benchmarks by providing background and objectives, description and discussion of comparative analysis of obtained results. The following benchmark activities are summarised: NEA/NRC Oskarshamn-2 BWR stability benchmark, and NEA Kalinin-3 water-water energetic reactor (VVER-1000) coupled code benchmark. Since the concept of benchmarks are used throughout this report, its meaning for the discussed NEA benchmarks is defined. Achieving the next level of credibility in computational simulations of nuclear reactor design and safety requires concerted and determined efforts. The goal of these efforts is to improve the reliability of the computer software, the estimation of numerical accuracy, the quality of the physics models used, and the quantification of uncertainty. This report focuses on one aspect of the needed improvements to software reliability and physics modelling, namely, the construction and use of highly demanding V&V benchmarks. The NEA benchmarks of interest are those related to the accuracy and reliability of physics models and codes. These benchmarks are combinations of verification and validation benchmark exercises which involve both use of experimental (measured) data and reference solutions i.e. code-to-data and code-to-code comparisons. When comparing code predictions to experimental data in these benchmarks usually the experimental uncertainties are provided.

3.3 Coupled thermal-hydraulics core/neutronics simulators

The previous name of NSC EGUAM was the Expert Group on Reactor Stability and LWR Transient Benchmarks. This expert group dealt throughout the 1990s with modelling and benchmarking issues in the field of 3D coupled neutronics/thermal-hydraulics transients for nuclear reactor cores. This was the first set of NEA multi-physics benchmarks for LWR cores mostly focused on multi-physics verification since no comparisons with experimental data were involved. Later coupling of core phenomena and system dynamics for nuclear reactor core design and safety analysis was introduced along with comparisons to experimental/measured data developing the second set of NEA multi-physics benchmarks. This set was discussed above along with the latest set of multi-physics benchmarks which added to validation, the aspects of sensitivity and uncertainty analysis.

As mentioned above the first set of benchmarks aimed at performing code-to-code comparisons although the benchmark reactor core models are based on real reactor data. The first benchmark is a PWR 3D core transient benchmark [46] based on a rod ejection accident. This is the ejection of a control assembly from the core, which may occur because of the rupture of the drive mechanism casing located on the reactor pressure vessel top. This event can produce significant, well localised perturbations of the neutronic and thermal-hydraulic core parameters, without exceeding the safety margins. Hence, a rather realistic standard reactor situation is defined, that efficiently utilises the neutronics and thermal-hydraulics sub-models of the reactor dynamics code. The second one is a BWR core benchmark. The BWR problems consist of sub-prompt critical reactivity excursions generated by rapid cold-water injection or core pressurisation events. This set of problems was chosen because it is felt that the analysis of two such cases − in which the interplays of the neutronic and thermal-hydraulic effects are markedly different − represents a direct and effective way to fulfil the objectives of the benchmark.

The third one applies the same core model as the PWR rod ejection benchmark and is based on modelling an uncontrolled withdrawal of control rods at zero power accident on a PWR [47]. The accident consists basically of a continuous reactivity insertion, limited by a reactor trip, which occurs a certain delay after high flux or high flux increase detection. Like the rod ejection accident, the peak power usually takes place before the scram and the

main factor limiting the consequences of the accident is the Doppler effect. The temperature rise, however, is stopped by the trip, that must therefore be considered. It should be noted that the peak power occurs while important power distribution changes take place in the core, because the rod extraction continues until reactor trip. Two prompt neutron groups, i.e. thermal and fast neutrons, and six delayed neutron groups are used for neutron modelling. The boundary condition for the solution of the neutron diffusion equation is flux vanishing at the outer reflector surface. A complete set of macroscopic cross-sections for transport, scattering, absorption and fission and their derivatives with respect to the boron density, moderator temperature, moderator density and fuel temperature is defined for each composition. The feedback or coupling between neutronics and thermal-hydraulics is characterised by definition of channel regions. In the benchmark, each FA must be defined as a channel region ("closed channels" model), ignoring inter-assembly cross-flow and mixing and using one TH feedback axial mesh per assembly. A flat profile of the radial distribution of the power density inside the fuel is assumed. The inlet mass flow through the core is distributed uniformly among the channels. The transient to be analysed as a function of time in 3D or 1D is generated by the withdrawal of control rod banks from an initially critical core at HZP. The withdrawal speed is a typical bounding value.

The fourth verification core benchmark addresses a rod ejection transient in a PWR core loaded partially with weapons-grade, MOX fuel [48]. The neutronics characteristics of plutonium are sufficiently different from uranium to significantly change the kinetics response of the reactor core. The reactor core chosen for the simulation is based on a four-loop Westinghouse PWR power plant like the reactor proposed for plutonium disposal in the United States.

In addition to the above core verification benchmarks the second exercises of the LWR core/plant benchmarks (PWR MSLB, BWR TT, V1000 CT, Kalinin-3 VVER-1000 transient and Oskarshamn-2 BWR stability benchmarks) described previously can be used for validation of multi-physics core models. These are benchmark exercises with provided core thermal-hydraulic boundary conditions from system calculations performed by the benchmark teams. The available measured data for integral parameters and local distributions inside LWR cores can be used for code-to-data comparative analyses.

3.4 Coupled neutronics/fuel performance simulators

The heat transfer phenomena inside the fuel rod are comprised of heat conduction in the fuel pellets, heat transfer across the gap between fuel pellets and cladding inside surface, and heat conduction across the cladding thickness. The combination of these effects, along with the geometrical fuel pin design, will influence the fuel pin overall time constant at power variations, though the heat transfer across the gap (gap conductance) will have the greatest influence. All the effects are dependent on the fuel pin burn-up and will consequently also have a variation in the axial direction.

Modelling of fuel rod behaviour in multi-physics calculations is mostly important for predictions of fuel temperatures for feedback purposes i.e. Doppler feedback modelling. Usually this is done by incorporating simplified fuel rod models in system thermal-hydraulics, or sub-channel (core) thermal-hydraulics, or neutronics core simulators. These models are efficient but need to be improved for accurate predictions of fuel temperatures. The list of heat conduction and fuel-related phenomena or related computational aspects that may require further investigation to validate the results of multi-physics calculations includes the following: minimum number of concentric rings for the fuel rod that bring to the convergence of results, pellet gap performance during the transient with main reference

to variations in physical properties and geometry, and fuel deformation and change in physical properties during the transient (namely steep power rise).

Currently there are two tendencies to improve the accuracy of predictions of Doppler (effective fuel temperature) feedback temperatures in multi-physics calculations: using higher-fidelity fuel performance codes to inform simplified fuel rod models [49] and to couple directly fuel performance codes with neutronics and thermal-hydraulic core models [50]. The issue with the second tendency is that usually the fuel performance codes model a single fuel rod, which requires many parallel calculations and affects computational efficiency.

Fuel performance codes analyses the thermal, mechanical and internal gas responses of fuel rod components with the goal of predicting rod condition and integrity. Modelling of thermal behaviour during normal and transient conditions includes surface heat transfer, the heat transfer across the fuel-to-cladding gap, thermal conductivity of fuel and cladding, power generation distribution in the fuel and solution of the conduction equation. These codes can model steady-state and cycle depletion as well as transient fuel behaviour [51].

One example of coupling simplified fuel rod models with neutronics codes are the coupling of INTERPIN with the Studsvik CMS codes − CASMO and SIMULATE [52] for steady-state and cycle depletion calculations as well as the development of SIMULATE-3K explicit fuel pin modelling [53] for transient calculations.

In traditional multi-physics calculations, the coupling is performed on a node/assembly basis and for the purposes of modelling thermal-hydraulic feedback effects (including Doppler feedback) the physical fuel pins within a node (assembly) are modelled by an average/lumped fuel rod. The capability to explicitly represent every fuel pin in the reactor core has been recently added to novel high-fidelity multi-physics calculations by coupling neutronics, thermal-hydraulics and fuel performance codes on fuel pin/sub-channel basis [54].

3.5 Multi-physics multi-scale code systems

The traditional multi-physics methodologies have reached maturity and have several common features [55]:

- the 3D core neutronics model is based on two-group (or few-group) coarse-mesh diffusion approach using nodal nuclear data (library of parameterised nodal equivalent parameters);
- the spatial neutronics/thermal-hydraulic coupling is performed on assembly/channel level;
- simplified fuel rod models are utilised as part of the core thermal-hydraulic codes;
- the temporal neutronics/thermal-hydraulic coupling is performed in the operator-splitting approach using nested loop iteration (fixed point iterations) for steady-state simulations and sequential parameter exchange (explicit coupling) at each time step for transient simulations;
- the evaluation of safety related parameters on pin/sub-channel level for the hot assembly/channel is performed via pin-power reconstruction combined with sub-channel calculations using boundary conditions provided by the coupled core model.

These multi-physics methodologies can predict the non-symmetrical core power perturbations in a more realistic manner and they can predict safety margins more accurately by means of 3D core model with a spatial resolution at fuel assembly level for a wide range of normal operation including cycle depletion, operational transients and postulated accidents. The approximation level is acceptable, however, the safety-relevant parameters, that determine the accident consequences, such as fuel rod enthalpy, departure from nucleate boiling ratio (DNBR), burn-out, maximum fuel rod cladding temperature, fuel rod centreline temperature, etc., must be evaluated at local conditions i.e. in terms of a single rod (pin) response rather than based on an assembly-wise response. Different approximated "hot channel" or "hot assembly" models are used for approximated predictions of local safety parameters. Usually coupled thermal-hydraulic system and neutronics codes are further coupled with sub-channel codes [56-58], extending the multi-physics coupling to multi-scale modelling.

An example of validation of such multi-physics multi-scale code systems for licensing applications is given in [58] for the RELAP5/PANTHER/COBRA code package. The validation of this package depends on the separate validation of each major component of the coupled package and on the validation of the coupling processes themselves (i.e. the data exchange interfaces). The RELAP5, PANTHER and COBRA codes have been validated separately as single physics codes for licensing applications. For the multi-physics multi-scale coupled code package the validation effort of the coupled code package is mostly focused on the coupling processes themselves.

In addition, the validation of the coupling interfaces is performed followed by validation of the whole coupling process. Specific demonstrations that the interface tools achieved in all cases the required data transfer is provided to show that:

- the transfer of the variables between the different codes perform exactly as designed and the code internal variables are consistently assigned to the required values;
- the coupled code solutions are identical to the separate stand-alone code solutions with the same imposed boundary conditions;
- the coupled code solutions are not influenced by the time advancement techniques chosen in the data transfer process.

4. Uncertainty quantification approaches

This chapter discusses experimental uncertainty and the impact of data calibration for computational models.

4.1 Overview of uncertainty methodologies

One of the most important terms in reactor safety is the safety margin and the licensing of nuclear power plants has been done by assuming conservative values for the computations. Nowadays, it is possible to estimate certain parameters using non-conservative data with the complement of uncertainty evaluation and these calculations can also be used for licensing. The uncertainty methods within the nuclear field are an important step to help increase production, while staying below the safety limits [59].

Several uncertainty methods have been developed for uncertainty evaluation of the system codes including:

Adjoint sensitivity analysis procedure [60]: The theory behind the method is to get sensitivity responses for all uncertain parameters and then use them to assess the uncertainty by propagation of error formulae. The method works for both linear and non-linear systems and this makes it appropriate for the case of a nuclear power plant. This method requires significant modifications of the code.

Propagation of input errors (PIE) [61]: This approach represents statistical variation of the input parameters, together with their uncertainties, to reveal the propagation of errors through the code. The method relies on real code calculations, but instead of calculating certain parameters with discrete values, it performs many times the same calculation using different values for these parameters. This approach allows evaluation of correlation coefficients between the uncertain parameters and the target output parameter, which can be used to determine the most influential parameters. The drawback of this method is that all uncertain parameters must be identified, and probability density functions must be assigned to them, which sometimes has to be an engineering judgement.

Propagation of output errors [62]: This methodology focuses on extraction of the errors from a suitable experimental database coming from integral test facilities and real plant data. The results calculated by the system codes are extrapolated with the uncertainty band, to obtain the uncertainty in the code prediction. The benefit is that the method does not require the identification of all uncertain input parameters. The drawback is that it relies on non-physical extrapolation of errors coming from all available relevant data and producing the final uncertainty band which is not necessarily directly related to the given case.

The second method (propagation of input errors) is the most used within the industry and it has been extensively verified. It provides the opportunity to identify the influence of each parameter on the results, which is not possible in the third method (propagation of output errors). Furthermore, the propagation of output errors requires extensive and relevant experimental data to implement the method, which is not available for example, in the case

of BWR stability studies. Moreover, the propagation of input errors method relies on the actual code calculations without using approximations such as fitted response surfaces.

4.2 Propagation of input errors methodology

The PIE method is based on statistical variation of input parameters and it does not require modifications of the code (except for the closure models and correlations). In principle there is no limitation on the number of uncertain parameters and range of variation of the perturbed parameters. In this method, every parameter is considered as a probability distribution, not as a discrete value, as shown in Figure 4.1. A random set of discrete values based on their probability density functions (PDFs), for all "suspicious" parameters needs to be generated. The sources of PDFs are literature (e.g. scientific papers) or an expert judgement. After all important parameters are identified and the random sample is set, N model runs should be performed with these randomly sampled parameters as input. The required number of runs (N) is given by the Wilks' formula, Equations (1) and (2) [63,74]:

$$1 - (\alpha/100)^N \geq \beta/100 \quad (1)$$

β% is the confidence level that the maximum code result will not be exceeded with the probability α% of the corresponding output distribution, which is to be compared to the acceptance criterion. The formula for the two-sided statistical tolerance intervals is given as:

$$1 - (\alpha/100)^N - \mathrm{N}\,(1 - (\alpha/100))\,(\alpha/100)^{N-1} \geq \beta/100 \quad (2)$$

Here, α and β have the same meaning as in the previous equation.

Depending on the requirements for the confidence interval, one can estimate how many calculations are needed to obtain the desired results. The minimum number of runs can be found in Table 4.1. Usually (95%/95%) one- or two-sided tolerance limit is used, which is taken as a best-estimate prediction requirement [63].

Table 4.1. Minimum number N of calculations

	One-sided statistical tolerance limits			Two-sided statistical tolerance limits		
β / α	0.9	0.95	0.99	0.9	0.95	0.99
0.9	22	45	230	38	77	388
0.95	29	59	299	46	93	473
0.99	44	90	459	64	130	662

Source: Triola, 2007.

In the PIE calculation, all parameters are varied simultaneously. The PIE uncertainty calculation provides the uncertainty of the output parameters which are to be examined. Comparing this result with the measurements provides a measure of the confidence of the code prediction.

The Spearman rank correlation coefficient between the output parameter and the input parameter value can be used to identify the most influential parameters. This coefficient provides a quantitative indication if the considered parameter (and its uncertainty, represented by its PDF) has a significant impact for example on the stability of the reactor

(in case of BWR studies). The criterion for "importance" consists of the so-called critical value of the Spearman correlation coefficient. If the absolute value of the estimated correlation coefficient is higher than the critical value, then this parameter is determined to have a statistically significant impact on the result. Otherwise, the parameter will be considered to have low or no importance. The critical values r_s for the Spearman rank correlation coefficient can be evaluated using Equation (3) [65].

$$r_s = \pm \frac{z}{\sqrt{n-1}} \tag{3}$$

For the confidence interval of 95%, z = 1.96 and n is the number of runs [65]. Another important outcome of the Spearman rank correlation is the sign of the correlation coefficient; if it is positive then increasing the input parameter increases the output parameter, if it is negative then increasing the input parameter decreases the output parameter.

Sources of uncertainties

The propagation of input errors method relies on the availability of the input uncertainty probability density functions. Without these functions PIE uncertainty calculation could not be performed. Several classifications of uncertainties can be found. In general, uncertainties can be divided in two broad categories.

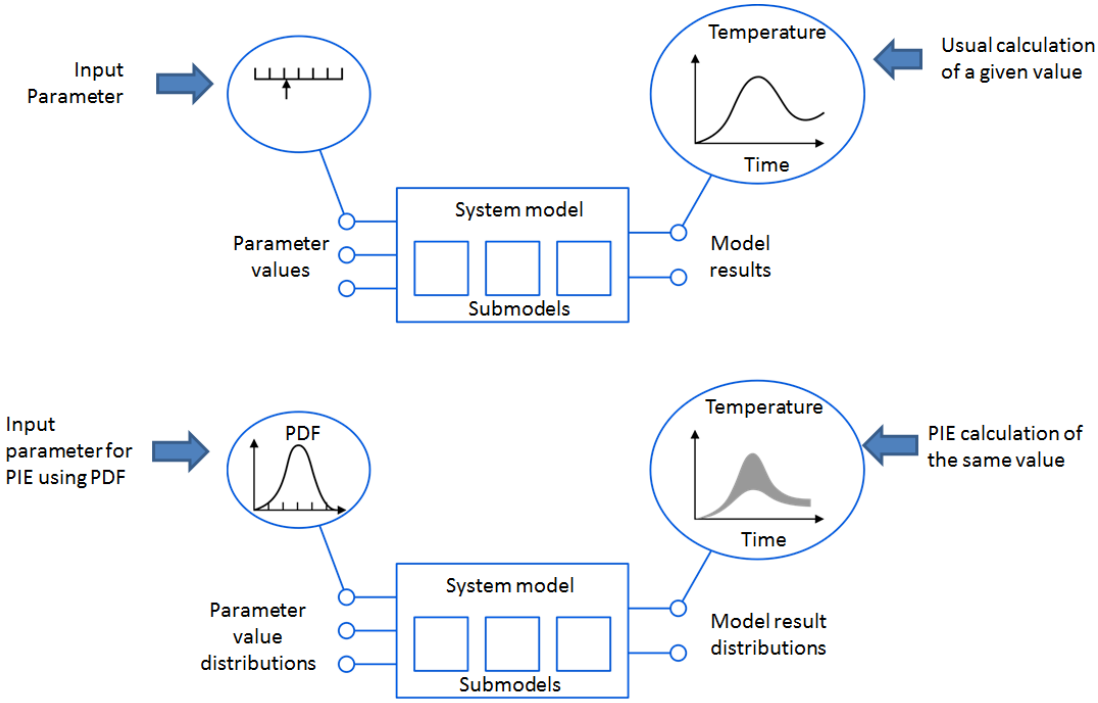
The first category is called aleatory (or stochastic) uncertainty. This uncertainty comes from the random nature of how a system behaves. An example of this uncertainty can be the measurement of the temperature in a room. Each time one measures, it will be different within the limits of the measuring instrument. This uncertainty is irreducible (cannot be reduced using the same technology) and is associated with the performance of an experiment or a measurement [64,65].

The second category is the epistemic (or subjective) uncertainty. This category stands for the lack of knowledge of a certain parameter. An example of this uncertainty can be a certain correlation in the analytical model, which might not be able to represent the reality in some ranges of other parameters during the simulation. This uncertainty is reducible (it could be reduced if new knowledge is provided) [64,65].

The three major sources of uncertainties in accident analysis have been identified in [64].

- Code or model uncertainty: Uncertainty associated with the models and correlations, the solution scheme, model options, un-modelled processes, data libraries and deficiencies of the computer program.
- Representation or simulation uncertainty: Uncertainty in representing or idealising the real plant, such as that due to the inability to model a complex geometry accurately, three dimensional effects, scaling, control and system simplifications.
- Plant uncertainty: Uncertainty in the measuring or monitoring of a real plant, such as reference plant parameters, instrument error, set points or instrument response, initial conditions.

Figure 4.1. Illustration of the PIE method and results interpretation



Source: Glaeser, 2008.

4.3 Summary of general frameworks for uncertainty quantification

This section provides a summary of common features and differences of the current uncertainty quantification (UQ) frameworks in use.

Code scaling applicability and uncertainty (CSAU)

In 1988, the United States Nuclear Regulatory Commission (US NRC) revised the emergency core cooling system (ECCS) rule that allowed the use of best-estimate codes in performing safety analyses with the estimation of uncertainty [66,67]. This alternative approach commonly is referred to as the Best Estimate Plus Uncertainty (BEPU) method. In this approach, various sources of uncertainties are combined to predict the aggregate uncertainty in the results of the analysis.

The US NRC developed the code scaling, applicability and uncertainty (CSAU) [67] evaluation methodology to illustrate, a systematic, auditable method of estimating uncertainty in the prediction of safety parameters from best-estimate computer codes and demonstrated the method by applying it to large break loss-of-coolant accidents (LBLOCAs) for a standard PWR. The methodology heavily relies on separate effects tests and somewhat on integral effects tests. The recognition of scaling distortion of these tests and their contributions to the overall uncertainty is an important aspect of the CSAU methodology.

The CSAU methodology is a 14-step procedure arranged in three elements as shown in Figure 4.2. Element 1 − Requirement and Code Capability − includes the first six steps. These steps identify the scenario or transient, power plant and important phenomena based on a phenomena identification and ranking table (PIRT) analysis. Then the code for safety

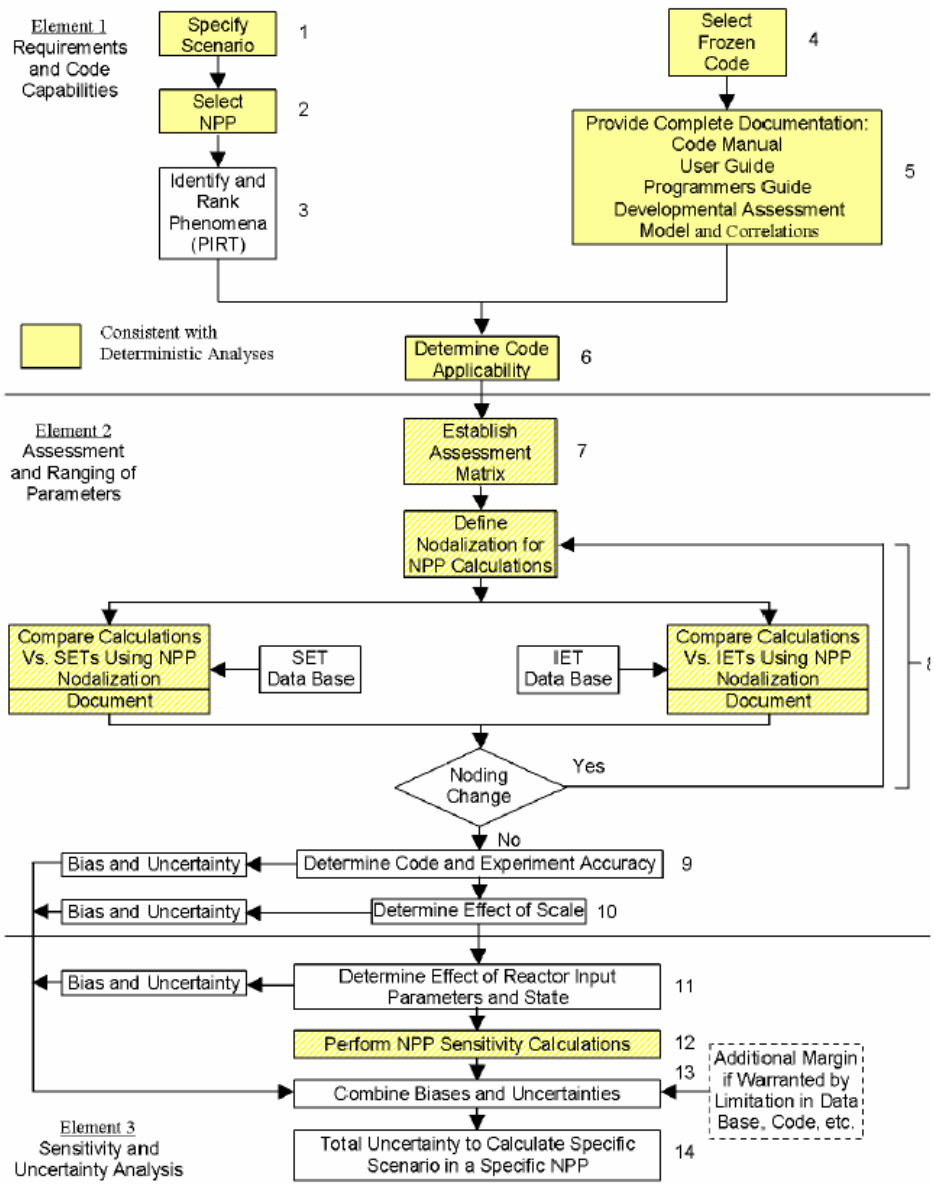
analysis is chosen for the transient. Based on the code manuals, the code applicability is determined. The code applicability is assessed in Step 6 of the CSAU methodology. The PIRT identifies the important phenomena for the given scenario and plant. The code's formulation, model, and correlations are reviewed to assess if the code has the model/correlations to simulate the important phenomena, and if the code has scale-up capability. It is recognised that while the formulation may be general, the correlations or constitutive relationships are empirical. The code's scalability will depend on these correlations and the underlying tests. If the tests scale to the plant for the phenomena of interest, then the correlation is applicable. However, if the correlation was derived from tests that do not scale to the plant, the code may not scale up to the plant. Code validation with scaled tests or counterpart tests is another way of assessing code's ability to scale and applicability.

Element 2 − Assessment and Ranging of Parameters − includes four steps. An assessment matrix is established based on a PIRT. Nuclear power plant nodalisation is established and safety calculations are performed. Based on comparing the calculation results with separate effect test (SET) and integral effect test (IET) data sets, the nodalisation is modified and iterated. Step 9 concerns estimating the code's uncertainty based on experiments, and Step 10 is for determining the effect of scaling and the resulting bias and uncertainty. With them, the uncertainties of code models are estimated and are input to Step 13 where all the uncertainties and biases are combined. In Step 9, the uncertainty in predicting phenomenon is estimated by identifying the appropriate parameters to represent it and selecting the separate effects tests. In cases where there are data for full-scale facilities with reactor thermal-hydraulic conditions, modelling the tests with the proper nodalisation, comparing the predictions with the data and accounting for instrument uncertainty, will suffice. However, for small tests, a scaling study will be needed to find any scaling bias, or counterpart tests must be used at different scales. Engineering judgement and sensitivity studies are also used to estimate the uncertainty range in the designated parameters representing the phenomenon, or the bias in the figure of merit (FOM).

There are two approaches for estimating uncertainties, based on using integral effects tests, or separate effect tests. If there are well-scaled integral facilities for the transient of interest, a comparison of the predicted and measured values of the FOM can provide an estimate of uncertainty. However, it is very difficult to design a single integral effects facility that can scale the transient for all phases. Also, as the uncertainty propagates with time, the initial lower-scale uncertainty will grow over time. Therefore, in general, the role of integral facilities is to verify an estimate of the overall uncertainty in the FOM attained by propagating uncertainties through the code and combining them. In this approach, the code uncertainty is estimated through the combination of uncertainties and biases of different phenomena as computed from separate effects tests. This overall uncertainty in the FOM should always be higher than the uncertainty estimated from integral effects test facilities. In them, the uncertainties of code models that are estimated and are input to Step 13 where all the uncertainties and biases are combined.

Element 3 − Sensitivity and Uncertainty Analysis − includes the remaining four steps. In this group, the overall uncertainty of the predicted FOM is evaluated. In the CSAU methodology, three uncertainty sources are quantified – the code and experiment accuracy (Step 9), the effect of scaling (Step 10) and the reactor input parameters and state (Step 11). The model uncertainties and reactor condition uncertainties are in the form of bias and distribution. These are propagated through code calculations for the plant and prediction of the FOM. These contributions to the FOM or safety parameter are combined in Step 13. The CSAU methodology ends with the estimation of total uncertainty.

Figure 4.2. The CSAU methodology flow chart



Source: Boyack. et al., 1989.

As an example, the CSAU methodology was applied to an LBLOCA in a standard PWR. The PIRT development in Step 3 identified five important phenomena; break flow, stored energy, pump performance under two-phase conditions, steam binding and the ECC bypass. Some of these phenomena were further broken into sub-phenomena.

Uncertainty in break flow prediction was estimated for subcooled and saturated conditions as the code has two different models. Marviken tests (Marviken Project, 1974) provided full-scale data, and so the uncertainty estimate did not need any additional scaling bias. The ranging of the parameter (surrogate for the critical flow model) and bias were estimated for subcooled and saturated choking.

The review of available counterpart tests for the primary pump showed scale-dependencies for the two-phase performance or degradation of the head. The two-phase flow has its own characteristic length, such as bubble size, and the larger the size of the flow channel, the smaller is the effect on the degradation of performance. In addition, specific speed also influences degradation. Larger specific speed-pumps have more axial flow and tend to degrade less. The largest size pump in the database is the Westinghouse pump at a 1/3 scale. The specific speed is around 5 200 rpm and is the same as a Westinghouse PWR pump. Comparing two-phase performances of the pumps at different scales, it was concluded that larger pumps experience smaller degradations. Therefore, Westinghouse's 1/3 scale data can be used for the nuclear power plant pump. It will have a slightly larger degradation than the nuclear power plant pump. However, this will be conservative as the pump flow will decrease sooner, at least for LBLOCA.

The stored energy in the fuel was rated very high in the PIRT. It was shown, through sensitivity analyses that the stored energy is the most sensitive to four parameters, namely, gap conductance, peaking factor, fuel thermal conductivity and convective-heat transfer. There are no scaling issues with the first three parameters since they are either independent of the length scale (thermal conductivity) or boundary conditions (peaking factor) or no scaled study is available (gap conductance). However, the convective-heat transfer was further broken into two parameters, minimum film-boiling temperature and the convective-heat transfer coefficient. It is recognised that a lower T_{min} will lead to an earlier transition to film boiling in the blowdown phase and delay the transitioning to subcooled boiling in the reflood phase and leading to higher peak cladding temperatures (PCT). There were data from many tests both for the tubes and the rods and for a large range in pressure. The TRAC models were compared with the available data. It was recommended that a homogenous nucleation temperature be used as it gave a lower T_{min} than that predicted by TRAC. The spread of all the data was 360°F and half of this value (180°F) was recommended for the range. Here, the approach is to use a conservative mean value and the range. The other contributor to heat transfer is the heat transfer coefficients. During the process of comparing the data it was found that TRAC over-predicted the heat transfer coefficient at void fractions greater than 0.75 and that the cause of this over prediction is the film-boiling heat transfer coefficient. In the actual code application, it is recommended that the Forslund-Rohsenow film-boiling correlation be removed and the uncertainty in the remaining heat transfer models is accounted for through a multiplier with a range of 0.75 to 1.25. The scaling effect was included in the overall uncertainty in the heat transfer model.

Another important phenomenon that affects the PCT is steam binding in the hot leg and the steam generator's u-tube. The liquid carried in the steam generator vaporises and creates a high pressure in the upper plenum, delaying the onset of reflooding, leading to a higher PCT. The sub-phenomena that control vapour-binding are the drops coming from the liquid interface in the core and the entrainment of these drops into the hot leg and steam generator. Modelling of two Slab Core Test Facility (SCTF − 1/21 size) tests with TRAC indicated that the code under-predicts the entrainment flow to the hot leg. A set of multipliers were developed to apply to TRAC models to increase the number of drops emanating from the interface and also to increase interfacial shear-stress to match the entrainment to the hot leg and the steam generator. The SCTF is a small facility. It is assumed that as correlations that are being affected are localised; they are not dependent on the size of the facility.

The phenomenon of ECC bypass is the most important phenomenon as it determines the refill phase and the flooding and quenching of the core. It affects the reflood PCT. The ECC injection is from the accumulator to the cold leg and to the down-comer. The steam up flow in the down-comer towards a break impedes the ECC flow through interfacial

shear, thus delaying the re-flooding phase. The other phenomenon that assists in refilling is the condensation of steam in the down-comer. When non-condensable gases are present in the down-comer, condensation is reduced and the ECC bypass is increased. The filling time of the lower plenum will depend on the combination of these phenomena. Many tests for ECC bypass phenomenon are available at different scales, such as CREARE (1/5), Battelle Columbus Laboratory (BCL) (2/15), and CREARE (1/15). A comparison of the predicted and measured lower plenum filling rates indicated that TRAC over-predicted the filling rates for small scale facilities and under-predicted them for a 1/5 scale facility. Data from a full-scale facility, Upper Plenum Test Facility (UPTF) [69], also became available. The TRAC code under-predicted the filling rate for UPTF [68]. As UPTF is full-scale test, the model's uncertainty and the corresponding bias in PCT were estimated directly. In addition, the TRAC code did not have a model for non-condensable gases. A separate analysis was performed to estimate the amount of non-condensable gas coming out of the coolant and its impact on delaying the reflood phase and the corresponding bias in reflood PCT.

In the CSAU methodology, many integral test facilities at different scales were reviewed; these scales included semi-scale, loss-of-fluid test (LOFT) [70], cylindrical core test facility (CCTF) [71], slab core test facility (SCTF) [71], and Primarkreislauf − large-scale test facility (PKL) [72]. It was concluded that all the blowdown PCTs were within the 95% tolerance limits when plotted as a function of the linear heating-rate. This finding indicated that this is the most dominant phenomenon in the core. However, there are other system-effects such as pump break that determine the time at which the heat transfer has degraded enough so that temperature rise is only a function of decay heat. In the case of reflood peak, the plots were made with the rise in core temperature as a function of the reflooding rate. It indicated that cores were well scaled in different facilities varying in size from Semi-scale (1/1700) to CCTF (1/21). However, the reflooding rate will be governed by system performance and any scaling distortion there will affect the rate of reflooding. The study showed, as expected, that temperature rise declines with an increase in the reflooding rate.

Facilities scale the blowdown phase well. However, the scaling effect becomes more pronounced for the refill- and reflood-phase due to the interaction of many scaled phenomena, such as the ECC bypass. To find scale similarities the PCT were plotted as a function of flow in the core. PCTs from different facilities correlated well. As the core thermal-hydraulic was decoupled from rest of the system in the refill/reflood phase in this study, the plot suggested that core was scaled well in all the facilities. A bias was estimated for the scaling effect of the ECC bypass phenomenon [62].

In estimating the uncertainty or bias induced by scale distortion in an integral test facility, the impacted parameter (e.g. peak cladding temperature in a LOCA) and the dominant contributing parameter (e.g. linear rate of heat generation in LOCA) are plotted for all available data points covering all scales. Then, the uncertainty in reaching the 95% confidence level is used as a confirmation of the CSAU procedure of aggregating important uncertainties in phenomena, resulting in total uncertainty in the FOM.

In evaluating the scale-up capabilities of correlations in the code, based on the PIRT result, one evaluates the processes that impact the parameter of interest e.g. the model of the reactor's coolant pump, the critical two-phase flow through breaks and liquid entrainment to steam generators in a LOCA. All available scaled data used to develop the correlation or the models in the code are compiled to determine the uncertainty or bias to reach a 95% confidence level.

If the distortion and scale-up capability are satisfied, the range of the nuclear power plant data needs to be compared to the conditions of the database experiments and the closure correlations in the code. If the nuclear power plant range is not covered, additional biases are needed. After this evaluation, all the uncertainties and biases are added together as the bias from scaling (Step 10). Both are combined with other sources of uncertainty from Steps 9 and 11 into the total uncertainty or bias (Step 13) for sensitivity calculation (Step 14,) using the nuclear power plant nodalisation. This will require many runs with the TRAC code. To avoid expensive runs, the TRAC code was replaced by a surrogate surface by running TRAC for different values of the uncertain parameters. Once a response surface is established, thousands of values of the FOM are estimated by sampling the uncertainty range for each parameter representing important phenomena. The large number of values is then plotted as a probability density function (distribution) and 95% values can be obtained. However, this approach of finding the 95% value using a response surface limited by the number of phenomena that can be considered.

GRS Uncertainty quantification methodology

The GRS method [73] is a probabilistic method based on the concept of propagating the input uncertainties. All relevant uncertain parameters including the code, representation and plant uncertainties are identified, any dependencies between uncertain parameters are quantified and ranges and/or PDFs for each uncertain parameter are determined. Expert judgement and experience from code applications to separate and integral test and full plant application are principal sources of information for uncertain parameters identification and quantification. Characteristics of the GRS method are:

- The uncertainty space of input parameters (defined by their uncertainty ranges) is sampled at random according to the combined "subjective" probability distribution of the uncertain parameters and code calculations are performed by sampled sets of parameters.
- The number of code calculations is determined by the requirement to estimate a tolerance/confidence interval for the quantity of interest (such as peak clad temperature). The Wilks formula [64,74] is used to determine the number of calculations needed for deriving the uncertainty bands.
- Statistical evaluations are performed to determine the sensitivities of input parameter uncertainties on the uncertainties of key results (parameter importance analysis).
- There are no limits for the number of uncertain parameters to be considered in the analysis and the calculated uncertainty has a well-established statistical basis.
- The method relies only on actual code calculations without using approximations like fitted response surfaces.

For the selected plant transient, the method is applied to an integral effects test simulating the same scenario prior to the plant analysis. If experimental data are not bounded, the set of uncertain input parameters must be modified. Experts identify significant uncertainties to be considered in the analysis, including the modelling uncertainties and the related parameters and identify and quantify dependencies between uncertain parameters. Subjective probability density functions are used to quantify the state of knowledge of uncertain parameters for the specific scenario. The term "subjective" is used here to

distinguish uncertainty due to imprecise knowledge from uncertainty due to stochastic or random variability.

Uncertainties of code model parameters are derived based on validation experience. The scaling effect must be quantified as model uncertainty. Additional uncertain model parameters can be included, or PDFs can be modified, accounting for results from the analysis of SET facilities. Input parameter values are simultaneously varied by random sampling according to the subjective PDF and dependencies. A set of parameters is provided to perform the required number n of code runs. For example, the 95% fractile and 95% confidence limit of the resulting subjective distribution of the selected output quantities is directly obtained from the n code results, without assuming any specific distribution. No response surface is used or needed.

Sensitivity measures by using regression or correlation techniques from the sets of input parameters and from the corresponding output values allow the ranking of the uncertain input parameters in relation to their contribution to output uncertainty. Therefore, the ranking of parameters is a result of the analysis, not of prior expert judgement. The 95% fractile, 95% confidence limit and sensitivity measures for continuous-valued output parameters are provided.

Upper statistical tolerance limits are the upper β confidence for the chosen α fractile. The fractile indicates the probability content of the probability distributions of the code results (e.g. $\alpha = 95\%$ means that PCT is below the tolerance limit with at least $\alpha = 95\%$ probability). One can be 95% confident that at least 95% of the combined influence of all the characterised uncertainties are below the tolerance limit. The confidence level is specified because the probability is not analytically determined. It accounts for the possible influence of the sampling error since the statements are obtained from a random sample of limited size. The smallest number n of code runs to be performed is given by the Wilks formula [74] (Equations 1 and 2). The minimum number n of calculations for both one-sided and two-sided can be found in Table 4.1. As a consequence, the number n of code runs is independent of the number of selected input uncertain parameters, only depending on the percentage of the fractile and on the desired confidence level percentage. The number of code runs for deriving sensitivity measures is also independent of the number of parameters. As an example, a total number of 100 runs is typical for the application of the GRS method. For regulatory purposes where the margin to licensing criteria is of primary interest, the one-sided tolerance limit may be applied, i.e. for a 95th/95th percentile 59 calculations should be performed. The FOM is arranged in decreasing order and the higher value represents 95% percentile with 95% confidence. The Wilks formula has been extended for more than one resulting output parameter in a recent work [75].

GRS Sampling-based uncertainty analysis codes

General method

For the investigation of the uncertainty of output quantities obtained by simulation programmes, sampling-based uncertainty analyses are performed. With this approach, input uncertainties are propagated through the calculation chain to output uncertainties for quantities of interest. At first, the uncertain input parameters must be identified. Furthermore, the corresponding probability distribution functions for each uncertain input parameter must be chosen (e.g. the normal distribution with a mean value and a standard deviation) and possible correlations between input parameters must be identified. Based on this information, a set of samples for each input parameter is generated such that new input

data sets are created. The simulations are then performed with these varied input data. For the output quantity of interest, a set of results is obtained which can be statistically analysed to determine a mean value and a standard deviation. The standard deviation corresponds to the uncertainty of the respective quantity due to the perturbed input parameters.

XSUSA

The XSUSA (Cross Section Uncertainty and Sensitivity Analysis) method [76,77] is based on the random sampling GRS method implemented in the code package SUSA "Software for Uncertainty and Sensitivity Analysis") [78]. The uncertain input parameters as described above are the neutron cross-sections that serve as input to neutron transport codes. When applying the random sampling method with neutron cross-section uncertainties, many nuclear data libraries are generated in which the quantities with available uncertainties (essentially inelastic and elastic scattering, the (n,2n) and capture cross-sections, the fission cross-section, the number of neutrons per fission and the fission neutron spectrum) are varied at the same time for a large number of nuclides. The basis for generating the data variations is the SCALE 6.1 covariance data library which contains uncertainties for relevant nuclides [79]. Correlations between the energy group data of each nuclide/reaction combination are considered as well as cross-correlations between data of different reactions or even data for different nuclides. It is furthermore assumed that the neutron cross-sections follow normal distributions with mean values and standard deviations from the cross-section library and the covariance data files, respectively. Any quantity that is output from the criticality or depletion calculation with the considered neutron transport code can be statistically analysed. These typically include the multiplication factor, reactivity coefficients, power distributions as well as homogenised macroscopic cross-sections generated for use in nodal diffusion codes [80,81].

SUSA

The software tool SUSA (Software for Uncertainty and Sensitivity Analyses) [82-84] guides through the main steps of a probabilistic uncertainty and sensitivity analysis. These steps can be summarised as follows:

- identification of all phenomena, modelling assumptions and parameters that are potentially important contributors to the uncertainty of the computational result and representation of all uncertainty sources by uncertain parameters;
- quantification of the state of knowledge on the uncertain parameters in terms of probability distributions and dependence measures;
- generation of a sample of values for the uncertain parameters according to a multivariate probability distribution which satisfies the input given in Step 2;
- computer code executions for each set of values sampled for the uncertain parameters − random sample from the unknown probability distribution of the computational result;
- quantification of the uncertainty of the computational result based on the sample resulting from Step 4;
- ranking of the parameters with respect to their contribution to the overall uncertainty of the computational result − sensitivity analysis;

- comprehensive documentation of the analysis steps for scrutinising the analysis results.

The last released version SUSA 4.0 is a powerful tool for uncertainty and sensitivity analyses of computational results and an important part of the GRS code system for nuclear reactor safety analyses. It provides support to quantify input uncertainties in terms of probability distributions, correlations and other appropriate dependence structures. For Monte Carlo simulation, the simple random and the Latin Hypercube sampling procedure are available. To prepare and launch computer code runs, a selection of code interfaces is implemented. In the field of nuclear reactor safety analyses many options exist for quantifying the uncertainty of a computational result. Options for performing a sensitivity analysis are also implemented. SUSA 4.0 combines well-established methods from probability calculus and statistics with a graphical user interface (GUI). The GUI guides through the main analysis steps, requests input data where necessary, checks for input errors and performs all other actions up to the final representation of results.

Automated Statistical Treatment of Uncertainty Method (ASTRUM)

Transients in nuclear power plants are simulated with large system codes that include best possible models and correlations for thermal hydraulics and neutronics. The predictions from these codes are best estimates of figures of merit or parameters of interest. However, there are many contributors to uncertainty in these predictions; thermal-hydraulic models, numerics and parameters of neutronics. The US NRC has allowed utilities and vendors to use best-estimate codes with an estimate of uncertainty with high confidence.

10 Code of Federal Regulations (CFR) 50.46 states that "uncertainty must be accounted for, so that, when the calculated ECCS cooling performance is compared to the criteria set forth in paragraph (b) of this section, there is a high level of probability that the criteria would not be exceeded." Paragraph (b) of 10 CFR 50.46 contains the list of the acceptance criteria. Clarification as to the US NRC expectations on the acceptable implementation of the "high probability" requirement is provided in Section 4 of Regulatory Guide 1.157 (Best-estimate Calculations of Emergency Core Cooling System Performance) that states "a 95% probability is considered acceptable by the NRC staff [· · ·]."

The CSAU methodology was the first to establish a systematic and auditable method to estimate uncertainty in best-estimate calculation with high level of confidence. Westinghouse developed Automated Statistical Treatment of Uncertainty Method (ASTRUM) in line with the CSAU methodology and followed two of the elements of the CSAU methodology. Reviews of ASTRUM have been provided by Frepoli [85] and for a method like ASTRUM by Martin and O'Dell [86].

The CSAU methodology has two important steps, PIRT in the first element that identifies important phenomena for the transient and the method of combining various contributors to uncertainty in code prediction for identified FOM in the third element. the individual uncertainties are in the form of distributions and biases. as the cost of each code run was high and number of calculations needed for high confidence was large, the CSAU methodology adopted a response surface approach. The response surface is a surrogate of the code. Because of the level of effort, PIRT was important to reduce the number of phenomena to a manageable number. The response surface approach restricted the method to a smaller set of contributors to the uncertainty. As the response surface can be sampled as many times as needed in a very short time, the results corresponding to the 95% percentile value has almost 100% confidence.

The ASTRUM uncertainty propagation method for uncertainty analyses is similar to the CSAU methodology and considers the effect of the uncertainties of input parameters, computer code models, the initial and boundary conditions, geometry, scale effect and other application-specific input data and solution algorithms on the predicted results for the FOM. ASTRUM differs in the way uncertainties are combined and the numbers of contributors to the uncertainty are considered. The most widely used method of this type is the methodology proposed first by GRS and based on well-established concepts and tools from probability and statistics given by Wilks. The main advantage to using these tools is that the number of calculations is independent of the number of uncertain parameters to be considered. The necessary number of code calculations is given by the Wilks' formula [74]. The number of calculations depends only on the chosen tolerance limits (confidence) or intervals of the uncertainty statements of the results. Wilks' formula does not need any assumption about the distribution of the result. The number code calculations, N, for given confidence (tolerance) of γ and percentile of β, for one parameter uncertainty is given by Wilk's formula:

$$\gamma = 1 - \beta^N \tag{6}$$

In case of multiple parameters, p, that are independent, the number of calculations is higher, and are given by following relationship [65]:

$$\beta = \sum_{j=0}^{N-p} \frac{N!}{(N-j)!j!} \gamma^j (1-\gamma)^{N-j} \tag{7}$$

For example, for a single parameter, the number of calculations needed for 95% confidence and 95% percentile is 59. In the case of three parameters, the number of calculations required for the same level of confidence and percentile increases to 124.

Modelling uncertainties are represented by specific parameters. These represent two possibilities:

- adding on, or multiplying correlations by a corrective term;
- a set of alternative model formulations.

Then, the respective state of knowledge is quantified by approximate probability distributions that includes the range and shape of the distributions. Such a distribution expresses how well the appropriate value of an uncertain parameter of the code application is known in the light of all available evidence. A state of knowledge based on minimum information at the parameter level is expressed by uniform distributions (state of maximum ignorance). The selection and quantification of these uncertain parameters are based on experience gained from validating the computer code by comparisons between the model's predictions and test data of integral tests and separate effects tests for the model parameters. These tests are based on phenomena identified in the PIRT. In addition, where the tests are at smaller scale, the uncertainty should be augmented to include the scale effect.

In the ASTRUM approach, values of uncertain parameters are randomly sampled and the code is run with a set of values representing all the uncertainties considered. For every run, a new set is randomly selected. The minimum number of code calculations depends on the requested probability content and confidence level of the statistical tolerance limits used in the uncertainty statements of the results. The required minimum number of these calculation runs is given by the Wilks' formula as stated earlier. The set of predicted values of the parameter are arranged from small to large value. In the case of PCT, the highest

value will represent the 95% percentile (that is 95% of values will be lower than this PCT) and 95% confidence. In the case of three parameters of interest, the set of values of three parameters from 124 runs are arranged in order. The top third value for each parameter represents 95/95 conditions.

It should be noted that the SET/IET matrix will be different for different transients. The range and distribution of each parameter representing the model uncertainty will be specific to the transient of interest. The PIRT will also be different. While the ASTRUM approach is not limited by the number of parameters representing the uncertainty, still the largest effort is in determining the range and distribution of these parameters. A PIRT helps in making problem manageable.

Frepoli [83] has shown through examples that the safety parameters predicted for the 95% percentile by CSAU-type approach and ASTRUM approaches are different and there is larger margin with ASTRUM predictions (lower PCT, lower maximum oxidation and lower core-wide oxidation).

Uncertainty Methodology based on Accuracy Extrapolation − UMAE

The UMAE [87] whose flow diagram is given in Figure 4.3, is the prototype method for the description of "the propagation of code output errors" approach. The method focuses not on the evaluation of individual parameter uncertainties but on the propagation of errors from a suitable database calculating the final uncertainty by extrapolating the accuracy from relevant integral experiments to full scale nuclear power plants.

Considering ITF of reference water cooled reactor and qualified computer codes based on advanced models, the method relies on code capability, qualified by application to facilities of increasing scale. Direct data extrapolation from small scale experiments to reactor scale is difficult due to the imperfect scaling criteria adopted in the design of each scaled down facility. So, only the accuracy (i.e. the difference between measured and calculated quantities) is extrapolated. Experimental and calculated data in differently scaled facilities are used to demonstrate that physical phenomena and code predictive capabilities of important phenomena do not change when increasing the dimensions of the facilities (see right loop FG in Figure 4.3).

Other basic assumptions are that phenomena and transient scenarios in larger scale facilities are close enough to plant conditions. The influence of user and nodalisation upon the output uncertainty is minimised in the methodology. However, user and nodalisation inadequacies affect the comparison between measured and calculated trends; the error due to this is considered in the extrapolation process and gives a contribution to the overall uncertainty. The method utilises a database from similar tests and counterpart tests performed in ITF that are representative of plant conditions. The quantification of code accuracy (step "f" in Figure 4.3) is carried out by using a procedure based on the Fast Fourier Transform Based Method (FFTBM, [88] and [89]) characterising the discrepancies between code calculations and experimental data in the frequency domain and defining FOM for the accuracy of each calculation. Different requirements must be fulfilled in order to extrapolate the accuracy.

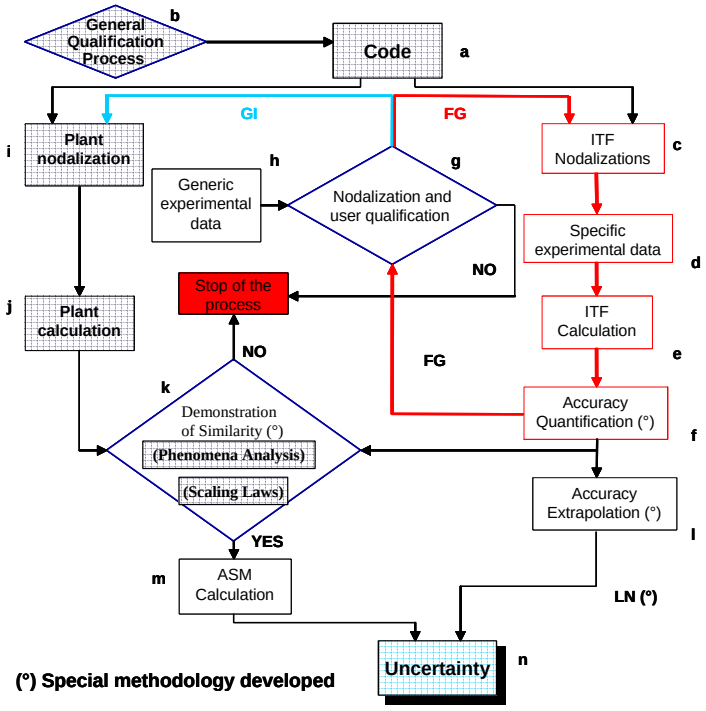
Calculations of both ITF experiments and nuclear power plant transients are used to attain uncertainty from accuracy. Nodalisations are set up and qualified against experimental data by an iterative procedure, requiring that a reasonable level of accuracy is satisfied. Similar criteria are adopted in developing plant nodalisation and in performing plant transient calculations (see left loop FG in Figure 4.3). The demonstration of the similarity of the

phenomena exhibited in test facilities and in plant calculations, accounting for scaling laws considerations (step "k" in Figure 4.3), leads to the analytical simulation model, i.e. a qualified nodalisation of the nuclear power plant.

The following three main differences between the CSAU methodology and the UMAE can be identified:

- Only expert (or engineering) judgement can stop the process of getting uncertainty in the case of the CSAU methodology, while a detailed comparison between measured and calculated trends may give the same results for the UMAE (path FG in Figure 4.3).
- Several sensitivity calculations using a plant nodalisation approved by expert judgements are necessary in the CSAU methodology to get uncertainty; one plant calculation through a qualified nodalisation is necessary in the UMAE.
- To get uncertainty from the UMAE, experimental data in ITF must be available and related to the assigned transient; this is not the case in the CSAU methodology. Furthermore, the code must be able to predict the measured scenario.
- Minor differences between the CSAU methodology and the UMAE are related to the following:
  - User qualification: unqualified users presumably will not get acceptable results from the block "f" in Figure 4.3, while they can perform sensitivity calculations in the CSAU methodology.
  - Errors that may be present in the plant nodalisations of both the CSAU methodology and the UMAE. The probability that this happens in the UMAE is minimised because of the analysis at block "k" in Figure 4.3.
  - The use of the response surface methodology is included in the CSAU demonstration and not in the UMAE.
  - The UMAE assumes that the ratio between experimental and calculated quantities (Y_E/Y_C) is a statistical quantity.

Figure 4.3. UMAE flow diagram (also adopted within the process of development and application of CIAU)



Source: D'Auria et al., 1995.

Code with capability of IAU (CIAU) and code with capability of IAU for coupled thermal-hydraulic/neutronics calculation (CIAU-TN)

All the uncertainty evaluation methods discussed in the previous section are affected by two main limitations:

- the resources needed for their application may be very demanding, ranging up to several man-months;
- the achieved results may be strongly method/user dependent (the so-called uncertainty-method-user effect).

The last item should be considered together with the code-user effect, widely studied in the past and may threaten the usefulness or the practical applicability of the results achieved by an uncertainty method. Therefore, the Internal Assessment of Uncertainty (IAU) was requested as the follow-up of international conferences ([89] and [90]). The CIAU and CIAU-TN approaches have been developed with the objective of reducing the limitations mentioned above.

The CIAU and CIAU-TN are extensively discussed in the available technical literature [91-95] and tens of additional relevant papers that provide comprehensive details about the method, can be found in the bibliography lists of the above references. Therefore, the present section supplies only "spot-information" about the CIAU, giving emphasis mostly to the idea behind the method and its main features.

The bases of the CIAU method can be summarised by the following steps:

- the use of a "systematic qualification process" [95] of thermal-hydraulic code calculations related both to ITFs and to nuclear power plants;
- the "accuracy extrapolation", i.e. the accuracy is not a function of the volume scaling ratio K_V and thus it can be extrapolated from facilities to nuclear power plants to get uncertainty;
- the "nuclear power plant status approach" to identify "phase spaces" (i.e. combinations of finite intervals of selected – driving – quantities) to which are associated single uncertainty values for each of the selected – output – quantities (i.e. responses);
- the separation and recombination of time and quantity "error" to split the physical (i.e. phenomena based) statistical treatment of the uncertainty in two contributions associated with the values of the selected – output – quantities (i.e. responses) and with the time when those values are reached during the transient;
- the "error filling process" and the "error extraction process" to generate the accuracy database (error filling process) and to use the derived uncertainty database (error extraction process) for the uncertainty evaluation of the qualified (following [95]) nuclear power plant code calculation.

In the next sub-sections, the word "error" has the same meaning of "accuracy", i.e. it refers to the discrepancy between experiment and code results.

The qualification process

The qualification process described in [95] involves the fulfilment of different "conditions of acceptability" for demonstrating the achievement of qualified ITF and nuclear power plant nodalisations and related code calculations (in this term it can be considered like the "engine" of the CIAU). Data coming from generic experiments in integral facilities and in separate effect test facilities, other than counterpart and similar tests and nuclear power plant transients can be processed. One condition for the application of the CIAU method is the similarity between the concerned plant scenario, in relation to which the uncertainty must be calculated, and the experimental/reference database originating the accuracy database (see also Figure 4.4).

The accuracy extrapolation

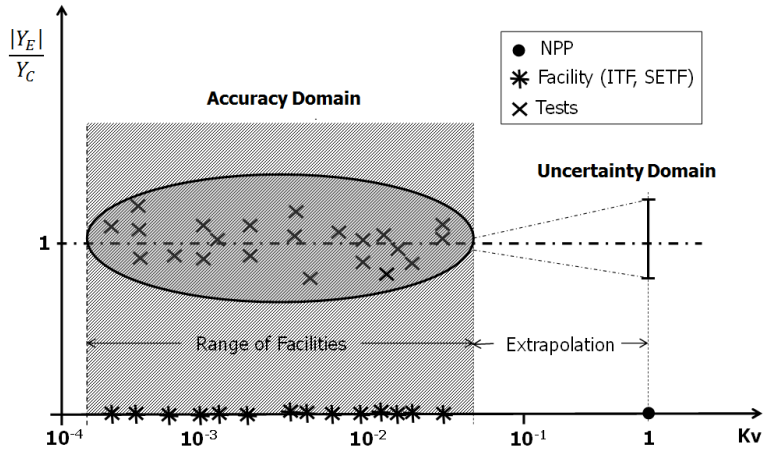
This step implies the demonstration that the code predictive capabilities of important physical phenomena in differently scaled facilities do not change when increasing the dimensions of the facilities. Figure 4.4 depicts the expected behaviour of the ratio between YE and YC of a generic response Y (e.g. PCT, minimum core collapsed level, etc.) as a function of KV where YE and YC are respectively the experimental and calculated values of Y. The expected behaviour of the ratio YE / YC is found, as shown in Figure 4.4 and confirmed by the analysis of several experiments and associated code calculations [96,97] derived from a database of similar tests and counterpart tests performed in ITF that are representative of the plant conditions. It should be noted that code-user effect and nodalisation inadequacies affect the comparison between measured and calculated trends and thus they are considered in the accuracy evaluation and consequently in the accuracy extrapolation process providing a contribution to the overall uncertainty.

The nuclear power plant status approach

The usual characterisation of any transient or event occurring or calculated in a typical LWR is through a number of time trends, e.g. pressures, levels, temperatures, mass flow rates versus time. The event time, or the time elapsed since the event beginning, constitutes the main way to characterise the transient together with the initial and boundary conditions. In this case, which can be identified as "time-domain", time is taken as the horizontal axis in the graphical representation of the transient evolution. Therefore, in the area of uncertainty evaluation, each transient becomes unique, thus requiring a specific evaluation of the uncertainty that characterises any of the time trends. This is true notwithstanding the possibility to consider key phenomena [98] that are common to classes of transients.

A different way to look at the same transients involves the use of the "phase-space". This approach consists of selecting a fixed, small group of quantities (called "driving quantities" Qd) and in describing any event taking place in a nuclear power plant not as a function of time, but by the group of values assumed by the selected quantities: each group of the selected variables represents a status of the plant. This approach is actually utilised to optimise the emergency procedures of nuclear power plants. In the graphical representation, any relevant quantity can be used in the vertical or horizontal axis.

Figure 4.4. Accuracy behaviour as a function of Kv



Source: Petruzzi, Giannotti and D'Auria 2004; Petruzzi and D'Auria, 2016; Bovalini et al., 1992.

Although the transients seem to be quite different in the time domain, when they are analysed in the phase-space domain it is possible to identify some areas or phenomenological regions through which the different kinds of transients pass through and in correspondence to which the same phenomena are expected to occur. The basic idea of the CIAU and CIAU-TN methods is that at any of these phenomenological regions, into which the "phase-space" is subdivided, one uncertainty value for the selected output quantities (called "object quantities", Y) can be assigned independently on the kind of transient. In other words, the nuclear power plant status is a region of phase space where the uncertainty in the code prediction is assumed to be "uniform".

The same idea, referring to specific thermal-hydraulic phenomena, is discussed in [98-100]. Those papers show that phenomenological areas or regions in the "phase-space" are suitable for use in scaling and extrapolation studies. Additional support for planning the method comes from the characterisation of generic plant status for the actuation of accident

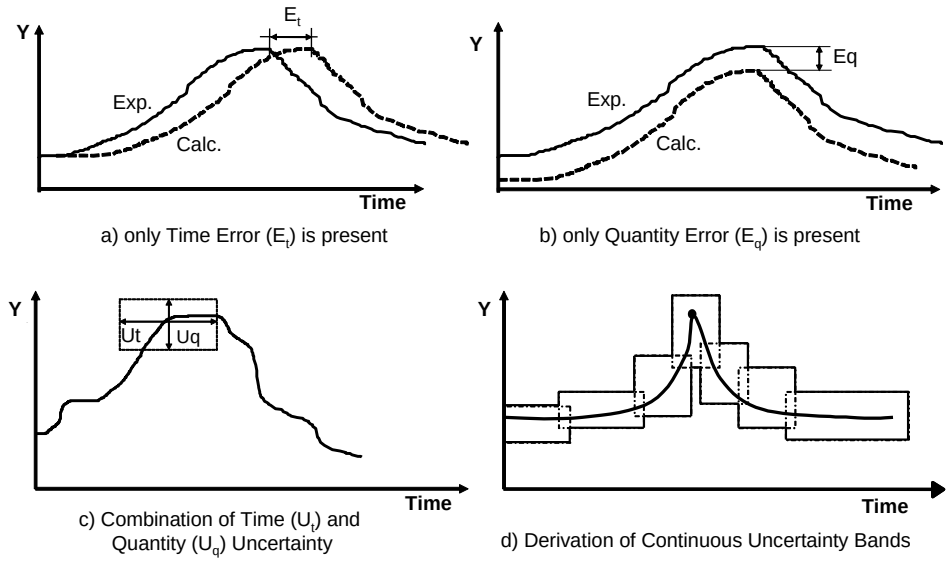
management countermeasures, as discussed in [101]. Finally, the pursued approach is similar to what is proposed by D.C. Groeneveld and P. Kirillov [102]: in that case, pressure, quality and flow rate are entries to the "look-up" table that provides a suitable value for the CHF. In the present case, proper "driving quantities" are entries to the matrix and vector which provide quantity and time uncertainty values respectively.

The separation and recombination of time and quantity errors

The definition of time and quantity error can be drawn from Figure 4.5. The dotted line is the result of a system code calculation: Y is a generic thermal-hydraulic code output plotted versus time. Each point value in the curve is affected by a time error (E_t in Figure 4.5a) and by a quantity error (E_q in Figure 4.5b). The availability of experimental data (measured in appropriate nuclear power plant simulators, i.e. ITFs) allows quantifying those errors and to generate the so-called (in the CIAU nomenclature) time and quantity accuracy database. Owing to the uncertainty affecting any thermal-hydraulic code calculation, each point value of the nuclear power plant code result may take any value within the rectangle (Figure 4.5c) identified by the time (U_t) and quantity (U_q) error (uncertainty).

The amount of the uncertainty value (i.e. each edge of the rectangle) can be defined in probabilistic terms consistently with what is recommended by current licensing approaches: e.g. a 95% probability level is considered acceptable to the US NRC staff for comparison of best-estimate predictions of postulated transients to the licensing limits in 10 CFR Part 50. The method used to combine the rectangles at the end of the CIAU process for generating the CIAU uncertainty bands can be seen in Figure 4.5d. The adopted process ensures a higher (still not quantified) level of probability with respect to the 95% probability usually associated with the edge of the rectangle.

Figure 4.5. Definition of quantity and time errors to be included into the quantity and time uncertainty database



Source: D'Auria and Giannotti, 2000; Petruzzi et al., 2005; Petruzzi and D'Auria, 2008; Petruzzi. D'Auria, Giannotti and Ivanov, 2004; Petruzzi, Giannotti and F. D'Auria, 2004.

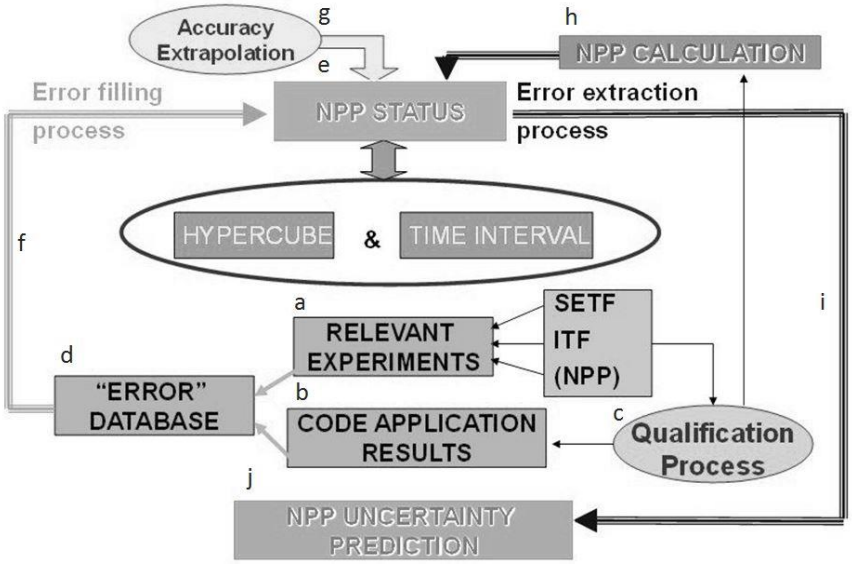
The error filling process and the error extraction process

Two processes are foreseen for the realisation of the CIAU and CIAU-TN methods: the "error filling" process and the "error extraction" process (see Figure 4.6). The former is dealing with:

- the selection (block a) of relevant experiments (ITF and SETF), i.e. of those experiments whose geometrical properties of the facility and boundary and initial conditions are similar to those of the concerned plant scenarios;
- the code calculation results (block b) qualified following the qualification procedure
  (block c) of [95];
- the derivation of the separate time and quantity accuracy (error) database (block d);
- the identification of the nuclear power plant statuses (block e);
- the storing of the time and quantity accuracy (error) values inside the selected (by the ITF and/or SETF experiment scenario) nuclear power plant statuses (block f).

After that a qualified nuclear power plant code calculation (block h) has been made available following the qualification procedure (block c) [95], the "error extraction" process (block i) is used to draw out from the selected (by the transient) nuclear power plant statuses the uncertainty values to be associated with the nominal (best-estimate) values of the object quantities for the uncertainty evaluation (block j). It should be noted that only one nuclear power plant best-estimate calculation per transient is sufficient for performing the uncertainty analysis. Between the two processes, the step dealing with the accuracy extrapolation (block g) ([96-98], see also Figure 4.6) is performed for passing from the accuracy database (output of the "error filling" process) to the uncertainty database (input of the "error extraction" process).

Figure 4.6. The error filling process and the error extraction process



Source: Petruzzi and D'Auria, 2016; Bovalini et al., 1992; D'Auria and Galassi, 1998.

A key feature of the CIAU and CIAU-TN approaches is the full reference to the experimental data. Accuracy from the comparison between experimental and calculated data is extrapolated to obtain uncertainty. A solution to the issues constituted by the "scaling" and "the qualification" of the computational tools is embedded into the method [100,101] through the qualification process that constitutes the engine for the development of CIAU and for the creation of the accuracy database.

Assigned a point in the time domain, the accuracy in predicting the time of occurrence of any point is distinguished from the accuracy that characterises the quantity value at that point. Quantity and time accuracies are associated to inaccuracies-in-code-models and uncertainties-in-boundary-and-initial-conditions including the time sequence of events and the geometrical model of the problem. Based on the above:

- The "transient-time-dependent" calculation by a code resembles a succession of steady-state values at each time step and is supported by the consideration that the code is based on a number and a variety of empirical correlations qualified at steady-state with assigned geometric discretisation. Therefore, quantity accuracy can be associated primarily with inaccuracies -in-code-models.
- Inaccuracy associated with the physical actuation of components (e.g. for a valve the time when the equivalent full flow area for the flow passage is attained) or the modelling of the I&C system (e.g. the scram signal) or inadequate nodalisation, can introduce time errors that cannot be associated to code model deficiencies. Therefore, time accuracy can be associated primarily with uncertainties-in-boundary-and-initial-conditions.

Once the time and quantity accuracy database has been derived, the overall accuracy and then uncertainty is obtained by the geometric combination of the two accuracies (and uncertainties) values, i.e. time and quantity, in the two-dimensional space-time plane.

4.4 New methods

CASUALIDAD method

The predictive modelling methodology constitutes a third approach for performing uncertainty analysis, different from propagation of input uncertainties or from propagation of code output accuracies.

The method is based upon powerful mathematical tools to perform sensitivity analysis and upon the Data Adjustment/Assimilation (DAA) methodology [103,104] by which experimental observations are combined with code predictions and their respective errors, to provide an improved estimate of the system state and of the associated uncertainty considering all input parameters $\boldsymbol{\alpha}$ that affect any prediction, being part either of the code models or of the input deck.

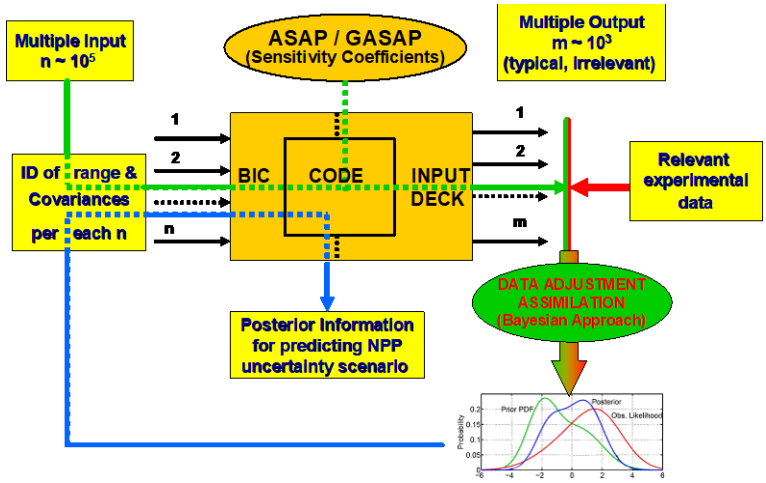
Since in most problems of practical interest, the number of input parameters $\boldsymbol{\alpha}$ exceeds the number of responses **R**, the method requires the most efficient deterministic method for computing local sensitivities **S** for large-scale systems, which is the Adjoint Sensitivity Analysis Procedure (ASAP) [105,106]. However, being large-scale systems frequently characterised by critical points like bifurcations, turning points, saddle points, response extrema or cliff-edge effects, local sensitivity tools cannot be properly used and a deterministic global sensitivity method has to be applied. In this context the Global Adjoint Sensitivity Analysis Procedure (GASAP, [105,106]) is one of the most advanced tools to deterministically compute the system's critical points **y** in the combined phase space formed by the parameters, forward-state variables and adjoint variables. Subsequently the local sensitivities of the responses **R** located at critical points **y** are analysed by the ASAP. Once the sensitivity matrix **S** of the responses **R** with respect to the parameters $\boldsymbol{\alpha}$ is available, the moment propagation equation is adopted to obtain the computed covariance matrix $\mathbf{C_R}$ of the responses starting from the covariance matrix $\mathbf{C}_{\boldsymbol{\alpha}}$ of the system parameters. The technique, by which experimental observations are combined with code predictions and their respective errors, to provide an improved estimate of the system state is known as DAA [104] and it is based on a Bayesian inference process. The idea at the basis of DAA can be made more specific as follows: the computed results **R** and the respective statistical errors $\mathbf{C_R}$ predicted by mathematical models and based on a "prior" or "first" guess PDF for the input parameters (i.e. $\mathbf{C}_{\boldsymbol{\alpha}}$) are combined with proper experimental observations **M** of the states of a system and associated uncertainty $\mathbf{C_M}$ to generate "adjusted" values for the system parameters ($\boldsymbol{\alpha}^{\mathbf{IE}}$, where the suffix Improved Estimate values (IE) and the respective input covariance matrix ($\mathbf{C}_{\boldsymbol{\alpha}}^{\mathbf{IE}}$, or "posterior" PDF). From this process, which can be considered as improved estimate analysis of the system's states, the responses $\mathbf{R}^{\boldsymbol{IE}}$ and the respective covariance matrix ($\mathbf{C_R}^{\mathbf{IE}}$) are finally derived. A short description of a method based on predictive modelling methodology is given hereafter.

The CASUALIDAD method (Code with the capability of Adjoint Sensitivity and Uncertainty AnaLysis by Internal Data ADjustment and assimilation) [107-109] has been developed as a fully deterministic method based on advanced mathematical tools for performing internally to the thermal-hydraulic system code the sensitivity and the uncertainty analysis. The availability of a suitable database of experiments (SETF and/or ITF) and related qualified code calculations constitutes a prerequisite for the development and the following application of the methodology. A simplified flow chart of the method is depicted in Figure 4.7.

Similar to the CIAU (see section above) method, the process to develop the database of improved estimations of input values and related covariance matrix is distinguished from

the application process where the database is used to produce the improved uncertainty scenario. Thus the information embedded in the set of experiments and related qualified code calculations is elaborated and transformed into suitable information for performing an improved (in the sense that is based on the experimental evidences) uncertainty evaluation. The general principles of the methodology together with brief descriptions of the main tools constituting the CASUALIDAD are given in the first sub-section below, whereas the structure of the method (i.e. the development process and the application process) is discussed in detail in the second sub-section below.

Figure 4.7. Uncertainty evaluation based on CASUALIDAD methodology



Source: Petruzzi, 2008; Petruzzi et al., 2010; Petruzzi and D'Auria, 2014.

The bases of the CASUALIDAD method

Establishing the range and probability distribution function of parameters is fairly easy for parameters which describe the condition of the plant (such as initial power or geometrical data) or for parameters describing physical data (such as thermal conductivity of UO_2). It is more difficult for parameters relative to the constitutive relationships (such as interfacial friction) because they cannot be directly measured in facilities. To this end, the results from SETF together with their experimental uncertainties are used for establishing or assessing these constitutive relationships. However, the models developed from SETF are applicable to a certain range of parameters, when often the correlations are extrapolated to more extreme conditions in correspondence of which the data is lacking. In order to justify these extrapolations, the ITF data, whose ranges of parameters are much closer to typical conditions, are used. However, the derivation of the PDFs of the input uncertainty parameters is never an easy and objective task and a common or agreed methodology is still not available to the nuclear community.

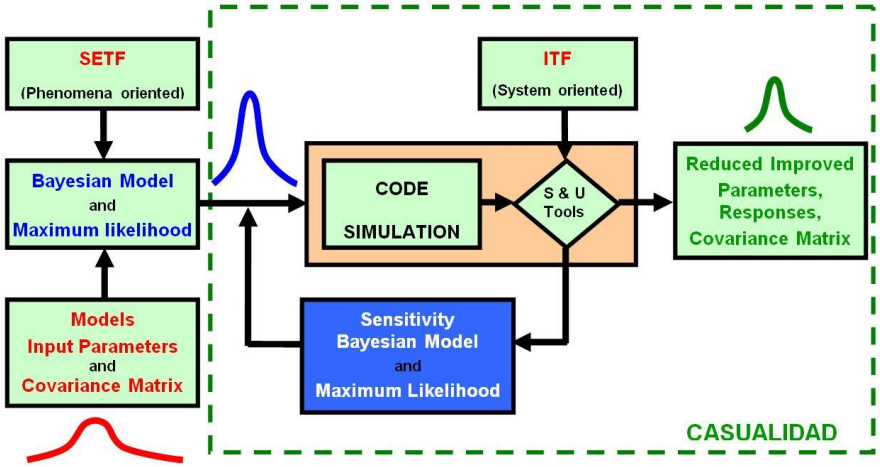
The fundamental principle of the methodology here proposed can be derived from Figure 4.8. The initial uncertainty distribution obtained from SETFs is shown coloured in red and represents the uncertainty in each of the model parameters (multiple model parameter distributions). After the application of the Bayesian Theorem (BT) and of the Principle of the Maximum Likelihood (PML), the uncertainty distributions (in blue), which are prior estimations for the code-simulation, are obtained. The code simulations are further constrained (using BT and PML) against the ITF for considering both the system behaviour and the use of the correlations (developed starting from SETFs) outside their range of

validity. At the end of this step, the key parameters, their contributions to the uncertainty of the system responses and the posterior parameter distributions (green curve in Figure 4.8) are obtained. It should be noted that if the extrapolation of the SETF conditions to the ITF conditions were not required and the various physics models employed in the ITF were truly uncoupled, then it is expected that the prior and posterior distributions resulting from the application of the BT & PML are very similar.

The framework for which the CASUALIDAD method has been developed deals with the dashed area in Figure 4.8, or in other terms the methodology is system oriented having as its main objective the improvements of the estimations of the system output responses and related covariance matrix (i.e. uncertainty) through the reduction and improvement of the input parameter values and covariance. Key elements for the methodology are:

- availability of a frozen qualified and internationally recognised thermal-hydraulic code;
- availability of a suitable large database of ITF containing different transient scenarios and different scales of facility (e.g. the set of tests belonging to the CIAU database [109,110]);
- use of a robust and rigorous procedure (i.e. set of acceptability criteria to be satisfied) for the qualification and acceptance of code calculations [95];
- availability of adequate (i.e. exact and efficient from computational resource point of view) methods for performing the local and global sensitivity analysis. The powerful tool based on ASAP is implemented for the derivation of the sensitivity matrix **S** containing the local derivatives of any response R_n (obtained by the code) with respect to any parameter α_i ($\partial R_n / \partial \alpha_i$). For large-scale systems, in which the number of system parameters and/or parameter variations to be considered exceeds the number of responses of interest, the ASAP is an effective method to employ. The global sensitivity analysis is performed through the implementation of the GASAP method aimed at determining all of the system's critical points and subsequently analyse them locally by ASAP. Thus, the strong non-linearities characterising the nuclear power plant system can be efficiently considered during the sensitivity analysis and taken into account for the following step dealing with the uncertainty evaluation;
- implementation of the DAA method based on the BT and the PML for updating the *a priori* PDF of the input parameters **α** and responses **R** with the available experiments **M** ("likelihood observations", see also Element 2 above) for getting the "posterior" IE of the input parameters, responses and related covariance matrices;
- use of the concept of status approach for grouping together the "posterior" IE of the input parameters, responses and related covariance matrices derived from similar transients, i.e. transients selecting the same path in the phase space of the selected driving quantities. A database of improved estimations is then generated and the appropriate information stored inside (i.e. the one in the phase space selected by the nuclear power plant calculation) can be used during the application process of the methodology.

Figure 4.8. The basic idea and framework of the CASUALIDAD method



Source: Petruzzi, 2008; Petruzzi et al., 2010; Petruzzi and D'Auria, 2014.

In addition to the above, the following assumptions are used in the methodology, including criteria and steps embedded in the methodology which itself allows either the detection when the assumptions are violated (and thus when the methodology cannot be applied) or the demonstration of their well-founded basis:

- Phenomena and transient scenarios in larger scale facilities will be close enough to plant conditions (see also similar discussion for the CIAU method in the Section above) − this assumption also supports Element 6 in the list above.
- Given that the discrepancy between measured and calculated responses (and not the absolute values) is used for evaluating the uncertainty, this difference is randomly dispersed around the zero-value independent of the volume scaling factors of the facilities ([111], see also Figure 4.6). Moreover, the methodology provides a consistent indicator χ^2 that quantifies the degree of consistency between calculation and experiment and allows neglecting the contributions of the related discrepancies to the uncertainty estimation when the consistency is poor (i.e. χ^2 far from unity value [112].
- The influence of user and nodalisation upon the uncertainty of the response is minimised in the methodology by the use of robust qualification procedures (see Element 3 of the previous list). The consistency indicator χ^2 contributes to minimise this influence discharging the cases where the consistency between calculation and experiment is poor.

The structure of the method

The CASUALIDAD methodology has been structured in two main steps. The former has the aim to generate the database of improved estimations starting from the available set of experimental data and related qualified calculations; the latter is dealing with the use of the selected (from the obtained database) set of improved estimations for the uncertainty evaluation of the predicted nuclear power plant transient scenario. More details about the two processes are given hereafter.

CASUALIDAD, Development process

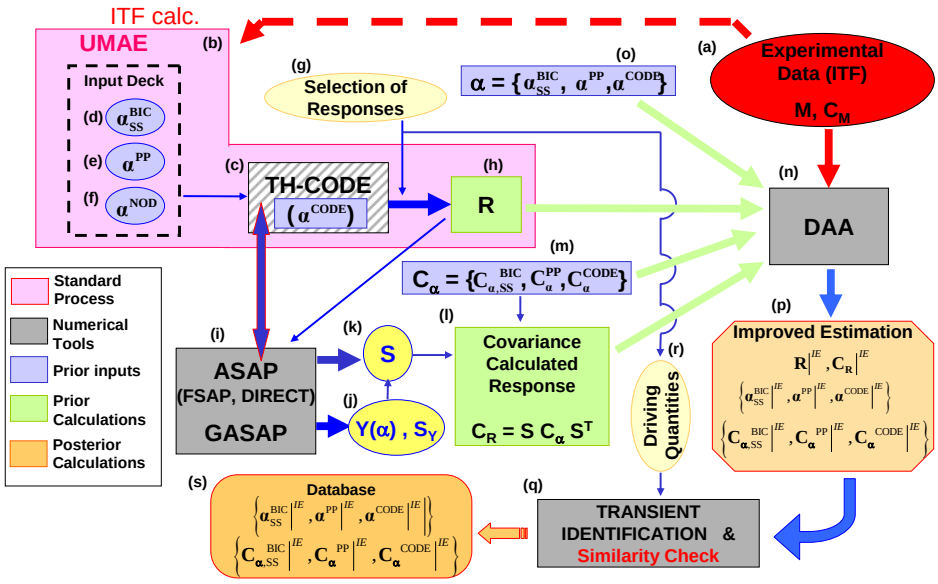
The development of the method and related database implies the availability of qualified experimental ITF data (block a in Figure 4.9), the use of a robust and consistent procedure for qualifying code calculations (block b) and the availability of a frozen version of the code (block c). These requirements constitute pre-requisites to the development of the methodology itself. Moreover, it is assumed that a steady-state (SS) condition is achieved before running the transient scenario, and consequently the values of input parameters characterising the BIC of the problem have to be considered after SS achievement. More precisely four different kinds of input parameters α are distinguished:

- the parameters α_{SS}^{BIC} (block d) which characterise the BIC, evaluated after SS achievement (e.g. the distribution of temperatures inside a core channel or the core inlet mass flow rates);
- the parameters α^{PP} (block e) used for specifying Properties and Phenomena (PP) of the system. They include for instance the geometrical properties of the system (e.g. the flow area of a pipe or the core active heat transfer surface area), the physical properties of the materials (e.g. the value of heat capacity at a certain temperature) and also parameters characterising complex thermal-hydraulic aspects, like the pressure drop distribution. With respect to α_{SS}^{BIC}, the α^{PP} parameters are those parameters whose values specified in the input deck do not change when the SS has been achieved;
- the parameters α^{NOD} (block f) which characterise the nodalisation (NOD), i.e. those parameters that constitute the discretisation of the real system into an ensemble of control volumes and junctions through the definition of the volume lengths and elevations, the volume flow areas, etc.;
- the parameters α^{CODE} (inside block c) that are part of the correlations inside the code. With respect to the other parameters, the α^{CODE} might not be directly accessible (modifiable) from the input deck.

The selection of the responses of interest (block g) among the thousands available from a code calculation implies an engineering judgement that must consider the relevance of the safety and licensing issues. No limitation exists when performing the sensitivity analysis (see blocks i and k). The situation is instead different when performing the uncertainty analysis (see blocks l and o), where practically the constraints derive from the available experimental responses (block a). Once the responses R have been selected (block g), they are passed to the sensitivity tools (block i) together with all input parameters α. The sensitivity analysis is then performed locally and globally in order respectively to obtain exact local derivatives of any response Rn with respect to any input parameter α_i ($\partial R_n / \partial \alpha_i$) and to determine the system's critical points $\mathbf{y}(\boldsymbol{\alpha})$ (bifurcations, turning points, saddle points, response extrema) and their derivatives ($\partial y_m / \partial \alpha_i$) with respect to any input parameter α_i (block j). The local sensitivity analysis is performed by ASAP [105,106] or alternatively can be carried out by Forward Sensitivity Analysis Procedure (FSAP) [105,106]. The global sensitivity analysis is performed by GASAP [105,106] and makes possible to efficiently deal with the non-linearities characterising the nuclear power plant system. Finally, the sensitivity matrix S (block k) is obtained and can be used for the following purposes (among others):

- to support the qualification process of the nodalisation through quantitative parameters that allow the verification of possible "unstable" behaviours of the developed nodalisation, i.e. if a small change in any of the input parameters $\boldsymbol{\alpha}$ causes a large variation in the selected relevant responses R. In fact, the matrix S providing the derivatives of any selected response respect with any parameter (e.g. the derivative of the core PCT with respect to the length of one node in the u-tube of the primary side of a steam generator) constitutes a large source of information for performing the qualification process;
- to understand the system by highlighting important data and eliminating the unimportant ones;
- to design and optimise the system (e.g. maximise the availability/minimise the maintenance);
- to perform the uncertainty analysis (see blocks l and o).

Figure 4.9: Flow chart of CASUALIDAD method: Development process



Source: Petruzzi, 2008; Petruzzi et al., 2010; Petruzzi and D'Auria, 2014.

While the sensitivity analysis is able to consider all parameters $\boldsymbol{\alpha}$, the uncertainty methodology here developed cannot deal "directly" with the $\boldsymbol{\alpha}^{NOD}$ parameters. The reason for such a limitation is due to the lack of information about the variance (and generally speaking about the covariance matrix) of the parameters characterising the nodalisation (e.g. the length of a volume in a nodalisation). However, as deducible from the word "directly", it should be emphasised that this limitation does not imply that the input uncertainties arising from the development of the nodalisation do not contribute to the final evaluation of the uncertainty of the responses. In fact, these input uncertainties affect the discrepancy between the experimentally measured values and the calculated values of the responses and thus finally affect the uncertainty evaluation.

The *a priori* knowledge (block m) of the covariance matrices $\boldsymbol{C}_{\alpha,SS}^{BIC}$, $\boldsymbol{C}_{\alpha}^{PP}$, $\boldsymbol{C}_{\alpha}^{CODE}$ (related to the BIC, PP and CODE parameters), deduced from SETFs, available literature or based

on engineering judgement, is then used in the "propagation of moments" equation to obtain the covariance matrix of the calculated responses (block l). The next step (block n) implies the use of the DAA as a methodology based on the BT and PML for consistently incorporating observed information into a predicting model. More specifically, the *a priori* knowledge of the:

- input parameters α_{SS}^{BIC}, α^{PP}, α^{CODE} (block o);
- input covariance matrices (block m);
- calculated response R (block h);
- calculated covariance matrix C_R (block l);

is combined in a statistically optimal way with "likelihood observations" (block a), i.e.:

- experimental measures of the responses **M**;
- covariance matrix of the measured responses C_M;

to consistently improve and reduce the posterior estimations (block p) of the:

- input parameters $\alpha_{SS}^{BIC}\Big|^{IE}, \alpha^{PP}\Big|^{IE}, \alpha^{CODE}\Big|^{IE}$;
- calculated responses $\mathbf{R}\Big|^{IE}$;
- input covariance matrices $C_{\alpha,SS}^{BIC}\Big|^{IE}, C_{\alpha}^{PP}\Big|^{IE}, C_{\alpha}^{CODE}\Big|^{IE}$;
- calculated covariance matrix $C_R\Big|^{IE}$.

Moreover, the DAA method supplies a quantitative measure of the consistency of the process through an indicator factor (χ^2) that allows quantification of the degree of the discrepancy between calculation and experiment and to not perform the adjustment and assimilation when the consistency is poor. As the CASUALIDAD methodology is system oriented, the experimental data to be incorporated in the DAA process are mostly dealing with ITF. However, SETF and also nuclear power plant operational transients can be processed if available.

The final step of the methodology has the goal to generate a database of (posterior) improved and reduced estimations of the input parameters and related covariance matrices. For each of the experimental test, the process up to the block p in Figure 4.9 has to be repeated for generating the posterior estimations. Considering that different kinds of scenario can be processed and that the same phenomena can occur in different transients, the concept of the "status approach" is adopted for generating the database. The idea here is to group together the improved estimations of the input parameters α^{IE} and related covariance matrices C_{α}^{IE} deriving from "similar" transients, i.e. transients selecting the same path in the phases space of the selected driving quantities. It is assumed that similar tests generate similar values of the percentages of parameters' variation between "posterior" and "prior" estimations (similarity check). Thus, if the similarity check is positively passed, the transient identification process (block q), based on the phase-space subdivision characterised by the selected driving quantities (block r), allows for

identification of the location inside the database where to store the obtained posterior estimations (block s).

CASUALIDAD, Application process

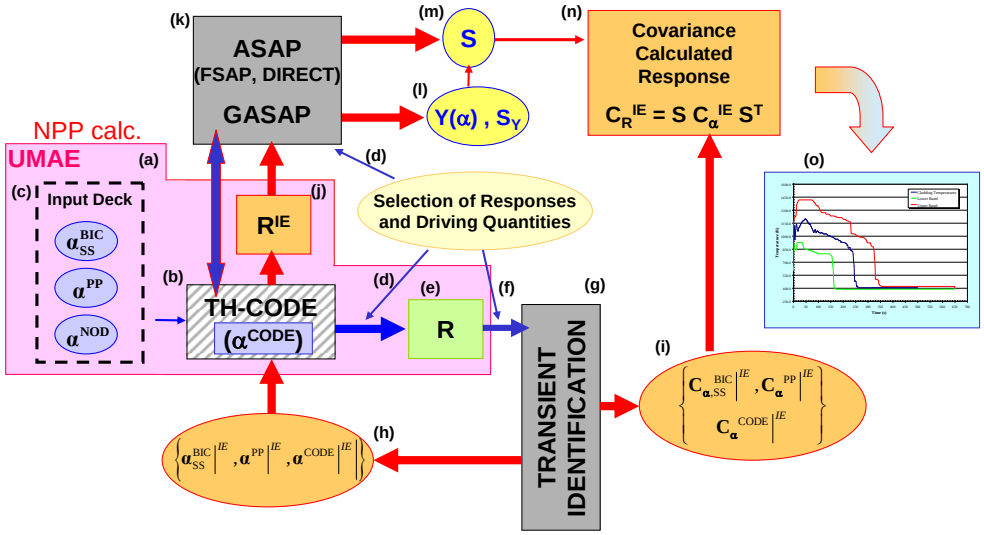
The application of the CASUALIDAD is straightforward once the database of the improved estimations of the input parameters and related covariance matrices is available.

After the nuclear power plant transient calculation has been qualified (block b in Figure 4.10), the input parameters characterising both the input deck (i.e. $\boldsymbol{\alpha}_{SS}^{BIC}$, $\boldsymbol{\alpha}^{PP}$, $\boldsymbol{\alpha}^{NOD}$, block c) and the correlations inside the code ($\boldsymbol{\alpha}^{CODE}$, inside block b) are evaluated on the "first-guess" basis (i.e. values deduced from SETFs, available literature or based on engineering judgement). The relevant responses from the safety and licensing point of view must be selected
(block d) in agreement with the selection process performed during the development of the methodology. The transient evolution, defined by the quantities **R** (block e), selects a path in the phase-space subdivision (characterised by the selected driving quantities, (block f) which can be identified through the transient identification process (block g). Thus, the posterior estimations of the input parameters (block h) and input covariance matrices (block i) associated to the selected path in the phase space can be drawn out from the database.

A second thermal-hydraulic system code calculation is set up using the posterior estimations of the parameters characterising both the input deck ($\boldsymbol{\alpha}_{SS}^{BIC}\big|^{IE}$, $\boldsymbol{\alpha}^{PP}\big|^{IE}$) and the correlations inside the code ($\boldsymbol{\alpha}^{CODE}\big|^{IE}$) in order to get an improved estimation of the responses $\mathbf{R}^{IE}$ (block j). The improved nuclear power plant transient calculation still undergoes the qualification process.

The sensitivity analysis is then performed locally and globally (block k) to derive the system's critical points (block l) and the derivatives of any response with respect to any input parameter (block m). The sensitivity matrix **S** can be used for the same purposes stated in the development process of the methodology having as reference the nuclear power plant instead of the ITF systems. Lastly, the uncertainty evaluation is performed by the "propagation of moments" equation where the improved estimations of the input covariance matrices $\boldsymbol{C}_{\alpha,SS}^{BIC}\big|^{IE}$, $\boldsymbol{C}_{\alpha}^{PP}\big|^{IE}$, $\boldsymbol{C}_{\alpha}^{CODE}\big|^{IE}$ are used (block i) to obtain the improved estimation of the covariance matrix of the calculated responses $\boldsymbol{C}_{R}^{IE}$ (block n). The diagonal values on the $\boldsymbol{C}_{R}^{IE}$ matrix allow finally the generation of continuous uncertainty bands for the selected responses $\mathbf{R}^{IE}$ (block o). A demonstrative application of CASUALIDAD method is given in [109].

Figure 4.10. Flow chart of CASUALIDAD method: Application process



Source: Petruzzi, 2008; Petruzzi et al., 2010; Petruzzi and D'Auria, 2014.

IMTHUA – Integrated Methodology for Thermal–Hydraulics Uncertainty Analysis

The basic idea behind IMTHUA [113] is to develop an uncertainty analysis methodology for best-estimate thermal-hydraulic codes (e.g. RELAP5) using and integrating all available evidence (i.e. experimental data, information and expert judgement). The methodology is quantitative and uses the Bayesian approach for evaluating the uncertainties associated with the thermal-hydraulic calculations.

Taking into account the limitations of the existing methodologies, the following factors are carefully considered in IMTHUA:

- Screening procedure for thermal-hydraulic phenomena: considering the extremely high number of phenomena that can contribute to the uncertainty, it is neither possible nor practical to explicitly quantify the impact of all such phenomena on output uncertainty. Consequently, a screening procedure is needed, but it creates non-trivial problems about the influence of sources of uncertainty neglected. In addition to this, it must be considered that different sources of uncertainty do not have equal influence.
- Use of experimental data: the available information should be carefully manipulated. Inference about physical models from experiments, credibility assessment and value of parameters and relevance of information strictly require sophisticated methodologies such as Bayesian methods. Moreover, the methodology has to be general, applicable to a wide range of scenarios and not tightly linked to peculiarities of specific cases.
- Assessment and propagation of uncertainties: the method for assessment and propagation of uncertainties must be efficient considering the available resources.
- Black box approach: using certain uncertainty procedures it is not possible to explicitly consider internal sub-model uncertainty.

Basic on the above, the idea of IMTHUA is to incorporate the best features of the existing methodologies into a new, more comprehensive method. The objective is to create an uncertainty method that:

- is general and applicable to a wide range of scenarios;
- treats all the important sources of uncertainty:
  - input parameters;
  - models and sub-models;
- considers an output adjustment based on integral performance information;
- uses a white box approach;
- is efficient with respect to cost and resources.

The main characteristics of IMTHUA are summarised in the following paragraphs.

Modified PIRT: In thermal-hydraulic calculations the number of phenomena that can contribute to the uncertainty is huge. Considering that it is not practical to explicitly consider all of these phenomena, a decision-making tool able to identify and rank the most important phenomena in certain scenario is necessary. This is the idea behind the PIRT. The problem of the traditional PIRT is that it only considers the effects of an input phenomenon on the magnitude of the output, without examining the credibility of the models and correlations related to the considered phenomenon. In order to avoid this limitation, a modified PIRT is used in IMTHUA. Phenomena are screened and ranked considering both their thermal-hydraulic and uncertainty importance. An analytical hierarchical process is used for thermal-hydraulic ranking while an expert judgement procedure is used to estimate the degree of credibility of the models and correlations used to represent the considered phenomena.

Input phase: Treatment of input parameters

The input data consists of model coefficients, boundary and initial conditions and it is necessary to evaluate the uncertainty of such data. Depending on the type of data and information available, the quantification of input parameter uncertainty can be done by the maximum entropy approach and by the expert judgement based on availability and type of data and information. A Bayesian methodology allows updating uncertainty distributions taking into account any new evidence.

Input phase: White Box approach

In addition to the input parameters, boundary and initial conditions, an important source of uncertainty that should be considered in the input phase is the uncertainty associated with the code models and sub-models. In this sense, a key objective of IMTHUA is the quantification of uncertainty due to model form. Firstly, the models, their alternative options and the structure of their engagement in the computation should be identified and documented. This is done by a method for measuring the contribution of model structural uncertainty to output uncertainty in addition to parameter uncertainties. Identified sources of uncertainties in code models and correlations are quantified by assigning probability distributions.

Efficient uncertainty propagation: Input parameter, model and sub-model uncertainties have to be propagated through code computations. A modified Wilks' tolerance limit

criteria sampling is used for the core of uncertainty propagation in IMTHUA, in order to reduce the number of Monte Carlo iterations for a given required accuracy.

Output correction phase: The output correction phase is necessary to account for user effects, numerical approximations and, in general, sources of uncertainty not considered in the input phase. In order to correct the output distribution, a Bayesian statistical method is used.

Firstly, an output database should be set up including all available test data on the FOM classified by applicability and degree of relevance. A Bayesian methodology can be implemented in the code for output automatic updating by comparing paired calculation and experimental data.

A key point of this step is that the experimental data should be evaluated for their degree of relevance to the conditions of the evaluated scenario. The data can be considered as:

- completely relevant: in this case the data is used directly for updating;
- partially relevant: in this case a Bayesian weighting process is needed and results in the evaluation of a factor assigned to the data before the updating process. The value of this factor is between 0 (non-applicable) and 1 (applicable) and should be quantified by an expert group for each test facility, considering the similarities and differences between it and nuclear power plant and the transient scenario.

This step, together with the treatment of input parameters and the white box approach, makes IMTHUA a hybrid input-output driven method.

SEC NRS Methodology

The Scientific and Engineering Centre (SEC) for Nuclear and Radiation Safety (NRS) in Russia has developed a regulatory approach for uncertainty analysis in the safety assessment of nuclear installations. Russian nuclear safety regulations require safety analysis to be supported with an evaluation of errors and uncertainties of the obtained results. SEC NRS is the technical and scientific support organisation of the Russian regulatory authority (Rostechnadzor). For nuclear power plants, this requirement is defined in [114]. Computer code calculation errors are to be assessed in a code verification and validation report, the requirements to which are given in [115]. However, [115] does not explain how exactly the code-calculated parameter errors should be evaluated; nor does it suggest how the error values obtained as a result of code validation should be used in a safety analysis of a nuclear facility (NF).

Code calculation error implies code output deviation from the measurement data obtained in the course of code validation experiments. Considering that results of any measurements feature uncertainty, one of the code calculation error components is the uncertainty of experimental measurements. Meanwhile, [116] requires obligatory justification of the sufficiency of experimental data used to validate a code, in addition to evaluation of measurement uncertainty. This aspect is discussed in detail in [117].

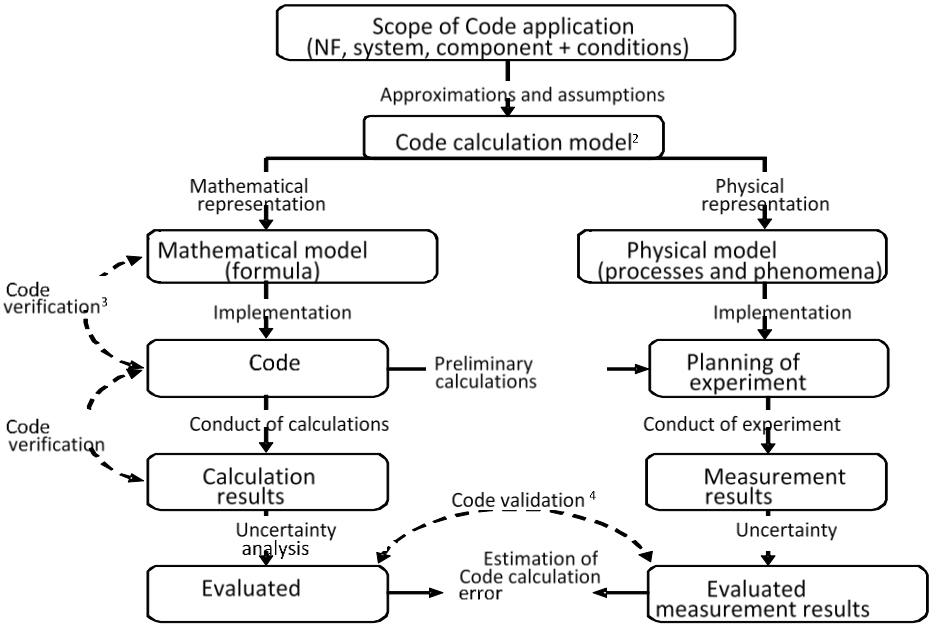
Another code calculation error component is uncertainties caused by the assumptions and simplifications adopted to build the code calculation model, including the uncertainties associated with model nodalisation (control volumes, finite elements, etc.), selection of numerical solution technique and integration step for the code's set of equations, and the adverse effect of an unskilled code user. According to [116], analysis and minimisation of such uncertainties is a prerequisite to demonstrate code model correctness. In fact, the detailed discussion covers only the following error components of code output: uncertainty

of code calculation model parameters that have a statistical nature and uncertainty of experimental measurements. Code calculation uncertainty caused by the uncertainty of code calculation model parameters is defined as code output variation due to uncertainty of model parameters having a statistical nature (e.g. physical and chemical properties of materials, geometry, empirical equation coefficients underlying the code calculation model, etc.). This uncertainty is presented as an interval (range) with certain probabilistic characteristics.

Key stages in the assessment of the influence of code model parameter uncertainty on code output are shown in Figure 4.12. For Stage 1 the PIRT methodology is utilised.

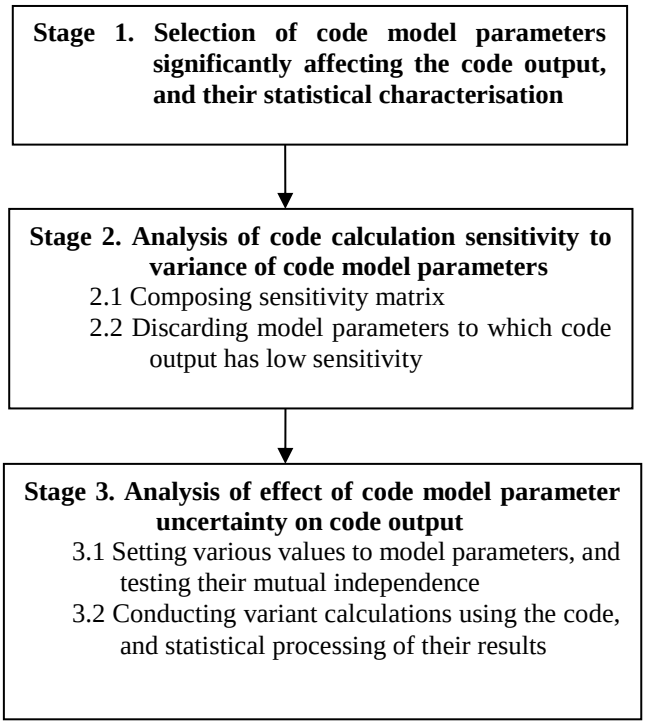
To obtain a sound value for code calculation error, code validation should use only those experimental data whose measurement uncertainty has been evaluated. The estimation of code calculation error during code validation consists first of estimation of error of steady-state calculations, and then followed by estimation of the error of transient calculations. During the code validation process, it is reasonable to use code output deviation from the measurement data as parameter calculation error, taking into account uncertainty of both code model parameters and the measurement data. These uncertainties are presented as intervals with specified probabilistic characteristics. Code calculations performed in the framework of a safety analysis of a nuclear facility may adopt only those error values that have been obtained in the experiments conducted at real nuclear facilities and integral experimental facilities, considering scaling factors. The number of such experiments is quite limited; therefore, in the safety analysis, the demanded conservatism of code output will be demonstrated with the help of one of the model parameter uncertainty evaluation methods. Of all numerous methods intended for evaluation of code model parameter uncertainty, the one that has found widest application in safety analysis of nuclear facilities is the approach based on the Wilks' formula. In order for uncertainty analysis (UA) to be accepted by the Russian regulatory authority (Rostechnadzor) the following is needed: verified and validated computer codes, experimental data used for validation should be properly assessed (measurement uncertainties, scaling applicability), safety objectives and UA methods should be well-defined and expert judgement should be minimised or at least formalised.

Figure 4.11. Process for evaluation of code output error



Source: SEC NRS, 2019.

Figure 4.12. Key stages in assessment of model parameters uncertainty



Source: SEC NRS, 2019.

IBRAE RAN Methodology

In the IBRAE RAN, the methodology for uncertainty-based best-estimate computer codes validation has been developed and implemented in the VARIA code [118,119]. It employs an approach, similar to one used in GRS method.

VARIA (from "variation") is a cross-platform application for mass computing that is used for uncertainty and sensitivity assessment in conjunction with best-estimate codes for modelling various aspects of nuclear power plant accident scenarios. It performs variation of input data for BE codes with desired parameter values distributions, controls execution of code instances on wide range of systems – from personal computers to large clusters consisting of multiple nodes and makes statistical analysis of the results. Due to the modular structure, it can be used with a variety of BE codes – adaptation for a new code requires just creation of a simple parser for input decks of this code. Meanwhile, the already existing parsers are sufficient for the majority of codes. Additional modules can be attached for advanced statistical analysis, visualisation of the arrays of results, etc.

Currently the VARIA functionality besides the basic statistical treatment of the results includes construction of uncertainty bands as well as calculation of sensitivity measures that include normalised multidimensional linear regression coefficients, Pearson, Spearman and Kendall correlation coefficients. These measures can be obtained for arbitrary time moments of the transients thus allowing observation of their temporal evolution. The results of the sensitivity study can be presented graphically both as bar charts and as scatter plots showing the dependence of the simulation results on given varied parameter with its linear approximation.

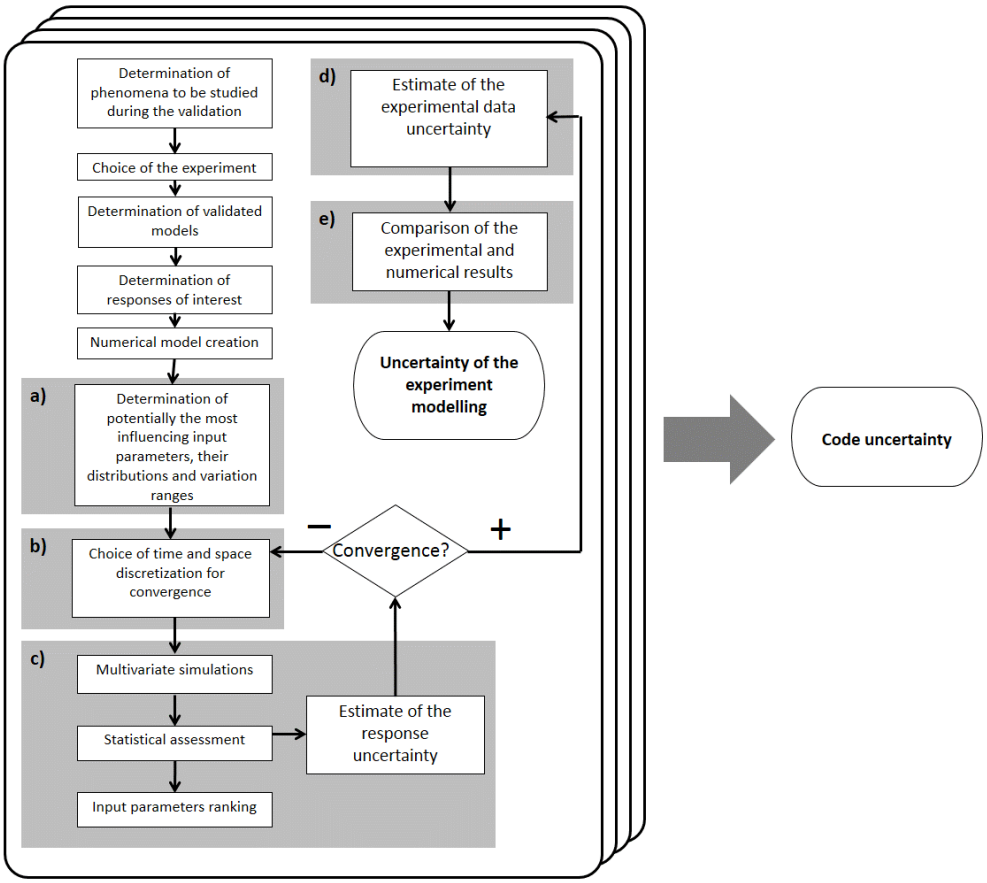
The IBRAE RAN validation methodology aims to estimate the uncertainty of the system response resulting from the (lack of) accuracy of the parameters of the system of interest and of the models implemented in the code. The representation uncertainties are minimised by the space and time step convergence testing. The uncertainties resulting from model scaling and from the user qualification are not accounted for. The validation procedure is outlined in Figure 4.12. It includes following main steps.

- The code input parameters that are supposed to influence the system response most are defined with their variation ranges and distributions. This is done by the experts; afterwards the sensitivity assessment will show their actual influence.
- Time and space convergence is tested to minimise the representation uncertainties.
- Multivariate simulations are performed. The number of code instances for uncertainty assessment is defined from Wilks formula [74] according to desired tolerance interval. Generally, it is 93, which corresponds to 0.95/0.95 probability for two-sided interval. For sensitivity study, the number on code instances N depends on the sensitivity measure taken. E.g. for multidimensional linear regression coefficients, it depends on the number of varied parameters n: $N >> n^2$. Uncertainty range of the response(s) of interest is found along with the mean value and the sensitivity coefficients.
- Uncertainty of the reference (experimental) data is estimated.
- Comparison of the multivariate simulations results with reference data is performed. Various measures can be used depending on the nature of the data (single point, several points, temporal dependence). These measures can include the uncertainty of the reference data and of the multivariate simulations results.

The overall code uncertainty for the validated models is obtained by combination of the uncertainties obtained for simulation of particular experiments.

This methodology is primarily aimed on the aleatory uncertainties. The question of applicability of such methods to the epistemic uncertainties is still open due to the subjectivity of its quantification, since it requires expert opinion [3,59]. However, the methodology authors argue that if sufficiently reliable estimates for epistemic uncertainties can be obtained, they can also be accounted for.

Figure 4.13. Validation procedure according to IBRAE RAN methodology



Source: IBRAE RAN, 2019.

4.5 Traditional single physics uncertainty quantification (UQ)

Concepts

Phenomena Identification and Ranking Table (PIRT)

The development and utilisation of PIRT is based on the following approaches:

- use of sensitivity and uncertainty analyses;
- use of expert opinion;

- use of non-dimensional parameters: benefits, cautions and consequences.

Calibration

The model form uncertainty is one of the most significant sources of uncertainties and the calibration step is used to improve models and to decrease model uncertainty. It is important to have a segregation of calibration data from validation data.

Experimental data uncertainties

The evaluation of experimental uncertainties and propagation of errors from "measured" data is a very important procedure. The evaluation of experimental uncertainty is performed in two ways:

- direct (e.g. measured flow rate) versus indirect (imaging of bubble formation in turbulent flow) experimental observations;
- propagation of error from "measured" data that is inferred from experimental observations from instruments (e.g. uncertainties in electronic signals from thermocouples or radiation detectors into "measured" quantities of interest).

Transposition and extrapolation

The transposition (interpolation within the validation domain) and extrapolation beyond validation domain using uncertainty analysis require:

- estimating the uncertainty in model input data for the application of interest;
- estimating model form uncertainty at the application of interest;
- identifying and distinguishing aleatory and epistemic uncertainties.

Propagation of uncertainties in single physics calculations

Various international benchmarks on BEPU applications to safety analysis have been organised and conducted. In this section the main outcomes from two NEA projects are summarised.

The BEMUSE benchmark

The BEMUSE (Best-Estimate Methods – Uncertainty and Sensitivity Evaluation) Programme – promoted by the Working Group on Accident Management and Analysis (WGAMA) and endorsed by the NEA Committee on the Safety of Nuclear Installations (CSNI) – represented an important step towards reliable application of high-quality best-estimate and uncertainty and sensitivity evaluation methods [120-123].

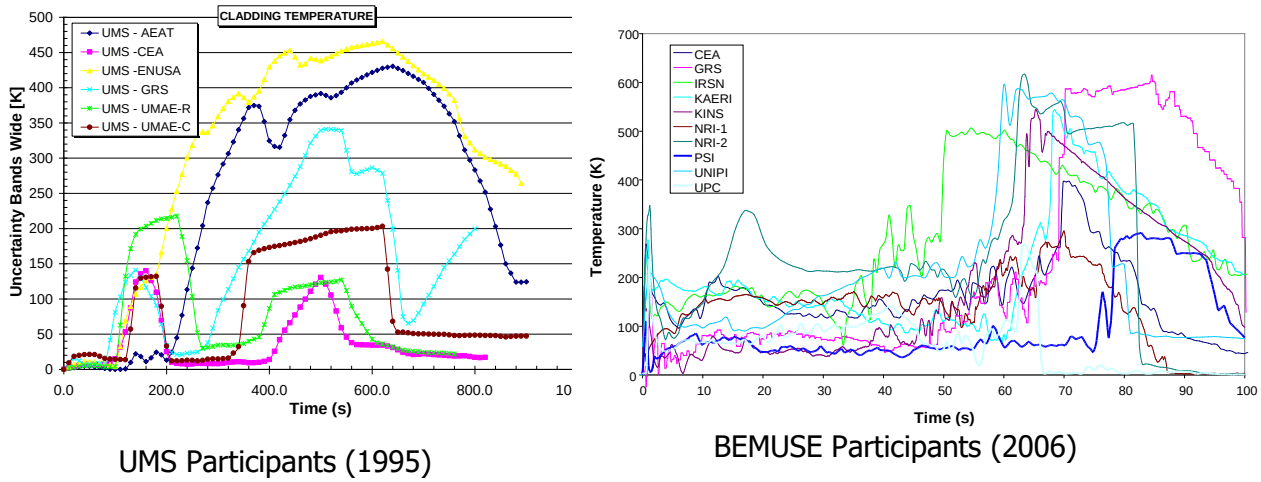
The programme was divided into two main steps (each one consisting of three phases) devoted to the uncertainty and sensitivity analysis related to an LBLOCA in the LOFT facility (L2-5 test) and in the ZION Nuclear Power Plant respectively. The programme started in January 2004 and ended in 2010.

The operational objectives included an assessment of the applicability of best-estimate and uncertainty and sensitivity methods to integral tests and their use in reactor applications. Both classes of uncertainty methods, were considered and investigated. Before summarising the lessons learnt, it might be useful to compare some of the final results of the BEMUSE Project Phase III with a previous (actually the first) international benchmark

on the uncertainty methods, the NEA Uncertainty Method Study (UMS, [124]), which focused on a small break LOCA experiment (LSTF SB-CL-18 5%) in the Japanese Large Scale Test Facility (LSTF). Figure 4.14 provides an idea about the magnitude of the discrepancy among the results predicted by different participants to the NEA UMS and BEMUSE ([124] and [122]) benchmark respectively, adopting very similar uncertainty methods (mostly of them applied methods based on propagation of input uncertainty parameters) and in some cases using also the same thermal-hydraulic code. It can be noted that the spread among the size of the uncertainty bands (for cladding temperatures in Figure 4.14) predicted by the UMS participants in 1995 was not reduced by the participants to the BEMUSE benchmark which was held more than 10 years later. The reasons that explain the differences between the results of users of the same code and (almost) same uncertainty method are several and coincide with some of the main outcomes from BEMUSE project [123]:

- differences between applications of statistical methods may mainly be due to procedures adopted:
  - to select the input parameters;
  - to properly estimate input parameter uncertainties;
  - to properly estimate the probability distribution functions.
- Some participants using statistical methods specified few important parameters or too narrow uncertainty ranges for important input uncertainties based on expert judgement and not on sufficient code validation experience. Therefore, skill, experience and knowledge of the users about the applied suitable computer code as well as the used uncertainty method are important for the quality of the results.
- An increased number of calculations for the statistical methods may be advisable because it decreases the dispersion of the tolerance limits.
- Differences between the methods based upon propagation of input uncertainties and methods based upon propagation of output errors may come from different experimental data bases used for the analysis.

Figure 4.14. Spread of uncertainty bands for cladding temperatures predicted by UMS and BEMUSE participants



UMS Participants (1995)

BEMUSE Participants (2006)

Sources: NEA, 2007; Wickett et al., 1998.

The PREMIUM Benchmark

In system thermal-hydraulics only few code input parameter uncertainties are obtained from experimental observations (mainly from separate effect test facilities), whereas for the major part of them engineering judgement is adopted for deriving ("first") guess values of ranges and PDF. This fact constitutes the source of a new user influence on the BEPU results (in addition to the code-user-effect) that can be named "uncertainty-method-user effect" and which has been found to be one of the lessons learnt from the BEMUSE project (see Section above and [115]). In this context, a new NEA benchmark called PREMIUM (Post-BEMUSE Re-flood Model Input Uncertainty Methods [125]) was launched in 2011 and completed in 2015.

Its main goal was the development, study, comparison and application of methods for quantification of the uncertainty of the physical models contained in thermal-hydraulic system codes used in nuclear safety. The application of these methods had the final goal to reduce the dependency on expert judgement in the input uncertainty quantification.

The benchmark application was focused on the physical models involved in the prediction of the core reflood, which is a fundamental stage in the LOCA scenario.

The PREMIUM benchmark has been a valuable exercise on methods for uncertainty quantification of physical computational models and their application to the models involved in the reflooding prediction. Different quantification methods and thermal-hydraulic codes have been used in the benchmark. Results have been found to be very dependent on the quantification method, rather than on the code. Furthermore, the results of the quantification process have shown a strong dependence on topics such as:

- the selected responses used in the quantification;
- the selected parameters to be quantified;
- the selected experimental database for the quantification;
- the code modelling and the numerical implementation;
- the quantified models, which, in general depend on the thermal-hydraulic code being used.

It was concluded that the quantification methods used in PREMIUM showed a strong user effect and the results of the quantified uncertainties had a large variability and discrepancy among the participants.

As a final outcome, the benchmark has revealed the necessity of further work on the quantification methods and on the development of "best practice" guidelines for the evaluation of model input uncertainty parameters. This is actually the goal of a new launched NEA project named SAPIUM (Systematic APproach for Input Uncertainty quantification Methodology), which started in 2017.

4.6 Traditional multi-physics uncertainty quantification (UQ)

Propagation of uncertainties in multi-physics calculations

The LWR Uncertainty Analysis in Modelling (UAM) benchmark

In recent years there has been an increasing demand from nuclear research, industry, safety and regulation for best-estimate predictions to be provided with their confidence bounds.

In addition to LWR best-estimate calculations for design and safety analysis, the different aspects of Uncertainty Analysis in Modelling (UAM) are to be further developed and validated on scientific grounds in support of its performance. There is a need for efficient and powerful analysis methods suitable for such complex coupled multi-physics and multi-scale simulations. The benchmark sequence addresses this need by integrating the expertise in reactor physics, thermal-hydraulics and reactor system modelling as well as uncertainty and sensitivity analysis and contributes to the development and assessment of advanced/optimised uncertainty methods for use in best-estimate reactor simulations.

In the comprehensive international LWR UAM benchmark activity different uncertainty analysis (UA) methods for coupled codes are being compared and their value assessed including the validation of the methodologies for uncertainty propagation. For the first time the uncertainty propagation is estimated through the whole simulation process on a unified benchmark framework to provide credible coupled code predictions with defensible uncertainty estimations of safety margins at the full core/system level. The benchmark allows not only comparing and assessing the current UA methods on representative applications but also stimulating the further development of efficient and powerful UA methods suitable for complex coupled code simulations and helps to formulate recommendations and guidelines on how to utilise advanced and optimised sensitivity analysis and UA methods in "best-estimate" coupled reactor simulations in licensing practices.

The approach described above is based on the introduction of nine steps (Exercises), which allows for development of a benchmark framework which mixes information from the available integral facility and nuclear power plant experimental data with analytical and numerical benchmarking. Such an approach compares and assesses current and new uncertainty methods on representative applications and simultaneously benefits from different methodologies to arrive at recommendations and guidelines. These nine steps (Exercises) are carried out in three phases as follows:

Phase I (Neutronics Phase):

- Exercise 1 (I-1): "Cell Physics" focused on the derivation of the multi-group microscopic cross-section libraries;
- Exercise 2 (I-2): "Lattice Physics" focused on the derivation of the few-group macroscopic cross-section libraries;
- Exercise 3 (I-3): "Core Physics" focused on the core steady-state stand-alone neutronics calculations.

Phase II (Core Phase):

- Exercise II-1: Fuel thermal properties relevant for transient performance;
- Exercise II-2: Neutron kinetics stand-alone performance (kinetics data, space-time dependence treatment, etc.);
- Exercise II-3: Thermal-hydraulic fuel bundle performance.

Phase III (System Phase):

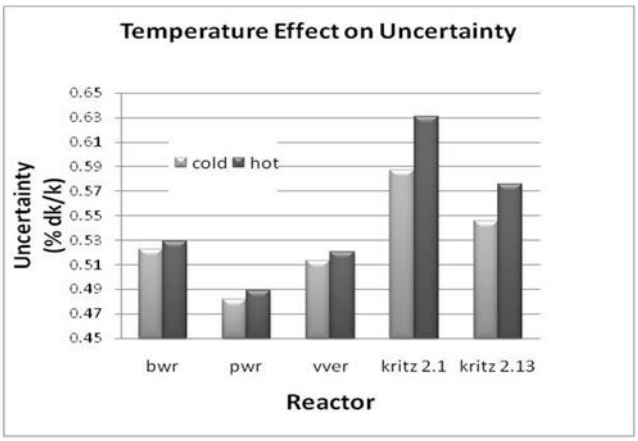
- Exercise III-1: Coupled neutronics/thermal-hydraulics core performance (coupled steady state, coupled depletion and coupled core transient with boundary conditions);

- Exercise III-2: Thermal-hydraulics system performance;
- Exercise III-3: Coupled neutronics kinetics thermal-hydraulic core/thermal-hydraulic system performance.

Separate specifications are prepared for each phase in order to allow participation in the full phase or only in a subset of the exercises [45]. Boundary conditions and necessary input information are provided by the benchmark team. The intention is to follow the calculation scheme for coupled calculations for LWR design and safety analysis established in the nuclear power generation industry and regulation.

One of the observations from analysis of the submitted results for Phase 1 [126] is the impact of spectral changes to the magnitude of nuclear data propagated uncertainties in neutronics integral parameters and local distributions. There are two major contributors to spectral changes – material compositions and temperatures. The latest impact is shown in Figure 4.15 for different LWR numerical test cases and the Kritz experimental test cases, where cold means hot zero power and hot means hot full power state with corresponding moderator/coolant and fuel temperatures.

Figure 4.15. Temperature effect on propagation of nuclear data uncertainties to multiplication factor uncertainty



Source: Bratton et al, 2014.

The expected impact and benefits of the LWR UAM benchmark activity for LWR safety and licensing are summarised in [45]. This benchmark project is challenging and responds to needs for estimation of confidence bounds for results from simulations and analysis in real applications. Among the expected results of this project are:

- systematic identification of uncertainty sources;
- systematic consideration of uncertainty and sensitivity methods in all steps; this approach will generate a new level of accuracy and will improve transparency of complex dependencies;
- all results will be represented by reference results and variances and suitable tolerance limits;
- the dominant parameters will be identified for all physical processes;
- support of the quantification of safety margins;

- the experiences of validation will be explicitly and quantitatively documented;
- recommendations and guidelines for the application of the new methodologies will be established.

The LWR UAM activity will establish an internationally accepted benchmark framework to compare, assess and further develop different uncertainty analysis methods associated with the design, operation and safety of LWRs. As a result, the LWR UAM benchmark will help to address current nuclear power generation industry and regulation needs and issues related to practical implementation of risk-informed regulation. The realistic evaluation of consequences must be made with best-estimate coupled codes, but to be meaningful, such results should be supplemented by an uncertainty analysis. The use of coupled codes allows avoidance of unnecessary penalties due to incoherent approximations in the traditional decoupled calculations and to obtain more accurate evaluation of margins regarding licensing limit. This becomes important for licensing power upgrades, improved fuel assembly and control rod designs, higher burn-up and others issues related to operating LWRs as well as to the new Generation III + designs being licensed now (ESBWR, AP-1000, EPR-1600 and etc.). As such, establishment of this internationally accepted LWR UAM benchmark framework offers the possibility to accelerate the licensing process when using best-estimate methods and contributes to establishing a unified framework to estimate safety margins, which would provide more realistic, complete and logical measures of reactor safety.

5. Summary of validation and uncertainty quantification state of practice

5.1 Summary of practices for validation and uncertainty quantification for single physics codes

System analysis codes

A key feature of the activities performed in nuclear reactor safety technology is the necessity to demonstrate the qualification level of each tool adopted within an assigned process and of each step of the concerned process [127-129]. Therefore, the qualification of best-estimate codes, models, "best modelling practices" and uncertainty methods must be considered of great importance in order to ensure the validity of performed BEPU system analysis. A consistent code assessment supported by a qualified experimental database is an important step for developing a solid basis for the uncertainty evaluation in the frame of a Best Estimate Plus Uncertainty (BEPU) approach. An example is The International Experimental Thermal HYdraulics Systems database, TIETHYS (www.oecd-nea.org/tiethysweb/).

The experiments available through the Nuclear Energy Agency (NEA) Committee on the Safety of Nuclear Installations (CSNI) Integral Test Facility (ITF) [123] and Separate Effect Test Facility (SETF) [124,125] matrix constitute a large experimental database for the nuclear thermal-hydraulic community. These databases collect over thirty years of experiments: separate effects test for individual phenomena, integral tests for large break loss-of-coolant accidents (LBLOCAs), small break LOCA, transients, beyond design basis accidents and accident management in pressurised water reactors (PWRs), boiling water reactors (BWRs) and water-water energetic reactor (VVER) types of reactor. The enormous amount of information has been used for the code assessment in the framework of verification and validation (V&V) activities. The availability of the experimental database constitutes also the prerequisite for the creation of a qualified accuracy database of system thermal-hydraulic responses to be used for the uncertainty evaluation in the methods based on "extrapolation of code output accuracies" but can contribute also to the V&V process of methods based on "propagation of input uncertainties".

An example of practice of validation and uncertainty quantification (VUQ) for System Analysis codes is the Standardised and Consolidated Calculated and Reference Experimental Database (SCCRED) [130] methodology which has been developed to generate a series of documents and tools to set up a qualified experimental and calculated database for V&V purposes of BEPU applications, i.e. best-estimate computational codes and associated uncertainty methodologies. Figure 5.1 depicts the SCCRED diagram: the information contained in the experimental reports together with the code input nodalisations are the elements to be elaborated in a systematic way by a qualified database made up of the following documents:

- the reference data set for the selected test of the facility;
- the qualification report;
- the engineering handbook.

The methodology has been developed in such a way as to allow for the collection, organisation, use and preservation of an exhaustive set of geometrical data, experimental results and qualified code calculation responses, ensuring finally (see Figure 5.1):

a. an exhaustive consolidated information set;

b. the traceability of the information, including the decisions taken during the activity;

c. the standardisation of the format by which the information is collected;

d. the application of a systematic approach for qualifying code calculations and associated nodalisation techniques;

e. the availability of a database of experimental and associated qualified calculated results (TIETHYS);

f. the availability of a database of accuracy (deriving from the differences between experiment and calculation results) to be used for:

   – V&V of the codes and associated nodalisation techniques; and

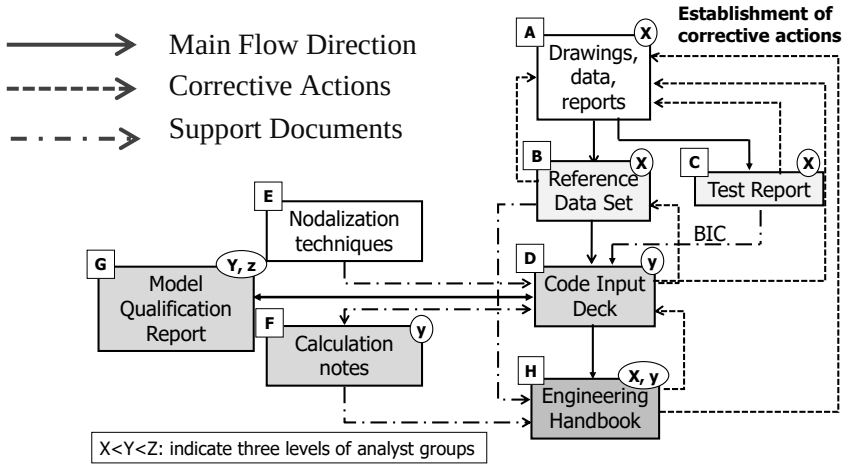
   – V&V of the uncertainty methods either based on the quantification of input uncertainty parameters or output responses.

More details about each step of the SCCRED methodology are provided in [130] and hereafter the focus is on the validation process of code calculations (see item d above).

The qualification process of a thermal-hydraulic system code calculation aims to demonstrate that the code results (obtained by the application of the code with the developed nodalisation) are a realistic approximation of the reference plant behaviour (a full-size nuclear power plant or a facility).

A major issue in the use of a mathematical model is the model's capability to reproduce the plant or facility behaviour under steady-state and transient conditions. These aspects are the two main verifications that must be passed in the qualification process. The first of them is related to the realisation of a nodalisation-schematisation of the reference plant or facility; the second one is related to the capability to reproduce and analyse the transient behaviour to derive the necessary information.

Figure 5.1. SCCRED flow chart



Source: Petruzzi and D'Auria, 2016

The qualification of the nodalisation is a mandatory process to take into account the effect of many different sources of approximations:

- the data of the reference plant or facility available to the code user are typically non-exhaustive to reproduce a perfect nodalisation-schematisation of the reference plant;
- the code-user derives, from the available data, an approximated nodalisation-schematisation of the plant or facility reducing the level of detail of the simulated hardware;
- the code capability to reproduce the hardware, the plant systems and the actuation logic of the systems further reduce the level of detail of the nodalisation-schematisation.

The needs for qualifying the code capability and the nodalisation features to perform the transient analysis derive from the following statements:

- the code options must be adequate;
- the nodalisation-schematisation solutions must be adequate;
- the simulation of some systems can be tested only under transient conditions (e.g. emergency core cooling system [ECCS]) that are not involved in the normal plant operation, i.e. during steady-state code condition;
- the capability of the "code-nodalisation" of the system to reproduce relevant TH phenomena expected in the transient must be tested.

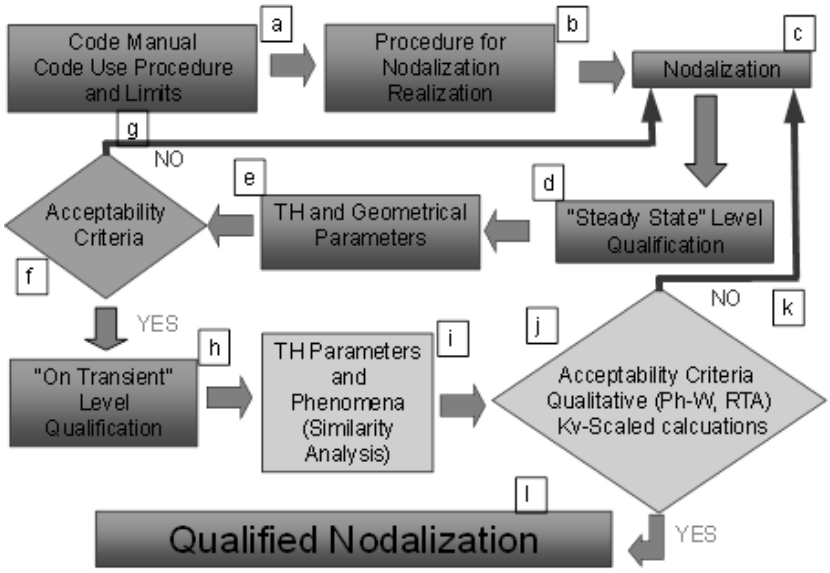
The qualification procedure has been developed including the necessary checks for the different aspects mentioned above and the criteria adopted to produce a judgement about the acceptability of the code analysis results.

The goal of the qualification procedure is to develop and obtain a qualified nodalisation considering the comparison with the hardware data, BIC and the time trends of relevant quantities. The procedure distinguishes between three main processes:

- the "geometrical fidelity";
- the "steady state";
- the "transient" level of qualification.

A scheme of the procedure can be seen in Figure 5.2 where the processes are represented by the steps "f" and "j" which constitute the checking points of the procedure. If the checking points are not fulfilled (paths "g" and "k") the nodalisation must be improved (step "c"). It must be pointed out that many cycles "c-d-e-f-g" could be necessary to gain the access to the step "h". Similarly every time the path "k" is activated the process goes again from "c" to "f" and then from "h" up to "j" (the path "c-d-e-f-h-i-j-k-c" could be actuated more than one time). The last step "l" is reached at the end of the procedure and this implies the qualification of the developed nodalisation. The above qualification process has been applied in several international benchmarks, including the NEA Best-estimate methods – Uncertainty and sensitivity evaluation (BEMUSE) [131].

Figure 5.2. Flow chart of the qualification procedure



Source: Petruzzi and D'Auria, 2016

Once the qualification procedure has been successfully passed, the quantification of the accuracy can be performed for the selected responses and phenomena and a database of accuracy values is then derived. The availability of such a qualified database constitutes the final outcome of the SCCRED steps and can be used:

- for the V&V demonstration of the codes and associated nodalisation techniques;
- for the derivation of the uncertainty values of the responses of interest following the methods based on propagation of accuracies;
- as a basis for deriving statements about the PDF and the ranges of variation of the input uncertainty parameters for the methods based on propagation of input uncertainties;
- for the derivation of a database of (posterior) improved and reduced estimations of the input parameters and related covariance matrices following the methods based on the predictive modelling approach.

Neutronics (reactor physics) codes

A summary of practices for VUQ for neutronics codes is given by the example of the work performed at Idaho National Laboratory (INL), which is focused on Transient Reactor Test Facility (TREAT) analysis and is summarised below:

- INL has employed the traditional Monte Carlo method to TREAT models [132] to compute the 95th percentile with a confidence level of 95%, sensitivities, output correlations and high-order statistical moments based on Wilks' formula. Regarding this method, both the nuclear data (e.g. multi-group cross-sections) and the system parameters (e.g. boron concentration, initial fuel temperature) can be perturbed based on given probability distributions. The TREAT models are then executed at each perturbed state and the output variations are recorded.

- INL has also employed some advanced methods to efficiently perform the SA/UQ for TREAT transient calculations, i.e. the stochastic colocations combined with generalised polynomial chaos (gPC) expansions and the high dimensional model reduction method combined with sparse grid and gPC expansions. The responses are represented via gPC expansions, while the gPC coefficients are determined via the Smolyak-like sparse grid quadrature. These methods will converge very fast with few model evaluations for a moderate number of input parameters (i.e. < 15). These methods are already applied to TREAT transient test #15 [132].
- INL has also developed an active subspace method to handle hundreds of input parameters. The input parameter space is reduced via principal component analysis and input-output correlation analysis. Once the input space is reduced, the methods mentioned above can be used to perform the UQ in the reduced space. This method has been applied for IAEA-2D PWR benchmark problem [133].
- INL has also developed an adjoint method inside the Rattlesnake transport code enabling use of generalised perturbation theory to perform SA/UQ. This method is very efficient if the number of inputs is very large and the number of responses is relatively small. For each given response, one needs to calculate the generalised adjoint solution that can be used to compute the response sensitivities with respect to all input parameters. Once the sensitivities are known, the uncertainties of inputs can be easily propagated via the "sandwich" equations. This method has already been applied to models of TREAT [134]. Similar capabilities are available in the NEWT code within the SCALE system.

Fuel performance codes

Over the past several years, an effort has been made for the evaluation of uncertainties associated with modelling and prediction of fuel behaviour using the best-estimate plus uncertainty approach [18-20]. There are several sources of uncertainty in fuel performance analysis. The rod's manufacturing parameters, system boundary conditions and experimentally determined material properties are never accurate but introduce various amounts of uncertainty into the system. These uncertainties will be propagated to model outputs such as the fuel centreline temperature, internal pressure and gap conductance. The primary parameter of interest is the fuel temperature, because most of the physical phenomena occurring in nuclear fuel during its irradiation in reactor are driven by temperature. In the simulation process, the response of the models describing these phenomena is mainly conditioned by the confidence in the calculated temperature of the fuel.

In best-estimate analysis quantifying both the magnitude and the source of the output uncertainties is necessary. The latter is known as the sensitivity analysis, where most studies are focused on the first-order effect of the input parameters on the output. A common approach is to evaluate, for example, the Spearman correlation coefficients or the first order Sobol' indices from the model output [18], although some studies have shown that the higher-order interactions between the input variables should not be completely neglected.

In the NEA Benchmark for Uncertainty Analysis in Best-Estimate Modelling (UAM) for LWRs Exercise II-1 [135] was developed to identify and propagate input uncertainties through fuel performance codes for PWR, BWR and VVER fuel designs. The example of the boundary condition uncertainties in terms of upper and lower bounds, as well as the type of distribution are provided in Table 5.1.

Tables 5.2 and 5.3 show the uncertainty of the boundary condition and the material properties, respectively that are currently used in the benchmark.

Table 5.1. Exercise II-1 core boundary condition variations

Parameter	BWR	PWR	VVER	Distribution
System pressure (%)	± 1.0	± 1.0	± 2.0	Normal
Coolant flow rate (%)	± 5.0	± 5.0	± 5.0	Normal
System power (%)	± 5.0	± 5.0	± 5.0	Normal
Inlet fluid temperature (K)	± 3.0	± 3.0	± 3.0	Uniform

Source: Hou et al., 2016

Table 5.2. Core boundary condition standard deviations

Parameter	Standard Deviations		
	BWR	PWR	VVER
System pressure	0.00333	0.00333	0.00667
Coolant flow rate	0.01667	0.01667	0.01667
System power	0.01667	0.01667	0.01667

Source: Hou et al., 2016

Table 5.3. Material properties recommended uncertainties

Parameter	BWR	PWR	VVER
Fuel thermal conductivity	± 0.5 W/m-K	± 0.5 W/m-K	± 0.5 W/m-K
Fuel thermal expansion	± 15%	± 15%	± 15%
Cladding thermal conductivity	± 5 W/m-K	± 5 W/m-K	± 5 W/m-K
Cladding thermal expansion	± 30%	± 30%	± 30%

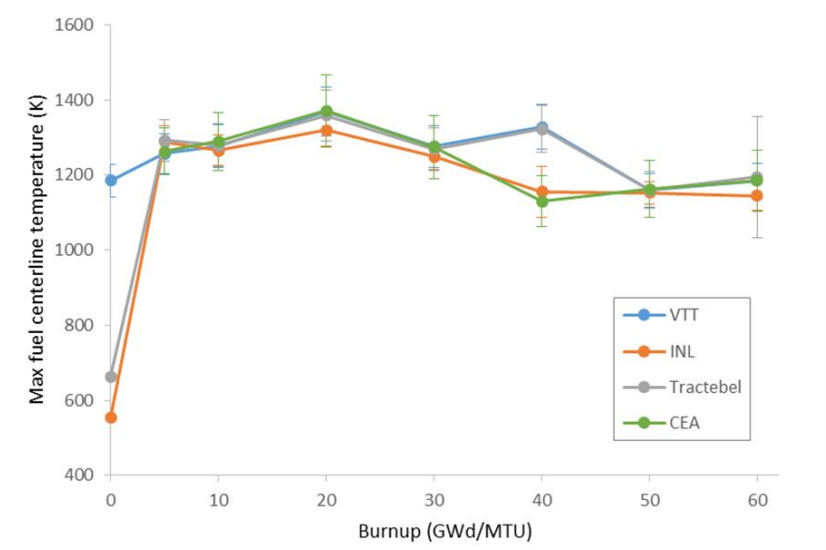
Source: Ikonen and Tulkki, 2014; Hou et al., 2016.

A list of output parameters calculated by fuel performance codes have been identified in the benchmark, as they are important to propagation to other types of codes. For example, the gap conductance is often specified in the input for the simplified fuel rod models in thermal-hydraulics codes, therefore it is vital to understand how it varies according to the prediction of fuel performance analyses. The uncertainty parameters to be propagated from the numerical cases are:

- gap conductance ($W/m^2/K$);
- fuel thermal conductivity (W/m/K);
- radial rod dimensions (rod outer diameter, rod elongation);
- gap width (μm);
- for transient cases, the heat transfer coefficient between cladding and coolant is also a requested propagated output ($W/m^2/K$).

As an example of uncertainty propagation in fuel performance calculations, a comparison between participants' results for the PWR depletion test case of Exercise II-1 for the LWR UAM benchmark [141] is shown in Figure 5.3:

Figure 5.3. PWR depletion test case



Source: Avramova and Ivanov, 2017.

Core thermal-hydraulics codes

The validation activities for core thermal-hydraulics codes are usually combined with a statistical uncertainty analysis framework. The input parameters include boundary conditions, geometry and modelling uncertainties, which are selected using a sensitivity study and then defined based on expert judgement. As an example, the methodology developed for the core thermal-hydraulic simulator CTF coupled via scripts with the statistical analysis tool, Design Analysis Kit for Optimisation and Tera-scale Applications (DAKOTA) is discussed in [136]. A forward uncertainty quantification method with Latin Hypercube sampling is used, where the sample size is based on available computational resources. The means and standard deviations of thermal-hydraulic quantities of interest are reported, as well as the Spearman rank correlation coefficients between the inputs and outputs. This allows the same interface to be used for many different statistical studies and enables automatic parallelisation of analyses. External Python scripts are used to prepare the CTF input deck with input parameters determined by DAKOTA and to extract quantities of interest from the CTF output. This CTF-DAKOTA interface is also used for the sensitivity studies [137]. The means and standard deviations are accompanied by their respective standard errors and the correlation coefficients are tested for statistical significance. The new element in this methodology is that given a specified amount of computational resources, it can be used to quantify statistical significance using fundamental statistical analyses. This is in contrast with the prevailing methods in nuclear engineering, which provide a sample size necessary to achieve a specified level of statistical certainty [139].

As mentioned above the LWR UAM benchmark is an ongoing project that is creating standard nuclear engineering problems for the application of uncertainty methods [135]. Although the goal of the UAM benchmark is to address uncertainties in

multi-physics and multi-scale simulations, its two first phases are composed of single physics problems. Phase II, Exercise 3 of the UAM benchmark provides 12 test cases for uncertainty quantification of core thermal-hydraulic codes for nuclear engineering applications. These cases are numerical and experimental cases for steady and transient applications based on representative PWR, BWR and VVER designs.

An extensive set of preliminary sensitivity studies were used to eliminate possible input parameters that have minimal influence on the quantities of interest. First, each potential input was varied over a small perturbation about its nominal value; the maximum change in each quantity of interest is a measure of sensitivity. These so-called "parameter studies" quantified the univariate effect of each input uncertainty on the outputs and gave one indication of whether an input should be included in future analyses. The second sensitivity study method used was Morris Screening, which is a valuable tool to provide information about input interactions with relatively little computational expense [138]. Essentially, Morris Screening creates a randomised set of finite differences throughout the parameter space. These finite differences, called "elementary effects", were used to quantify both the univariate and multivariate effects between the inputs and outputs.

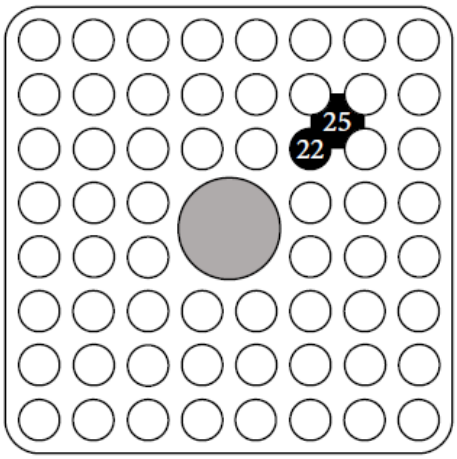
Both parameter studies and Morris Screening were completed for all four LWR UAM test cases for a large set of potential input parameters. The results are prohibitively large and are therefore excluded from this report; an overview can be found in [136]. Thresholds were set for the parameter study and Morris Screening results and those input parameters that did not exceed the threshold for at least one quantity of interest were excluded from the study. Based on the sensitivity studies, 21 input uncertainties were selected. Each input uncertainty is either normal or uniform. Both normal and uniform distributions are characterised by their bounds. Uniform distribution bounds correspond to their minimum and maximum value. The normal distributions are bounded to avoid unphysical input parameter ranges; the bounds correspond to a perturbation of three standard deviations.

The validation metric is important for experimental test cases where computational results are compared to experimental data. Two validation metrics are chosen, the first is a simple difference between the mean code result and the reported experimental value. This metric maintains the units of the original measurement and is therefore very intuitive, but it cannot give any indication of similarity between two distributions. To compare code results with uncertainty to experimental results with measurement error, it is necessary to use a validation metric which can compare two distributions. A large variety of such metrics are available and one of these metrics is the Kolmogorov/Smirnov (KS) Test. The KS test measures the maximum vertical distance between the two cumulative density functions (CDFs) through dKS. The two CDFs represent the code and experimental distributions when the KS test is used for validation.

Results are presented for the BFBT-based experimental steady-state test case (see Figure 5.4) from Exercise II-3 of the LWR UAM benchmark. The calculated results as requested by the benchmark include: (1) three global quantities of interest (maximum void fraction, maximum cladding surface temperature and pressure drop), (2) axial distributions of temperature and void fraction and (3) an exit void fraction distribution. The axial distribution of void fraction in channel 25, the cladding surface temperature distribution of rod 22 and the exit distribution of void fraction are shown in Figure 5.6. The dips in the exit void distribution for this case are due to the influence of the unheated water rod at the centre of the assembly. The exit void fractions given in Figure 5.6(c) are compared to the BFBT experimental results. The difference between the experiment and the mean code results are shown in Figure 5.5(a), where darker colour channels indicate that the CTF

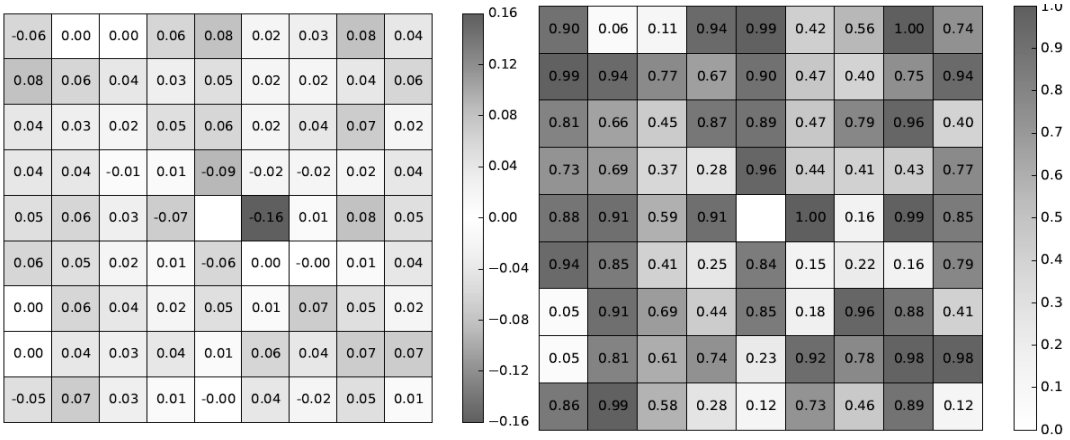
prediction is further from the experiment. The BFBT measurements are assumed to have a normal distribution with a mean of the experimental measurement and two standard deviations equal to 3% void. This value is the measurement error of the X-ray CT scanner used in the BFBT Facility. The code distribution is compared to the experimental distribution using the KS test and the results are shown in Figure 5.5(b). Lighter colours indicate that the two distributions are closer together. Figure 5.6 presents quantified validation results for the BFBT case. To draw further conclusions, this same data is presented in Figure 5.7 with a distinction made between four different types of subchannel. Corner subchannels are channels that contact the assembly wall on two sides, side subchannels contact the wall on one side, and unheated channels are those that are in direct contact with the centre water rod on one side. The rest of the channels are considered centre subchannels. A colour-coded map is included in the figure. The absolute difference between the prediction and measurement (x-axis in Figure 5.7) only indicates how close the means of the two distributions are, whereas the KS metric (y-axis) gives an indication of closeness for both the mean and the data spread. The code and experimental standard deviations are of the same magnitude and vary only slightly, therefore the two metrics are closely related. Figure 5.7 indicates that the unheated rods are less accurately modelled in CTF compared to the other subchannels. This is likely because the CTF model used does not explicitly account for the centre water region, so any thermal inertia of the water rod is completely neglected.

Figure 5.4. Exercise II-3 – BFBT experimental test case



Source: NCSU, 2019.

Figure 5.5. Quantified validation of exit void fraction distribution for the BFBT tests case

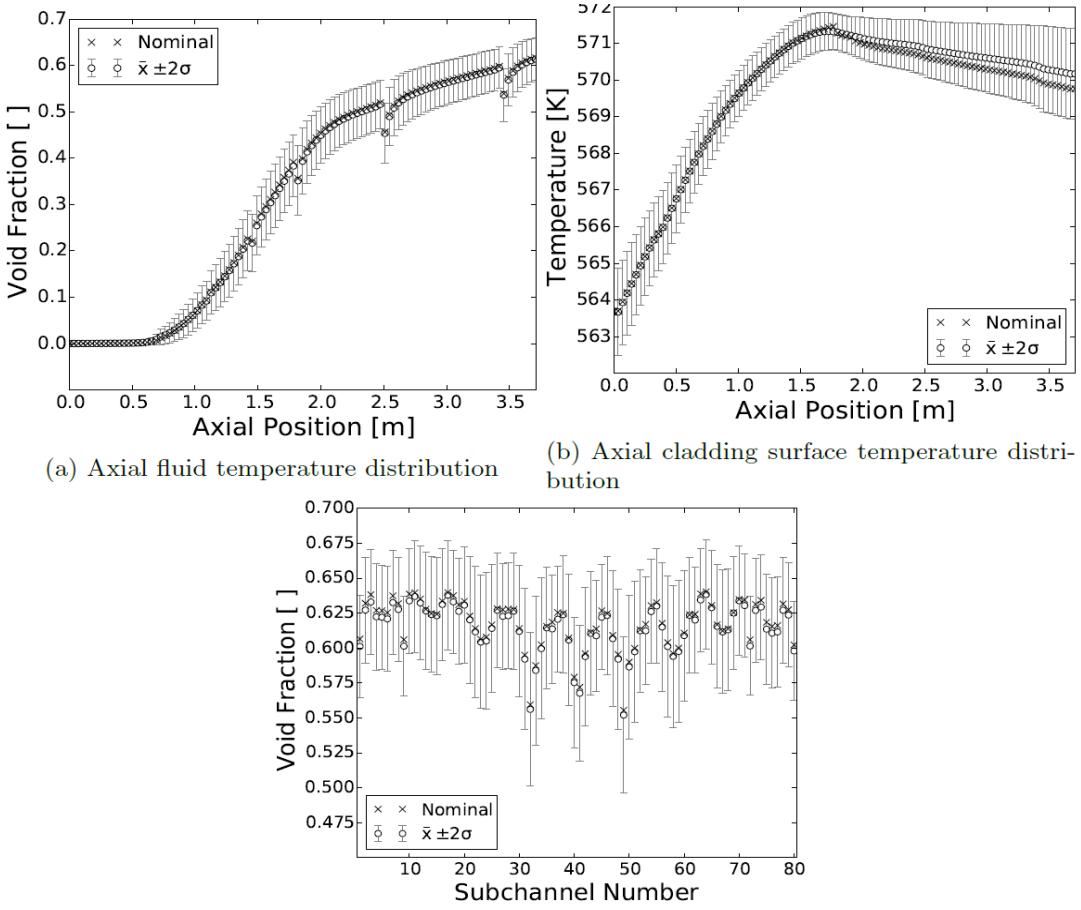


(a) Difference between experiment and predicted values ($\alpha_{exp} - \alpha_{code}$)

(b) Kolmogorov-Smirnov metrics (d_{KS}) for comparison of two distributions

Source: NCSU, 2019.

Figure 5.6. Results for the BFBT test case



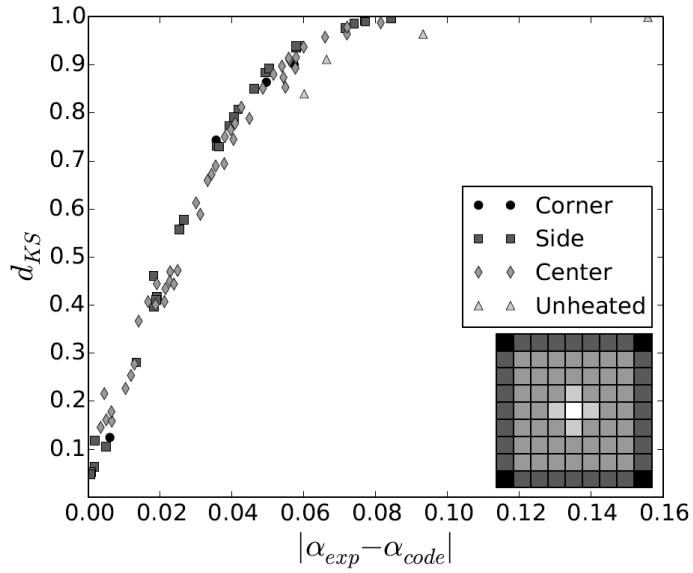
(a) Axial fluid temperature distribution

(b) Axial cladding surface temperature distribution

(c) Exit void fraction distribution

Source: NCSU, 2019.

Figure 5.7. Relationship between the absolute difference (between experimental value and code results) and dKS for different subchannel types



Source: NCSU, 2019.

5.2 Summary of practices for validation and uncertainty quantification for multi-physics codes

The qualification procedure of traditional coupled multi-physics code systems is based on the qualification framework (V&V) of separate single physics models/codes and includes in addition V&V of the coupling methodologies of the different physics models. The extended V&V procedure involves testing the functionality, the data exchange between different physics models and their coupling, which is designed to model combined effects determined by the interaction of models. The extended validation procedure compares the predictions from coupled multi-physics code systems to available measured data and reference results. It is important to emphasise that such validation should be based on a multi-level approach like the one utilised in validating coupled neutronics/thermal-hydraulics codes in international standard problems. Appropriate benchmarks have been developed in international co-operation led by the NEA that permits testing the neutronics/thermal-hydraulics coupling and verifying the capability of the coupled (traditional multi-physics) codes to analyse complex transients with coupled core/plant interactions. These benchmarks provide a validation basis for the current generation of coupled best-estimate codes.

The current tendencies in coupled code developments are towards systematic integration of uncertainty and sensitivity analysis with simulations for safety analysis. Sensitivity and uncertainty analysis capabilities must be further developed for comprehensive coupled code simulations with non-linear feedback mechanisms as well as tested for uncertainty propagation through multi-physics multi-scale calculations on comprehensive benchmark frameworks, such as the LWR UAM benchmark described previously in this report [141].

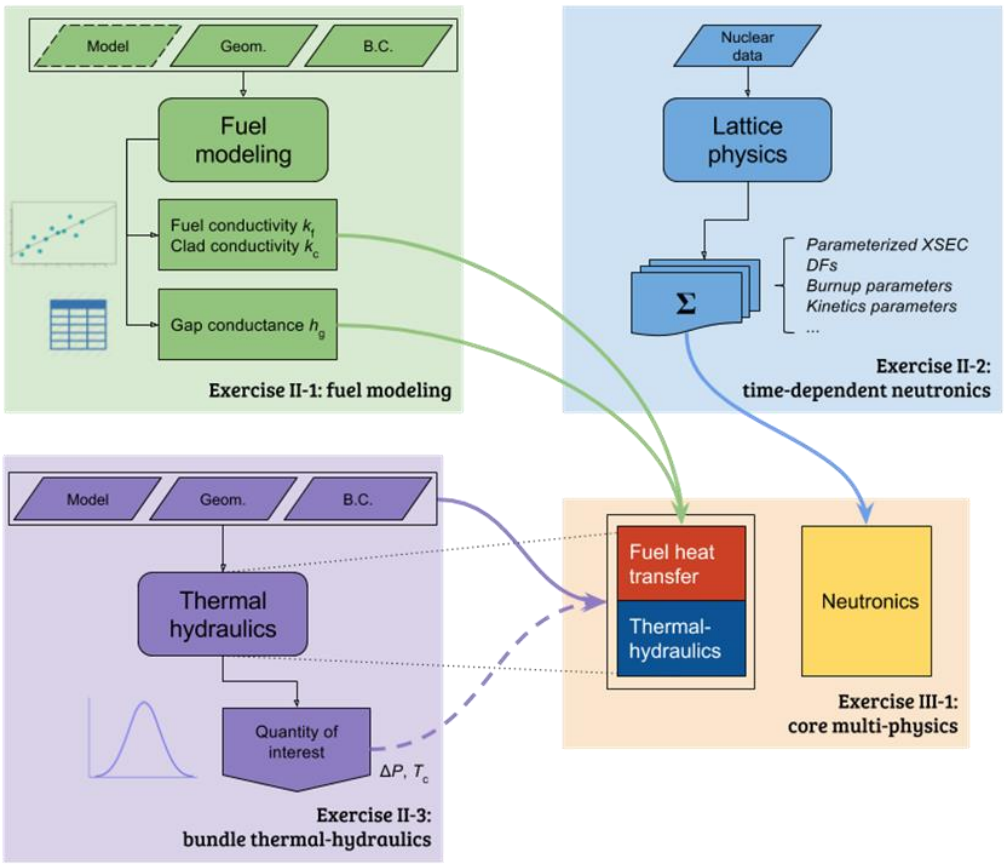
Phase III of the LWR UAM benchmark is focused on propagation of multiple uncertainties in coupled multi-physics steady-state, cycle depletion and transient calculations. The

interactions between Phase III and Phase II (which is focused on uncertainty propagation in single physics models which are components of the coupled multi-physics calculations) are shown in Figure 5.8.

One of the LWR core test problems in Exercises III-1 of the LWR UAM benchmark is based on the Three Mile Island Unit 1 (TMI-1) PWR. An uncertainty propagation mechanism has been developed using a stochastic sampling method by considering the uncertainties from neutronics, fuel modelling and thermal-hydraulics modelling in the coupled multi-physics simulations. The LWR UAM Phase III benchmark specification has been modelled using the coupled neutronics/thermal-hydraulics code system TRACE/PARCS, which consists of a 3D neutronics model and a 3D thermal-hydraulics core model (with integrated simplified fuel rod model). The input uncertainties of the neutronics simulation include the few-group cross-sections and kinetics parameters, generated using the Sampler/Polaris sequence of SCALE 6.2.1. The parametrised cross-section and other nodal parameters uncertainty libraries have been generated following the methodologies developed in Exercise II-2 (see Figure 5.9). The most important heat transfer related variables were considered as sources of input uncertainty in the simplified fuel rod modelling, including the thermal conductivity of fuel and cladding and the gap conductance. The calculations performed within the framework of Exercise II-1 with the higher-fidelity fuel performance code FRAPCON as well as utilising the available experimental data helped developed parametrised values and associated uncertainty bounds for these three parameters to be used in the coupled multi-physics calculations in Exercise III-1. For thermal-hydraulic parameters a mini-PIRT for the envisioned initial steady-state and transient application has been performed to identify which parameters plus uncertainties are to be propagated. For such propagation the experience accumulated in the Exercise II-3 PWR test problems was utilised. The envisioned transient applications are the TMI-1 PWR Rod Ejection Accident (REA) scenarios. DAKOTA was used to sample the resulting single physics input parameters to the coupled multi-physics code system and to perform the uncertainty analysis. Two types of simulations have been conducted: steady-state HZP and hot full power (HFP) core conditions at BOC and EOC and transient core behaviour initiated by the spatially asymmetric REA scenarios. Quantities of Interest (QoI) for the steady-state calculation, which includes core multiplication factor and power peaking factors, were calculated with associated uncertainties and analysed by normality test. For transient calculations, best-estimate results of the time evolution of core reactivity, core power and peak fuel and cladding temperature were generated with 95%/95% tolerance limits.

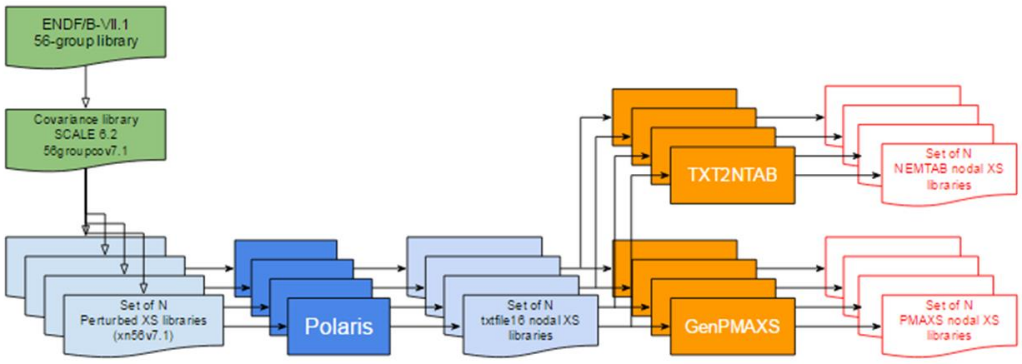
Figure 5.10 illustrates values and statistical error (as a result of using a statistical sampling method with 150 samples in this study) in predicting multiplication factors for different initial steady states while Figure 5.11 through Figure 5.13 show the predicted axial and power distributions with propagated uncertainties. Note that larger uncertainties were observed at BOC than EOC and the propagated uncertainties of HZP states are more pronounced than those of the HFP states.

Figure 5.8. Interactions of Phase II and Phase III of the LWR UAM benchmark



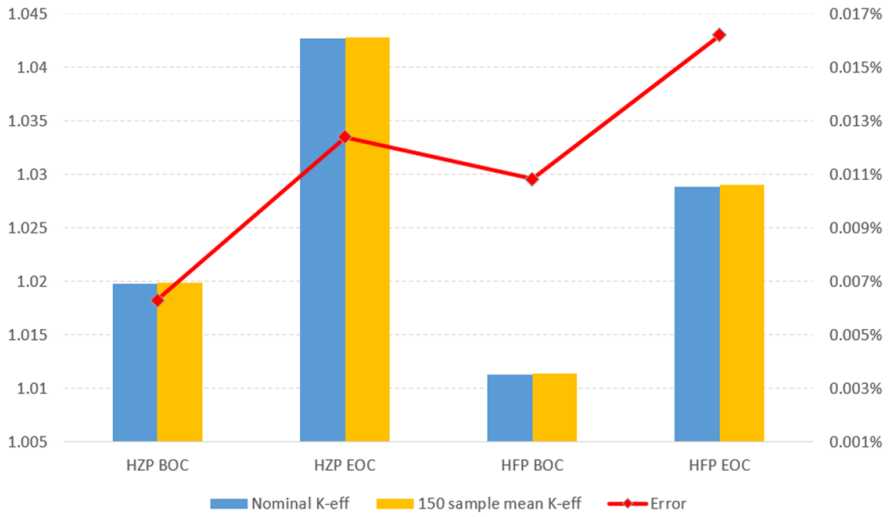
Source: NCSU, 2019.

Figure 5.9. Process of generation of parametrised cross-section libraries plus uncertainties



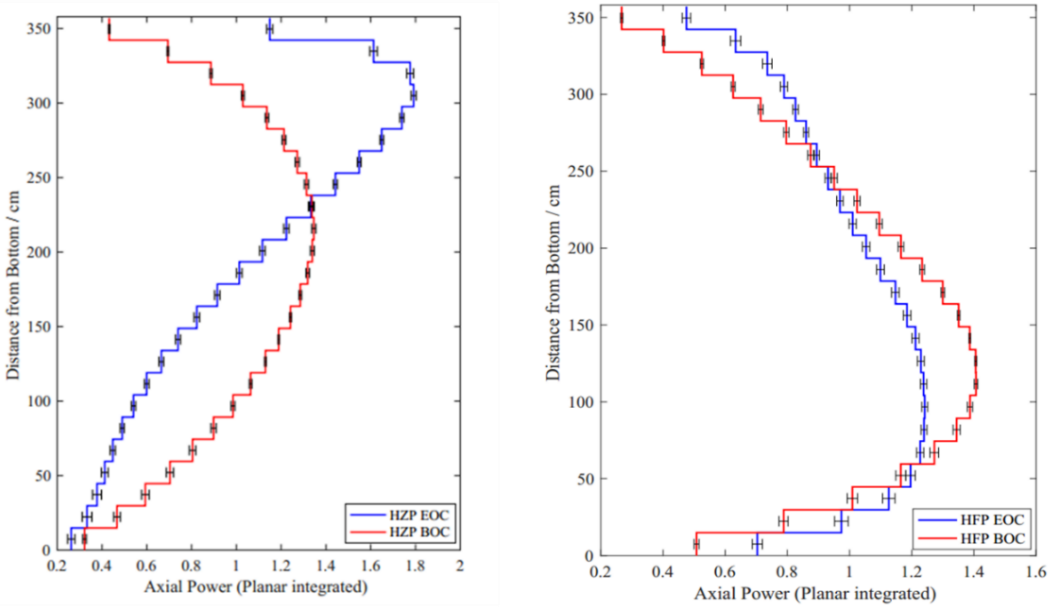
Source: NCSU, 2019.

Figure 5.10. Statistical errors of 150 samples mean k_{eff} compare to the unperturbed (nominal) k_{eff}



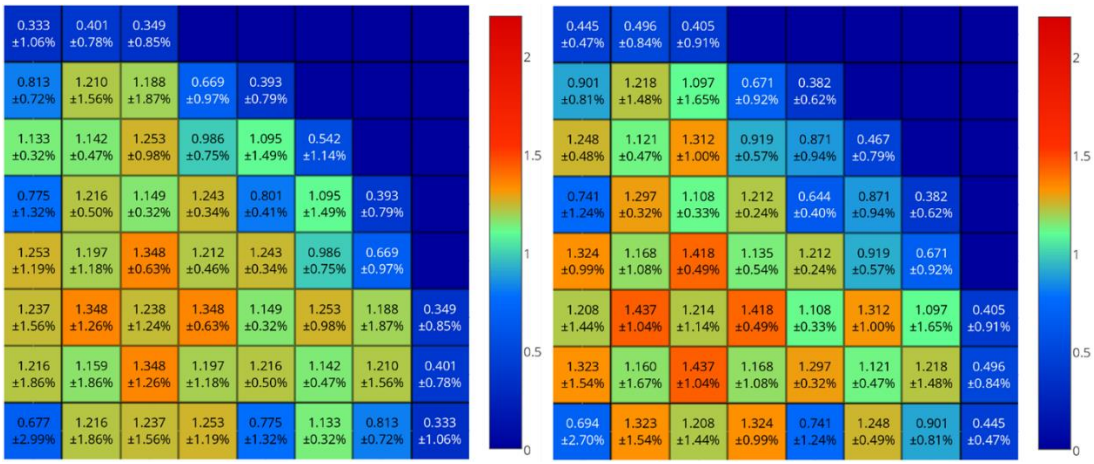
Source: NCSU, 2019.

Figure 5.11. Axial power distributions plus uncertainties at different states



Source: NCSU, 2019.

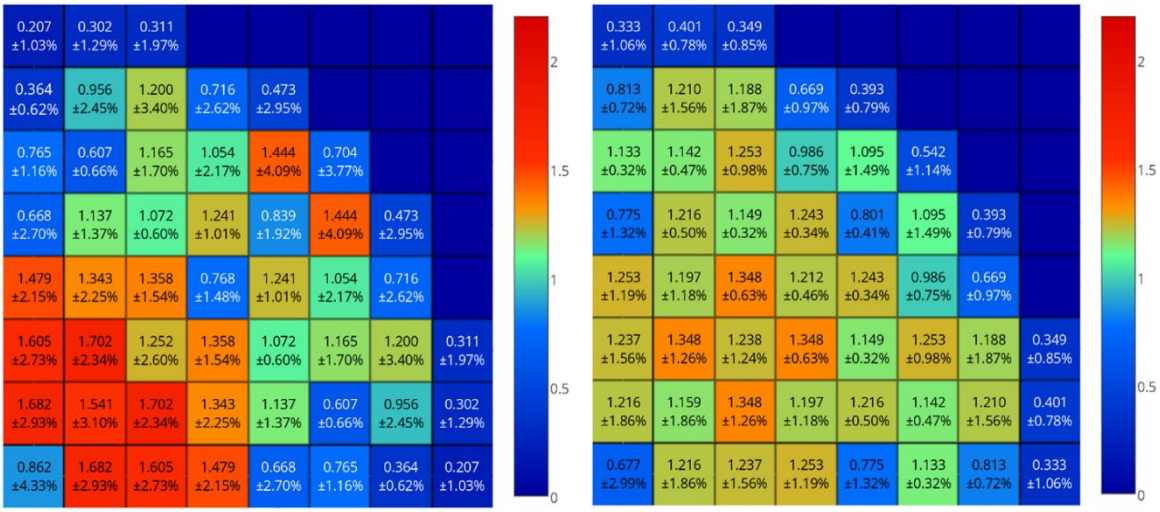
Figure 5.12. Radial power distributions plus uncertainties for HFP states



HFP BOC state HFP EOC state

Source: NCSU, 2019.

Figure 5.13. Radial power distributions plus uncertainties for HZP states



HZP BOC state HZP EOC state

Source: NCSU, 2019.

5.3 Use of Best Estimate Plus Uncertainty (BEPU) by regulation in licensing calculations

Realistic methods currently in use in industry and regulation are referred to as "best-estimate" calculations, implying that they use a set of data, correlations and methods designed to represent the phenomena, using the best available techniques. The risk-informed regulations also require that the uncertainty in these calculations be evaluated. These calculations are based on traditional multi-physics tools and are usually named as best-estimate plus uncertainty.

The traditional multi-physics tools have been used in two different ways in current licensing practices depending on the country and associated regulatory framework: best-estimate bounding and BEPU. The traditional multi-physics codes (for example coupled neutron kinetics/thermal-hydraulics codes) have been utilised in licensing applications in Europe in a best-estimate approach for transient and accident conditions with relevant changes of the power density distribution and a tight coupling of neutronics and thermal-hydraulics effects. Examples of such conditions are REA in PWRs or Rod Drop in BWRs, MSLB and boron dilution in PWRs, Anticipated Transient Without Scram (ATWS) cases, etc. In the US nuclear power generating industry, best-estimate methodologies supplemented with uncertainty analysis have been applied for thermal-hydraulics LBLOCA analysis. The US NRC accepts coupled 3D kinetics/thermal-hydraulics calculations for accidents with strong space-time effects such as PWR REA and MSLB for licensing power uprates, but these calculations have been applied in a bounding manner. The international trends in using traditional multi-physics (best-estimate or realistic) codes in licensing applications is summarised in Table 5.4.

Table 5.4. Trends in using traditional multi-physics codes in licensing applications

Applied codes	Initial and boundary conditions	System availability	Approach	Application
Conservative code	Conservative	Conservative assumptions	Deterministic	Old approach
Best-estimate (realistic) code	Conservative	Conservative assumptions	Deterministic	Current practice
Best-estimate code + uncertainty	Realistic + uncertainty; partly most unfavourable conditions	Conservative assumptions	Deterministic	New international trend; approach recommended by IAEA
Best-estimate code + uncertainty	Realistic + uncertainty	PSA-based assumptions	Deterministic + probabilistic	Risk-informed future standard?

Source: Petruzzi et al., 2016.

Recently, within the licensing process of the Atucha II Pressurized Heavy Water Reactor (PHWR) the BEPU approach has been selected for issuing of Chapter 15 of the Final Safety Analysis Report (FSAR) [142]. The complexity of a nuclear power plant and of the accident scenarios may be a challenge for a conservative analysis and may justify the choice of a BEPU approach in the licensing process. This implies two main needs: (1) the need to adopt and to prove (to the regulatory authority) an adequate quality for the computational tools and (2) the need to account for the uncertainty. The BEPU process was aimed at the licensing of the Atucha II (can-II) Nuclear Power Plant in Argentina operated by Nucleoeléctrica Argentina (NA-SA). Among the general attributes of a methodology to perform accident analysis of a nuclear power plant for licensing purposes, the very first one should be compliance with the established regulatory requirements. A second attribute deals with the adequacy and the completeness of the selected spectrum of events that should consider the combined contributions of deterministic and probabilistic methods. The third attribute is connected to the availability of qualified tools and analytical procedures suitable for the analysis of accident conditions envisaged for the nuclear power plant of concern. The execution of the overall analysis and the evaluation of results in relation to slightly fewer than 100 scenarios revealed the wide safety margins available for the nuclear power plant of concern, which was licensed in 2014.

Phenomena identification and ranking table (PIRT) Process

Introduction

Computer codes are used to design reactor systems and to analyse abnormal situations and transients. The process of system modelling consists of mathematical numerical methods and computer programs. The final product is a computer code. A computer code consists of formulations and numerical methods. The formulations consist of conservation equations for mass, momentum and energy for fluid, energy for fuel and equations for neutronics. The formulations also include hundreds of constitutive relationships characterising different transfer terms between gas, liquid and solid (wall, clad etc.). In addition to traditional multi-physics codes, there are other issues such as the effect of radiation on fuel composition, out-gassing, fuel-clad gap properties, corrosion and clad deformation leading to fuel-clad interaction. There are many issues related to normal and abnormal conditions for the reactor operations that challenge safety barriers and there are surrogate parameters that determine the effectiveness of the barrier. Some of these are clad temperature, clad oxidation and containment pressure. In addition, codes also address design related issues such as performance and power uprate.

For computer codes to be credible, they should have physics-based models that have properly adjusted parameters based on appropriate tests and have undergone rigorous validation, where code results are compared with the test data. These tests are separate effect tests and different levels of integral effect tests. Codes are applied to a variety of reactor problems and the sub-models of physical phenomena have different levels of impact on the QoI. Therefore, requirements for models for phenomena and component will be specific to an application. This leads to a need to prioritise the model development and tests for each application. In addition, the uncertainty quantification methods must also be appropriately chosen to characterise important physical phenomena and their interactions. This is important as there are hundreds of models and it is expensive to quantify uncertainty for each of them. Therefore, a method of identifying important phenomena is essential and it was first developed under the US NRC programme of code scaling, applicability and uncertainty (CSAU) quantification [67], called phenomena identification and ranking table (PIRT). There are two parts to PIRT, first, identification of phenomena and components at different levels. Second, ranking them based on their impact on the QoI or a FOM QoI.

In the past, phenomena identification and ranking tables (PIRTs) were developed on the basis of expert opinion. However, this becomes subjective. There are other approaches based on scaling or sensitivity analyses that quantify the impact of phenomena on the FOM; these are described in the next section.

Description

As PIRT is application dependent, the first step is to identify the reactor and the problem. The problem could be steady state or transient. In the case of a transient, the duration of the transient is divided into periods based on important events such as valve opening or operator action, or some significant change in important phenomenon.

Once the problem and the period of the transient have been established, the phenomena are decomposed from a top-down approach. The reactor system is first decomposed into larger components or sections with groups of phenomena. Each of these sections is then further decomposed. Finally, the decomposition leads to single basic phenomena. This step assures that all the phenomena and their hierarchy has been accounted for. This step depends on the expertise of the PIRT participants.

The next step in a PIRT is to rank the phenomena on the basis of their impact on the FOM. There are two approaches for ranking. The first approach is based on expert opinion. This was earlier developed in the CSAU methodology and applied to PWR LBLOCA events. This approach requires broad expertise among the participants of the PIRT. However, it has been adopted in different fields since it was introduced in the CSAU methodology. The weakness of this approach is that it is subjective and depends on expert opinion and resulting consensus.

The second approach is based on the relative quantitative impact of phenomena/component on the FOM; a so-called Quantified Phenomena Identification and Ranking Table (QPIRT). There are two ways to quantify the impact of different phenomena on the FOM. The first approach requires an order of magnitude analysis based on the conservation equations and reference values of the variables for each phase of the transient or for steady state. Examples of this approach are the hierarchical two-tiered scaling (H2TS) and the fractional scaling analyses (FSA). In this approach the initial or average values of reference quantities are used to nondimensionalise the system level balance equations for each phase of the transient. This method provides a quantitative approach for phenomena/component ranking.

The second approach for QPIRT is based on sensitivity analyses using the computer codes. In this approach the sensitivity of output parameters or the FOM to model parameters or initial and boundary conditions are estimated. Models with higher sensitivity have a higher magnitude of change or rate of change. However, the impact will be measured by net change of the parameter of interest or FOM over the variation of the model or input parameters during period of interest. The weakness of this approach is that sensitivity and ranking will be based on the models in the code that are themselves the target of code validation.

There is another addition to a traditional PIRT, which is inclusion of the status of knowledge. Knowledge will include an appropriate database and basic models. The combination of PIRT ranking and the status of knowledge sets the priorities for future experiment and model development. This new information was first incorporated into a PIRT for the advanced CANDU Reactor in Canada. It has now also been included in the DOE Consortium for Advanced Simulations of LWRs (CASL) programme.

Examples

Three examples representing the approaches described earlier are documented below.

The US NRC first applied the PIRT process in the CSAU for LBLOCA. A group of experts with knowledge of PWR LBLOCA analyses and tests was assembled. First, the transient was divided into periods based on either dominant phenomena or valve or operator action. A list of phenomena was identified. In the second iteration the phenomena are ranked based on their impact on an identified FOM. In the case of LBLOCA, peak clad temperature was selected as the FOM. The PIRT requires decomposition of the transient into phases and of the system into components and phenomena. An example of this is shown in the CSAU report [143].

LBLOCA was also analysed with the FSA methodology [144]. The approach is similar to the CSAU methodology. The system level balance equations were nondimensionalised with reference quantities estimated at the beginning of the phase of the transient. The net rate of change of state variables is the sum of the contributions from the different agents of change (phenomena). This approach identifies the phenomena through the agent of change

and the magnitude of the contribution to the net rate of change (frequency) is the measure of the ranking of the phenomena (see Table 5.5).

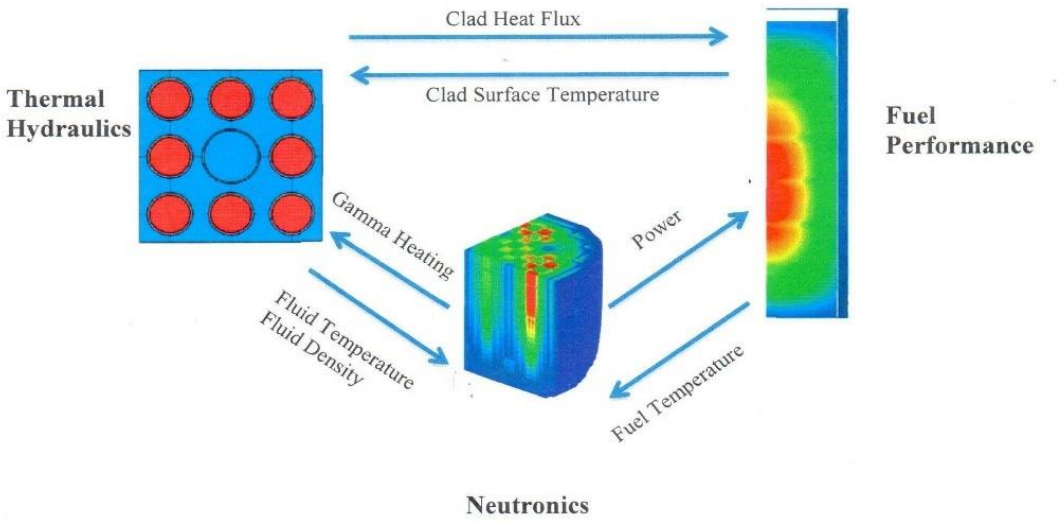
Table 5.5. FSA applications to LOFT and semi-scale

ω is in %/s	Net break flow	Net heating of two-phase mixture	Net heating (cooling) of liquid	Pumping power	Non-condensable gases
	ω_{bk}	$\omega_{\dot{Q}_{2\phi}}$	$\omega_{\dot{Q}_{1\phi}}$	$\omega_{P_{PP}}$	ω_{N_2}
LOFT	-577.3	1.41	-0.63	0.63	N.A.
Semi-scale	-602.6	1.41	-0.52	0.52	N.A.

Source: Wulff et al., 2009.

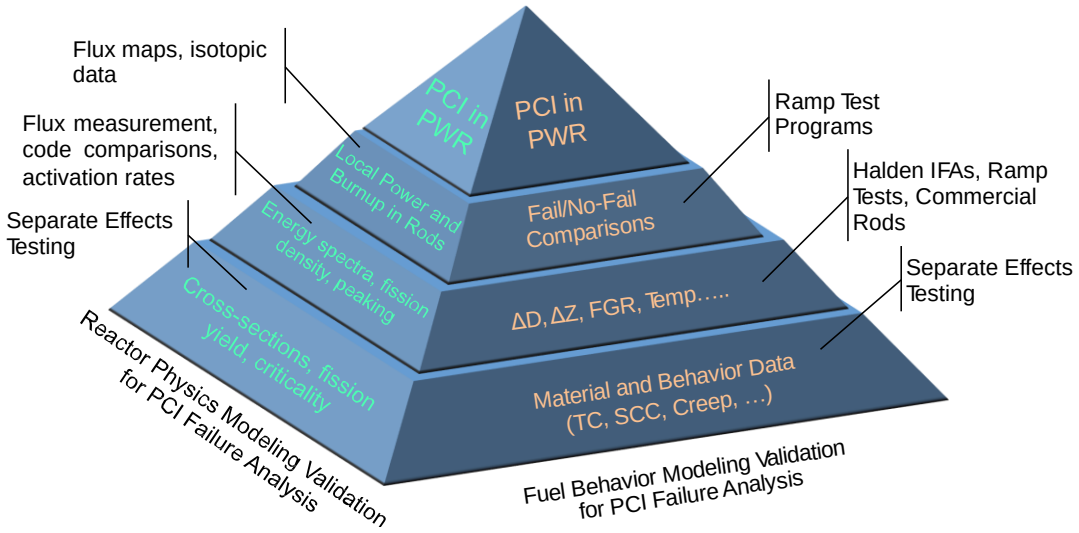
The second example is from the CASL programme. CASL has identified several challenge problems. One of the problems is pellet-clad interaction (PCI). In this case the simulation requires interaction of multiple physics, namely, neutronics, thermal hydraulics and fuel performance as shown in Figure 5.14. The envisioned validation pyramid is shown in Figure 5.15 while the level PIRT for this multi-physics problem is depicted in Figure 5.16. Figure 5.17 illustrates the bottom-up multi-scale validation approach with the lowest level phenomena associated to modelling of subcooled boiling.

Figure 5.14. Coupling of physical phenomena for PCI



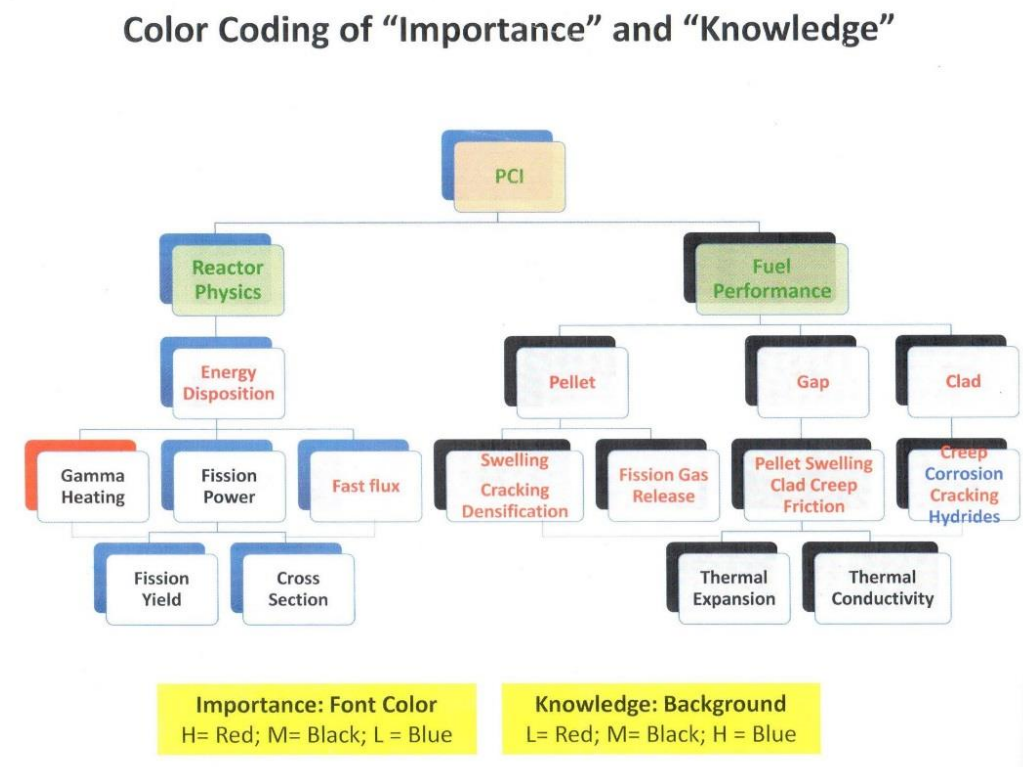
Source: N.IN.E., 2018.

Figure 5.15. PCI validation pyramid showing different physics



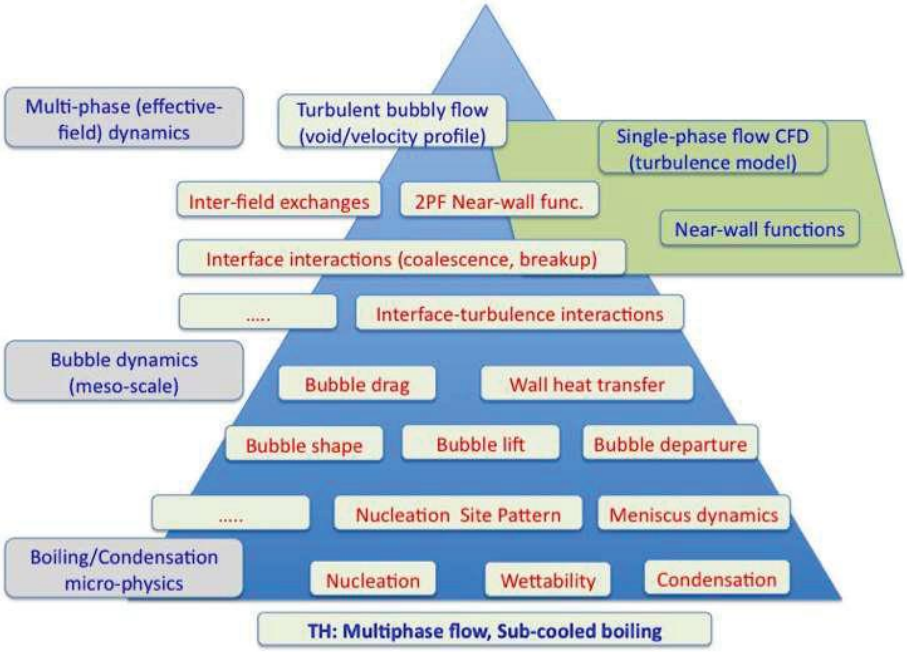
Source: CASL, 2018.

Figure 5.16. Decomposed level PIRT for PCI



Source: CASL, 2018.

Figure 5.17. Bottom-up approach with lowest level phenomena associated to modelling of subcooled boiling



Source: CASL, 2018.

Oregon State University has developed a QPIRT for a 2-inch break in an AP1000 reactor cold leg [145]. The method is based on the H2TS approach with the help of RELAP5 analyses. The starting formulation was based on a RELAP5 two-fluid approach. It yielded 28 non-dimensional groups. A simplified drift flux formulation yielded a smaller batch of eight non-dimensional groups. The study was applied to the core region for a 2-inch break for the Advanced Plant EXperiment (APEX) facility designed for the AP600 plant. RELAP5 results of the transient were used to estimate values for 14 non-dimensional groups for two phases. As expected, the non-dimensional groups change during different phases of a small break LOCA and so does their ranking. Table 5.6 shows that for the vapour phase, the pressure drop and interfacial heat transfer are the top two processes during In-Containment Refuelling Water Storage Tank (IRWST) injection. Pressure drop and interfacial drag are the top two processes for the sump injection phase. However, for the liquid phase, gravity and pressure are top two process groups (see Table 5.7). The two-fluid formulation based PIRT is useful for prioritisation for code development. However, this approach is not as useful for developing integral level tests. The alternate approach is to use a mixture level formulation for each phase of the transient. This led to eight Π groups, two in mass balance, four in momentum balance and two in energy balance. Figure 5.18 shows the π group values for five phases of the transient. Ranking of different phenomena can therefore be established.

In addition, the study compared the QPIRT with a standard PIRT. The emphasis is different between the QPIRT, which looks at balance equations and the PIRT where the effect of phenomena on a FOM is considered. It should be noted that H2TS could be structured to go from the balance equations to any FOM. This study showed that for system and component levels there was similarity in the ranking between the two approaches, except for a few phenomena.

Table 5.6. Vapour Phase Π Groups for APEX facility 2-inch break

Physical processes		∏ Groups	∏ Group values in transient	
			IRWST injection phase	Sump injection phase
			4 100 (sec)	9 300 (sec)
Mass	Vapour generation	∏gΓ	0.21	1.93
Momentum	Pressure difference	∏gP	813.0	153.7
	Gravity	∏gB	19.5	3.26
	Wall friction	∏FWG	2.58	0.41
	Interfacial phase change acceleration	∏ΓIG	5.58	2.68
	Interfacial drag	∏FIG	165.9	83.4
	Virtual mass	∏VMG	20.8	5.85
Energy	Vaporisation transient	∏GVT	0.00	0.00
	Pressure work	∏PG	0.01	0.00
	Wall heat transfer	∏Qwg	0.15	0.00
	Interfacial heat transfer	∏Qig	244	55.8
	Interfacial phase change acceleration	∏Γig	3.13	0.04
	Wall phase change	∏Γwg	2.91	2.10
	Dissipation	∏DISSg	0.00	0.00

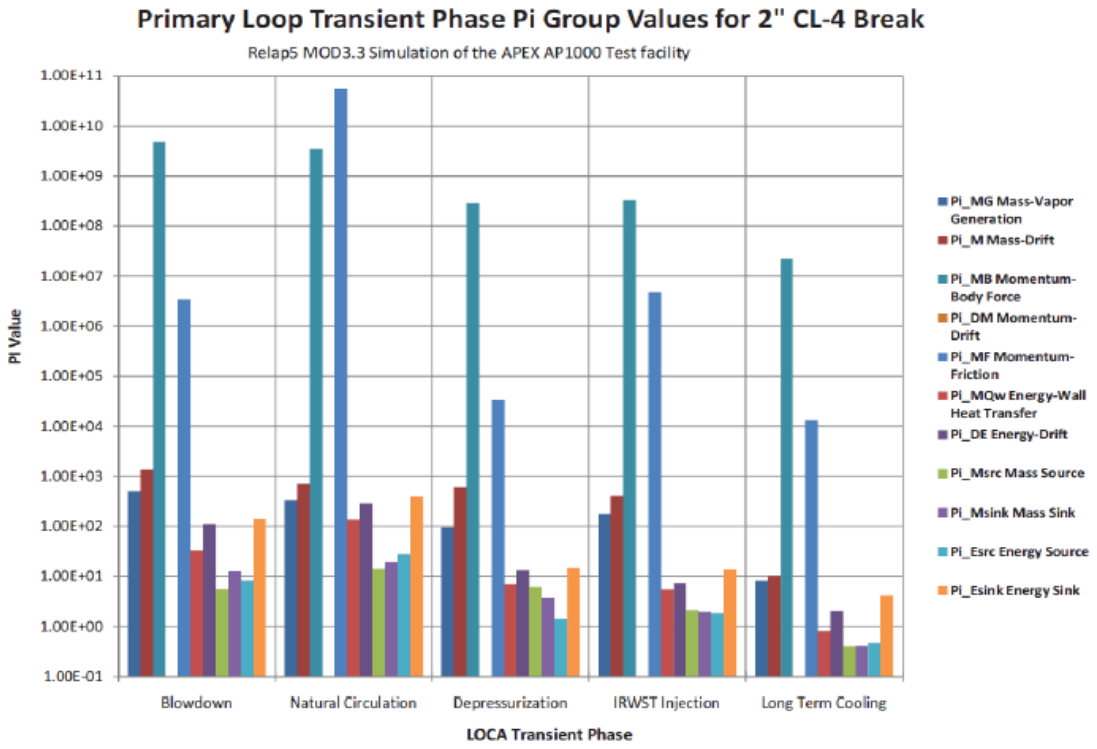
Source: Luo, 2012.

Table 5.7. Liquid Phase Π Groups APEX 2-inch break

Physical processes		∏ Groups	∏ Group Values in Transient	
			IRWST injection phase	Sump injection phase
			4 100 (sec)	9 300 (sec)
Mass	Vapour generation	∏fΓ	0.00	0.02
Momentum	Pressure difference	∏fP	397	153
	Gravity	∏fB	7 055	7 647
	Wall friction	∏FWF	0.64	10.26
	Interfacial phase change acceleration	∏ΓIF	0.01	0.00
	Interfacial drag	∏FIF	10.6	60.3
	Virtual mass	∏VMF	1.33	4.23
Energy	Vapourisation transient	∏FVT	0.00	0.00
	Pressure work	∏PF	0.00	0.00
	Wall heat transfer	∏Qwf	0.27	0.15
	Interfacial heat transfer	∏Qif	4.39	4.83
	Interfacial phase change acceleration	∏Γif	0.01	0.29
	Wall phase change	∏Γwf	0.06	0.14
	Dissipation	∏DISSf	0.00	0.00

Source: Luo, 2012.

Figure 5.18. Values of Π groups for different phases of the transient



Source: Luo, 2012.

Code validation and uncertainty analyses in licensing

All countries with operating and/or planned nuclear power plants have regulatory bodies that ensure that the reactor design is safe and is operated safely during its life. Safety decisions are made based on simulation of the reactor under design basis accident scenarios. Each of the countries has either their own codes or internationally recognised codes such as RELAP5, TRACE, CATHARE, ATHLET, etc.

Nuclear reactors are regulated by the US NRC based on analyses or simulation of reactors under hypothetical accident scenarios. The analyses predict safety parameters that are essential in protecting the public from the release of radioactive materials from the fuel. The safety criteria are related to ensuring that the fuel clad is not breached. The acceptance criteria that will ensure the integrity of the fuel clad are documented in 10 CFR 50.46 and they are: (1) peak cladding temperature (PCT) should be less than 2 200 F; (2) local maximum oxidation (LMO) should be less than 17%; (3) core-wide oxidation (CWO) should be less than 1% (to limit the maximum amount of hydrogen generated); (4) the core should maintain a coolable geometry; and (5) long-term cooling should be demonstrated.

The US NRC has developed guidelines for development of an evaluation model (EM) for safety studies and it is called the evaluation model. The EM consists of a reactor model, nodalisation and the codes. These guidelines are suggestions and are not requirements.

The principles of an evaluation model development and assessment (EMDAP) were developed from a study on quantifying reactor safety margins, based on the CSAU evaluation methodology for a large break LOCA.

The purpose of the CSAU methodology was to demonstrate a method that could be used to quantify uncertainties as required by the best-estimate option described in the NRC's 1988 revision to the ECCS Rule (10 CFR 50.46) [146]. The code uncertainty evaluation will involve the entire process of EMDAP. Since the publication of the CSAU report in December 1989, the CSAU process has been applied in many examples.

EMDAP is a multiple-step procedure, as shown in Figure 5.19. It has four elements and each element has multiple steps, giving 20 steps in total. The process addresses the question of the adequacy of an evaluation model (code and nodalisation) to simulate the scenario of interest in predicting safety parameters or a FOM.

The four elements of EMDAP address four topics; requirements of evaluation model, assessment base to support identified requirements, development of evaluation model and assessment of adequacy of EM.

The following description is summarised from US NRC regulatory guide 1.203 [148].

Evaluation Model Development and Assessment Process (EMDAP)

The basic elements of EMDAP are shown in Figure 5.19. This regulatory position addresses the four elements and the adequacy decision as shown in Figure 5.19. Adherence to an EMDAP for new applications or a completely new EM could involve significant iterations within the process. However, the same process applies even if the new EM is the result of relatively simple modifications to an existing EM.

Element 1: Establish requirements for evaluation model capability

Figure 5.20 illustrates four steps within this element and is described here.

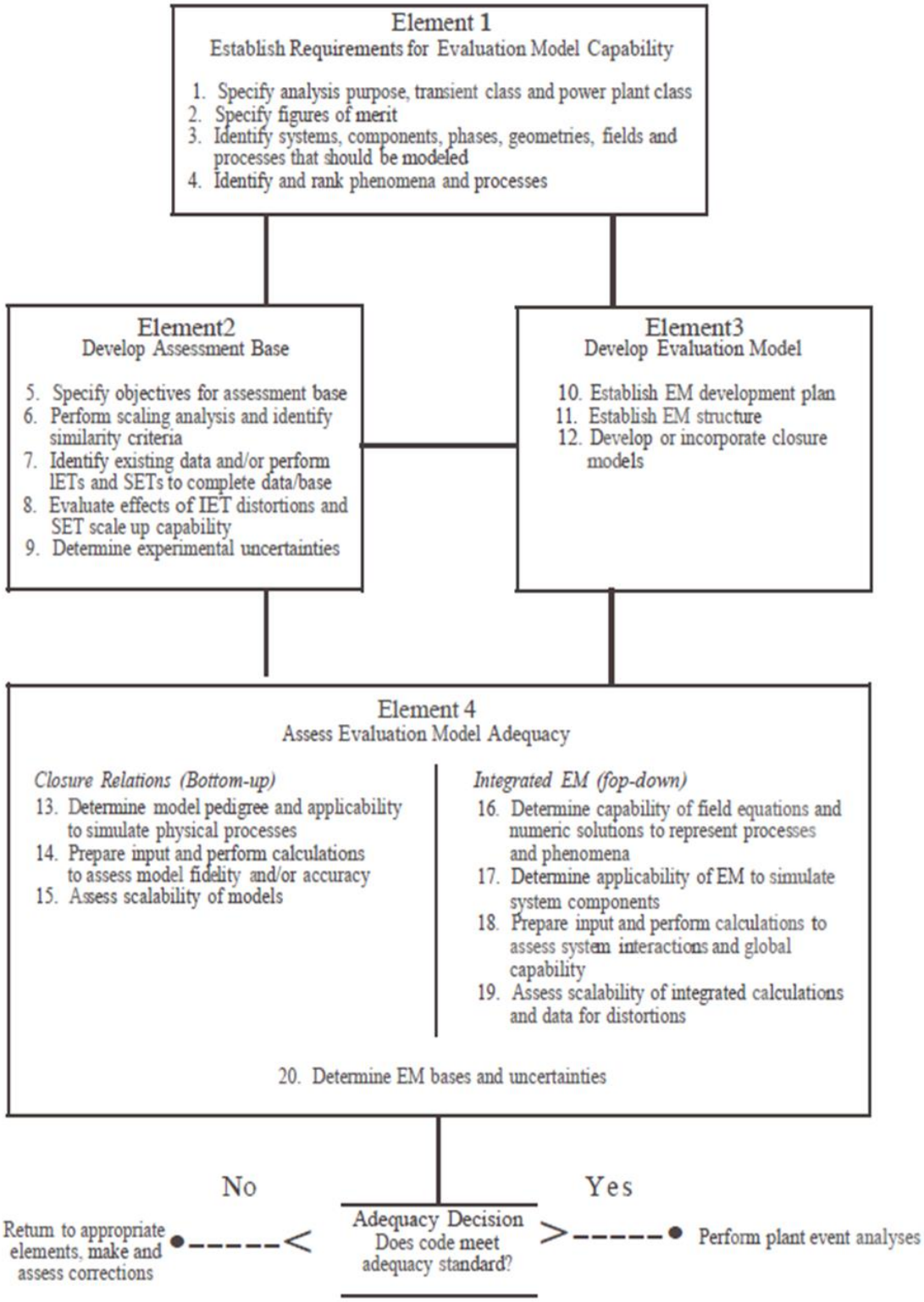
Step 1 is to specify the plant, scenario and the purpose of analyses. Specifying the purpose is important because any given transient may be analysed for different objectives. A SBLOCA may be analysed to assess the potential for pressurised thermal shock (PTS) or compliance with 10 CFR 50.46.

A LOCA may be analysed for load on containment. The statement of purpose influences the entire process of development, assessment and analysis for the prediction of FOM.

The evaluation model applicability is scenario-dependent because the dominant processes, safety parameters and acceptance criteria change from one scenario to another. The transient scenario, therefore, dictates the processes that must be addressed. A complete scenario definition is plant-class-specific or sometimes even plant-specific because the dominant phenomena and their interactions differ in varying degrees with the reactor design or a plant-specific configuration such as a specific fuel type or core loading.

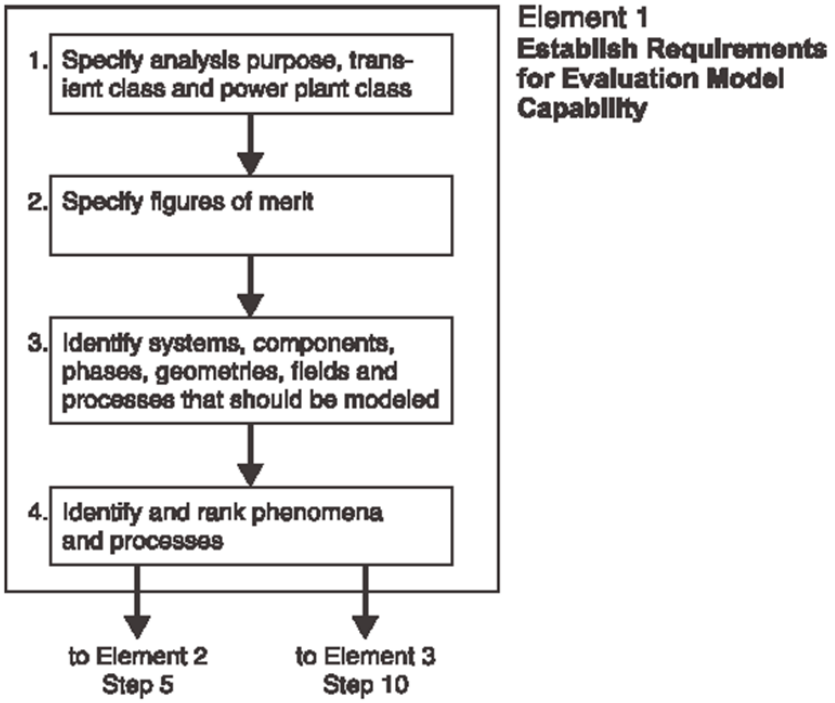
The licensee or applicant and the EM developer are responsible for justification of the use of EM and their applicability to plants and plant types.

Figure 5.19. The EMDAP process (US NRC 2005)



Source: NRC, 2005.

Figure 5.20. Steps in Element 1



Source: NRC, 2005.

Step 2 identifies the FOM based on the scenario and purpose of analyses. FOM are those quantitative that can be used to define acceptable answers for a safety analysis. The requirements for maintaining the reactor in a safe condition during normal operation and during transients and accidents are translated in terms of quantitative fuel and reactor system design limits (DNBR, fuel temperatures, etc.) for the events of interest. For ECCS design, five specific criteria described in 10 CFR 50.46 must be met for LOCA analysis. During evaluation model development and assessment, a temporary "surrogate" FOM may be used in evaluating the importance of phenomena and processes. In the case of SBLOCA, vessel inventory was deemed more valuable in defining and assessing code capability. Justification for using a surrogate FOM should be provided.

Because compensating errors in the code can unintentionally lead to correct answers, additional performance measures serve as physical tracking points and additional proof of accuracy. While the code may calculate the correct PCT, for example, incorrect or physically impossible parameter values could evolve in other areas of the calculation.

Step 3 identifies systems, components, phases, geometries, fields and processes that should be modelled in the EM. Hierarchical system decomposition methods were used to investigate scaling in complex systems [149,150]. These methods can also be valuable in identifying EM characteristics. The hierarchical level are as follows:

- *system:* the entire system that must be analysed for the proposed application;
- *subsystems:* major components that must be considered in the analysis; for some applications, these may include the primary system, secondary system and containment; for other applications, only the primary system would need to be considered;

- *modules:* physical components within the subsystem (i.e. reactor vessel, steam generator, pressuriser, piping run);
- *constituents:* chemical form of substance (e.g. water, nitrogen, air, boron);
- *phases:* solid, liquid or vapour;
- *geometrical configurations (phase topology or flow regime):* the geometrical shape defined for a given transfer process (e.g. pool, drop, bubble, film);
- *fields:* the properties that are being transported (i.e. mass, momentum and energy);
- *transport processes:* mechanisms that determine the transport of and interactions between constituent phases throughout the system.

Ingredients at each hierarchical level can be decomposed into the ingredients at the next level down. This process is described as follows:

- each system can be divided into interacting subsystems;
- each subsystem can be divided into interacting modules;
- each module can be divided into interacting constituents;
- each constituent can be divided into interacting phases;
- each phase can be characterised by one or more geometrical configurations (phase topology or flow regime);
- each phase can be described by field equations (e.g. conservation equations for mass, energy and momentum);
- the evolution of each field can be affected by several transport processes.

By carefully defining the number and type of each ingredient at each level, the evaluation model developer should be able to establish the basic characteristics of the EM. It should be noted that a deficiency at a higher level, is usually not resolvable by fixing ingredients at lower levels.

Step 4 describes the process of identification and ranking of phenomena and processes as they affect the FOM.

The scenario can be divided into distinct phases based on the events taking place such as valves, or operator action. Each of these phases will have a different set of important components and phenomena with respect to the FOM. It should be noted that the FOM could be a surrogate for safety parameters and the PIRT will reflect that. The PIRT can follow decomposition of the model starting from plant level, moving down through component and process levels.

The PIRT should be used to determine the requirements for physical model development, scalability, validation and sensitivity studies. Ultimately, the PIRT is used to guide any uncertainty analysis or in the assessment of overall EM adequacy.

The initial phases of the PIRT process described in this step can rely heavily on expert opinion, which can be subjective. Therefore, it is important to validate the PIRT using experimentation and analysis. Scaling methods can also be used to validate the PIRT. Sensitivity studies can help determine the relative influence of phenomena identified early in the PIRT development and for final validation of the PIRT as the EMDAP is iterated. Some examples of sensitivity studies used for this purpose are shown in [146,151-153].

The highly ranked phenomena and processes require greater modelling fidelity. The role of the PIRT process in experiments, code development, and code applications associated with reactor safety analysis are shown in [151,154].

Element 2: Develop assessment base

Element 2 and its associated five steps are shown in Figure 5.21. In this element the validation matrix for specific scenario is established. Scaling methods and evaluation of scale distortions in different tests are also performed.

Step 5 identifies that the test matrix is consistent with the PIRT and with the requirements in Element 1 for code validation. The database should include the following:

- separate effects experiments needed to develop and assess empirical correlations and other closure models;
- integral systems tests to assess system interactions and global code capability;
- benchmarks with other codes (optional);
- plant transient data (if available);
- simple test problems to illustrate fundamental calculation device capability.

It should be noted that code-to-code comparison and fundamental tests are only supplements and cannot replace SET, IET and plant data.

Step 6 is an import step in determining the adequacy of the validation test matrix for intended use. A scaling approach is developed in this step and non-dimensional groups are identified.

Scaling analyses should be conducted to ensure that the data and the models based on those data, will be applicable to the full-scale analysis of the plant transient. All tests, SETS and IETs are designed to simulate some phases of some scenarios. Even there, the tests include compromises and scale distortion. In some cases, tests designed for one phase of a scenario may be used for a different scenario and may incur additional scale distortions. The scaling analyses identify any such scale distortions. Knowledge of scale distortions is important in making a judgement about scalability of the EM. These distortions will add to biases and uncertainty in models and correlations in Element 4.

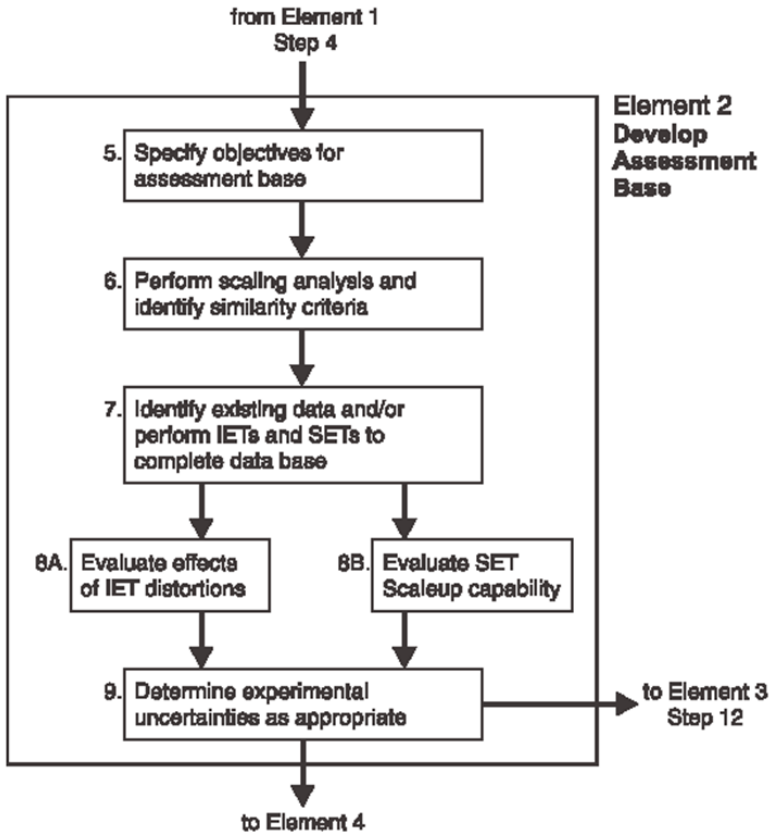
The scaling analyses employ both top-down and bottom-up approaches [150]. The top-down scaling approach evaluates the global system behaviour and systems interactions from integral test facilities that can be shown to represent the plant-specific design under consideration. A top-down scaling methodology is developed and applied to achieve the following purposes:

- derive the non-dimensional groups governing similitude between facilities;
- show that these groups scale the results among the experimental facilities;
- determine whether the ranges of group values provided by the experiment set encompass the corresponding plant- and transient-specific values.

The bottom-up scaling analyses address issues raised in the plant- and transient-specific PIRT related to localised behaviour. These analyses are used to explain differences among tests in different experimental facilities and to use these explanations to infer the expected

plant behaviour and determine whether the experiments provide adequate plant-specific representation.

Figure 5.21. Steps in Element 2



Source: NRC, 2005.

In Step 7, actual relevant SETS, IETS and plant data are selected based on the PIRT developed in Step 4. This set of tests is called the assessment matrix. It is important that there be multiple tests for the same phenomenon and components to avoid the effect of code tuning or calibration. Ideally, both the data that will be used to develop the correlation and the data that will be used to assess the correlation should be identified. This would help to ensure that the correlation is not tuned to a particular data set and that the data used to assess the correlation have not been deliberately selected to make the correlation appear to be more accurate than it truly is.

The data used for development and assessment should cover the full range of conditions for which the correlation will be used. For integral behaviour assessment, counterpart tests (similar scenarios and transient conditions) in different experimental facilities at different scales should be selected. Assessments using such tests lead to information about scaling capability of the codes.

In Step 8, effects of IET distortions and SET scale-up capability are evaluated (US NRC Regulation guide 1.203 [148]):

- *IET Distortions:* Distortions in the IET database may arise from scaling compromises (missing or atypical phenomena) in subscale facilities or atypical initial

and boundary conditions in all facilities. The effects of the distortions should be evaluated in the context of the experimental objectives determined in Step 5. If the effects are important and distortions are significant, new tests should be sought or performed.

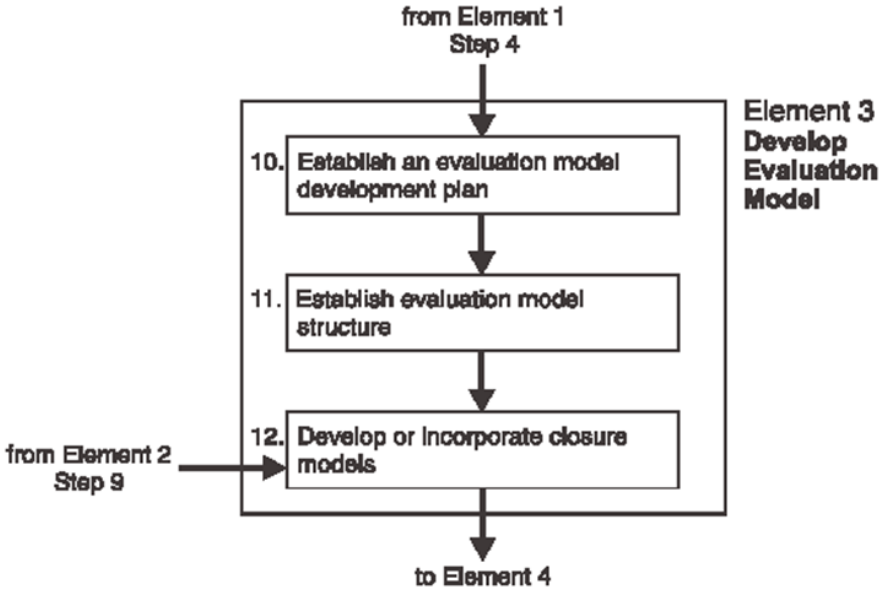
- *SET Scale-up:* As noted in Step 7, correlations should be based on separate effects tests (SETs) at various scales. In the case of poor scale-up capability, it may be necessary to return to Step 6.

In Step 9, the experimental uncertainties in the database are documented. These uncertainties arise from measurement errors, experimental distortions and other aspects of experimentation. If the quantified experimental uncertainties are too large compared to the requirements for evaluation model assessment, the data set or correlation should be rejected. A code should not be penalised due to bad data. These uncertainties are added to code calculation uncertainties determined from these tests.

Element 3: Develop evaluation model

Figure 5.22 depicts Element 3 with the three steps for developing the desired EM. This element reviews the documentation to determine the adequacy of the calculation devices for formulation, closure relationships and coupling between different codes. No calculations with codes are part of this element.

Figure 5.22. Steps in Element 3



Source: NRC, 2005.

Step 10 is needed to assure that the EM is developed under quality control and with proper documentation. Based on the requirements established in Element 1, an EM development plan should be devised. Such a plan should include development standards and procedures that will apply throughout the development activity and should address the following specific areas of focus:

- design specifications for the calculation device;

- documentation requirements;
- programming standards and procedures;
- transportability requirements;
- quality assurance procedures;
- configuration control procedures.

In Step 11, the code is assessed for adequacy of models and coupling for the intended application based on requirements established in Element 1. The EM includes the models of the individual component calculation devices, as well as the coupling of the calculation devices.

The structure for an individual device or code consists of the following six ingredients which are consistent with the scaling approach in Step 6:

- *Systems and components:* The EM structure should be able to analyse the behaviour of all systems and components that play a role in the targeted application.
- *Constituents and phases:* The code structure should be able to analyse the behaviour of all constituents and phases relevant to the targeted application.
- *Field equations:* Field equations are solved to determine the transport of the quantities of interest (usually mass, energy and momentum).
- *Closure relations:* Closure relations are correlations and equations that help to model the terms in the field equations by providing code capability to model and scale particular processes.
- *Numerics:* Numerics provide code capability to perform efficient and reliable calculations.
- *Additional features:* This addresses code capability to model boundary conditions and control systems.

The coupling of different codes in space and time should be described. Coupling should be consistent with the requirements and decomposition described in Step 3. Since most codes include user options, all selections made should be justified as appropriate for the EM.

Step 12 is for review of adequacy of closure models. Models or closure relationships that describe a specific process are developed using SET data. This includes models that can be used in a stand-alone mode or correlations that can be incorporated in a calculation device (usually a computer code). On rare occasions, sufficient experimental detail may be available to develop correlations from IET experiments. The scalability and range of applicability of a correlation may not be known (*a priori*) the first time it is developed or selected for use in this step. An iteration of the scale-up evaluation (Step 8) and adequacy assessment (Element 4) may be needed to ensure correlation applicability.

The basis, range of applicability and accuracy of incorporated phenomenological models should be known and traceable. Justification should be provided for extension of any models beyond their original bases.

Element 4: Assess evaluation model adequacy

Evaluation model adequacy can be assessed after the previous elements have been established and the EM capability has been documented. Figure 5.23 is a diagram of Element 4 and its eight related steps.

The EM assessment is divided into two parts as shown in Figure 5.23. The first part (Steps 13-15) pertains to the bottom-up evaluation of the closure relations for each code. In the first part, important closure models and correlations are examined by considering their pedigree, applicability, fidelity to appropriate SET data and scalability. The term bottom-up is used because the review focuses on the fundamental building blocks of the code.

The second part (Steps 16-19) pertains to the top-down evaluations of code-governing equations, numerics, the integrated performance of each code, coupling and the integrated performance of the overall EM.

In the second part of the assessment, the EM is evaluated by examining the field equations, numerics, applicability, fidelity to component or integral effects data and scalability. This part of the assessment is called the top-down review because it focuses on capabilities and performance of the EM.

The third group of data is the actual plant transient data and it provides confirmatory supporting assessments. It is important as there are no scale issues. Plant data can be used for code assessment if it can be demonstrated that the available instrumentation provides measurements of adequate resolution to assess the code.

It is important to note that any changes to an EM should include at least a partial assessment to ensure that these changes do not produce unintended results in the code's predictive capability.

Step 13 is needed to review the database behind correlations and component models in the codes. The pedigree evaluation relates to the physical basis of a closure model, assumptions and limitations attributed to the model and details of the adequacy characterisation at the time the model was developed. The applicability evaluation relates to whether the model, as implemented in the code, is consistent with its pedigree and can cover the range of the conditions expected during the transient. This step will indicate if further assessment with SETs should be done.

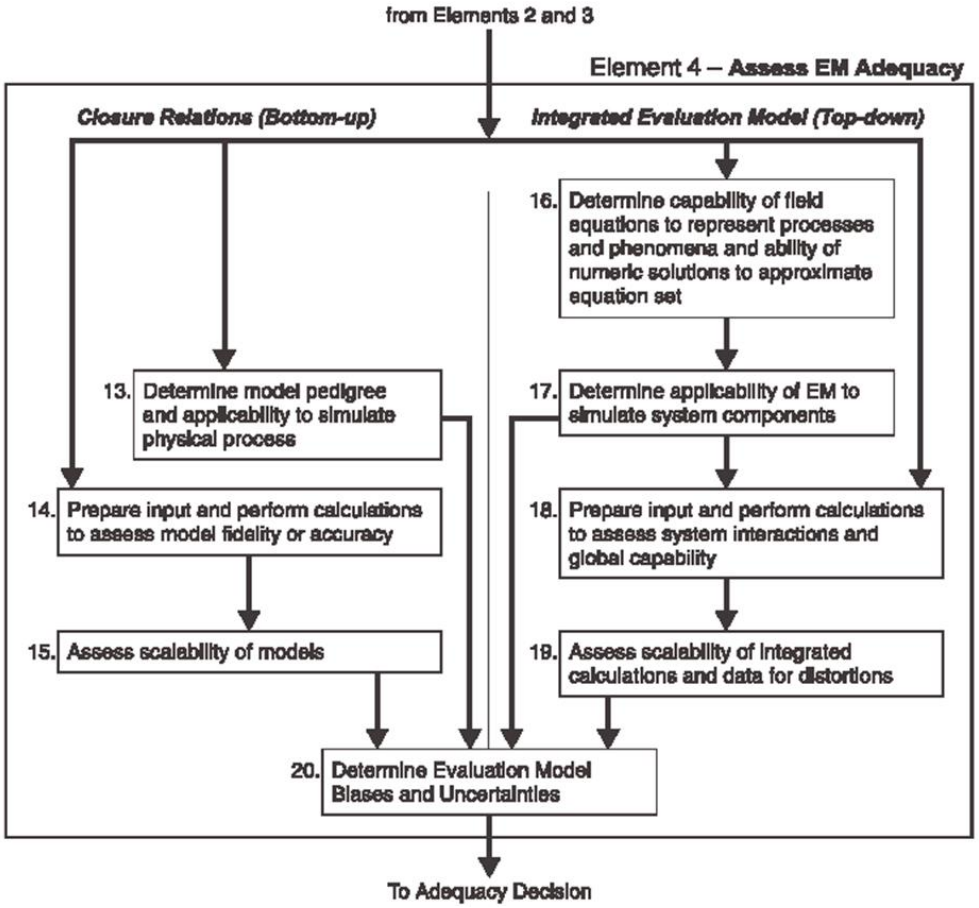
In Step 14, the relevant SETs are modelled and predictions are compared with the data.

SET input for component devices used in the model assessment (usually computer codes) should be prepared to represent the phenomena and test facility being modelled, as well as the characteristics of the nuclear power plant design. Nodalisation and option selection should be consistent between the experimental facility and similar components in the nuclear power plant.

Convergence studies should be performed to the extent practicable in both the test facility and plant models. Some models are essentially lumped parameter models and, in those cases, a nodalisation convergence study cannot be performed. In such cases, care should be taken to ensure that the model is applicable to both the test facility and the plant. It should be noted that for the most system codes, the predictions depend on nodalisations and code options and for assessment results to be applicable to plant calculations, the modelling should be consistent with the plant model.

When the calculations of the SETs are completed, the differences between calculated results and experimental data for important phenomena should be quantified for bias and deviation.

Figure 5.23. Steps in Element 4



Source: NRC, 2005.

Step 15 determines the scalability of the specific model or correlation is appropriate for application to the configuration and conditions of the plant and transient under evaluation. There are many references that illustrate this process [149,155-158]. In addition, counterpart tests could also be used to assess scalability of the correlations and component models.

Step 16 is part of the four steps that assess the ability of the codes to integrate different phenomena and components. This step deals with review of the adequacy of the code formulations and numerics for the intended application.

The numeric solution evaluation considers convergence, property conservation and stability of code calculations to solve the original equations when applied to the target application. The objective of this evaluation is to summarise information regarding the domain of applicability of the numerical techniques and user options that may impact the accuracy, stability and convergence features of each component code.

This step like Step 13, will indicate if further calculations must be performed. A complete assessment within this step can only be performed after completing a sufficient foundation of assessment analyses.

Step 17 addresses the review of code capability before the simulation of IETs. This applicability evaluation considers whether the integrated code is capable of modelling the plant systems and components. Before performing integrated analyses, the various EM options, special models and inputs should be determined to have the inherent capability to model the major systems and subsystems required for the particular application.

Step 18 prepares input and performs calculations to assess system interactions and global capability.

Step 19 assesses scalability of integrated calculations and data distortions.

At the end Step 20 determines biases and uncertainties in the evaluation method.

Adequacy decision

EMDAP provides a logical and auditable method to assess the applicability of an EM to an intended scenario. This approach also provides a method of quantifying the uncertainty in important phenomena and component models. These uncertainties can then be combined to provide an aggregated estimate of the uncertainty in the FOM. All 20 steps will be followed.

6. Conclusions

This report summarises basic concepts of validation and uncertainty quantification for single and multi-physics multi-scale codes. It includes a review of validation and uncertainty quantification (UQ) for single physics codes such as – core reactor physics, fuel performance, core thermal hydraulics and system thermal hydraulics. In addition, it addresses the validation approach for multi-physics codes consisting of thermal-hydraulics codes coupled with neutronics codes and fuel codes coupled with neutronics code.

The uncertainty quantification methods identified the source of uncertainty in prediction as initial condition, boundary condition and model form uncertainty. The majority of methods propagate uncertainties in initial conditions, boundary conditions and model form uncertainty through the codes to estimate the aggregate uncertainty in the quantity of interest. There are few methods that predict uncertainty in final quantity by propagation of output uncertainty from simulation of integral facilities. One method is a hybrid of these two approaches. In licensing space, the code scaling, applicability and uncertainty (CSAU), evaluation model development and assessment (EMDAP) and Gesellschaft für Anlagen- und Reaktorsicherheit gGmbH (GRS) methodologies are widely used.

The common elements of all the approaches for validation and uncertainty quantification are as follows:

- specification of plant and transient;
- frozen code with good documentation;
- a phenomena identification and ranking table (PIRT) process based on experts, scaling or sensitivity analyses;
- a test matrix consisting of separate effects and integral effects tests that represent the phenomena in the plant for the transient of interest;
- definition of plant input based on user guidelines and feedback from models for separate effect tests (SETs) and integral effect tests (IETs);
- contributors to uncertainty in figures of merit (FOMs) are initial and boundary conditions, approximation in representation of actual geometry, model form uncertainties and numerical methods. Model form uncertainty evaluation should account for scale distortion.

References

[1] Finck, P.,T. Valentine, J. Dyrda, J. Gulliford, J. Hudelot and U. Rohatgi (2016), "OECD/NEA Expert Group on Multi-Physics Experimental Data, Benchmarks and Validation", *PHYSOR 2016 Conference*, Sun Valley, ID, 1-5 May 2016.

[2] Oberkampf, W. and T. Trucano (2004), *Applied Mechanics Reviews*, Vol. 57, no. 5, pp. 345-384.

[3] Oberkampf, W. and C. Roy (2010), *Verification and Validation in Scientific Computing*, Cambridge University Press, Cambridge.

[4] Smith, K. (2008), "Studsvik Scandpower's s V&V approach for LWR reactor physics software", *Verification and Validation for Nuclear Systems Analysis Workshop*, 21-25 July 2008, Idaho Falls, Idaho, United States.

[5] Briggs, B. (2008), "The anatomy of a benchmark – Status of ICSBER and IRPhEP", *Verification and Validation for Nuclear Systems Analysis Workshop*, 21-25 July 2008, Idaho Falls, Idaho, United States.

[6] Mayhue, L., R. Milanova, H. Huria, B. Zhang, F. Franceschini, M. Ouisloumen, E. Mueller and P. Forslun Guimaraes (2008), "Qualification of NEXUS/ANC nuclear design system for PWR analysis", *PHYSOR08: International Conference on Reactor Physics, Nuclear Power: A Sustainable Resource*, Interlaken, Switzerland, 14-19 September 2008.

[7] NEA (2017), *International Handbook of Evaluated Reactor Physics Benchmark Experiments*, OECD/NEA Nuclear Science, 2017 Edition.

[8] NEA (2016), *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, OECD/NEA Nuclear Science, 2016 Edition.

[9] Hutton, J., D.J. Powney, P.K.Hutt, M.P. Knight, P. Bryce, A. Goddard, C.R. Schneidesch, D. Vantroyen, S. Bosso and O. Ergo (2000), "Comparisons of WIMS/PARTNER calculations with measurements of a range of operating PWRs", *Proceedings of PHYSOR-2000 Conference.*

[10] Cunningham, M., C. Beye, F. Panisko, P. Medvedev and G. Bema (2001), FRAPTRAN: A Computer Code for the Transient Analysis of Oxide Fuel Rods − NUREG/CR-6739, PNNL-13576, Pacific Northwest National Laboratory, Richland, WA.

[11] Moal (2010), "Advanced models for the simulation of post-DNB phenomena during reactivity initiated accidents with SCANAIR", *LWR Fuel Performance/TopFuel/WRFPM*, Orlando.

[12] Lassmann, K. (1992), "TRANSURANUS: A fuel rod analysis code ready for use", *Journal of Nuclear Materials*, Vol. 188 pp. 295-302.

[13] Veshchunov, M.S., A.l Boldyrev, V. Ozrin, V. Shestak and V. Tarasov (2011), "A new mechanistic code SFPR for modeling of single fuel rod performance under various regimes of LWR operation", *Nucl. Eng. Design*. 2011. Vol. 241. pp. 2822-2830.

[14] Veshchunov, M.S., V. Ozrin, V. Shestak, V. Tarasov, R. Dubourg and G. Nicaise (2006), "Development of the mechanistic code MFPR for modelling fission-product release from irradiated UO_2 fuel", *Nucl. Eng. Design*. 2006. Vol. 236. pp. 179-200.

[15] Geelhood, K., W. Luscher and C. Beyer (2011), "FRAPCON-4.0: A computer code for the calculation of steady-state", *Thermal-Mechanical Behavior of Oxide Fuel Rods for High Burnup* (NUREG/CR-7022, Vol. 1, PNNL-19418).

[16] NEA (2013), *RIA Fuel Codes Benchmark*, Vol. 1. No. NEA-CSNI-R-2013-7. OECD, 2013.

[17] Geelhood, K., W. Luscher, C. Beyer, J. Cuta and M. Flanagan (2011), "FRAPTRAN 1.4: A computer code for the transient analysis of oxide fuel rods", Pacific Northwest National Laboratory (PNNL), Richland, WA, US, *NUREG/CR-7023* 1 (2011).

[18] Bouloré, A., C. Struzik and F. Gaudier (2012), "Uncertainty and sensitivity analysis of the nuclear fuel thermal behavior", *Nuclear Engineering and Design* 253 (2012): 200-210.

[19] Ikonen, T. and V. Tulkki (2014), "The importance of input interactions in the uncertainty and sensitivity analysis of nuclear fuel behavior", *Nuclear Engineering and Design* 275 (2014): 229-241.

[20] Geelhood, K., W. Luscher, C. Beyer, D. Senor, M. Cunningham, D. Lanning and H. Adkins (2009), "Predictive bias and sensitivity in NRC fuel performance codes", *NUREG/CR-7001*, PNNL-17644, PNNL, Richland, WA.

[21] Rashid, J., S. Yagnik and R. Montgomery (2011), "Light water reactor fuel performance modeling and multi-dimensional simulation", *JOM* 63.8 (2011): 81.

[22] Geelhood, K. and W. Luscher (2014), "FRAPCON-3.5: A computer code for the calculation of steady-state", *Thermal-Mechanical Behavior of Oxide Fuel Rods for High Burnup, NUREG/CR*-7022, Vol. 1, Rev. 1, PNNL-19418, Vol. 1, Rev. 1.

[23] Geelhood, K.J.and W.G. Luscher (2014), "FRAPCON-3.5: Integral assessment", NUREG/CR-7022, Vol. 2, Rev. 1, PNNL-19418, Vol. 2, Rev. 1.

[24] Geelhood, K.J., W.G. Luscher and J.M. Cuta (2014), "FRAPTRAN-1.5: A computer code for the transient analysis of oxide fuel rods", NUREG/CR-7023, Vol. 1, Rev. 1 PNNL-19400, Vol. 1, Rev. 1.

[25] Geelhood, K.J. and W.G. Luscher (2014), "FRAPTRAN-1.5: Integral assessment", NUREG/CR-7023, Vol. 2, Rev. 1, PNNL-19400, Vol. 2, Rev. 1.

[26] Toptan, A., R. Salko, M. Avramova, D. Kropaczek, K. Clarno (2017), "Development and assessment of CTFFuel", CASL-U-2017-1418-000.

[27] Avramova, M. (2003), *COBRA-TF Development, Qualification, and Application to LWR Analysis*, MS Thesis, Pennsylvania State University.

[28] Salko, R. et al. (2016), *CTF Validation and Verification*, CASL-U-2016-1113-000.

[29] NEA (2006), *NUPEC BWR Full-size Fine-mesh Bundle Test (BFBT) Benchmark Volume 1: Specifications*, ISBN 92-64-01088-2, NEA No. 6212.

[30] Lahey, R.T., Jr., B.S. Shirlakar and D.W. Radcliffe (1970), *Two-Phase Flow and Heat Transfer In Multi-rod Geometries: Subchannel and Pressure Drop Measurements in a Nine-Rod Bundle for Diabatic and Adiabatic Conditions*, Technical report, GEAP-13049, General Electric.

[31] NEA (2010), *OECD/NRC Benchmark Based on NUPEC PWR Subchannel and Bundle Test (PSBT)*, NEA/NSC/DOC(2012)1.

[32] Smith, K.A., A.J. Baratta and G.E. Robinson (1995), "Coupled RELAP5 and CONTAIN accident analysis using PVM", *Nuclear Safety* 36, No. 1., 94-108.

[33] Weaver, W. (2005), *Programmers Manual for PVM Coupling Interface in RELAP5-3D Code*, INL-EXT-05-00203.

[34] Ofstun, R. and J. Scobel (2006), *Westinghouse Containment Analysis Methodology*, WCAP-16608-NP.

[35] Murata, K., D. Williams, R. Griffith, R. Gido, E. Tadios, F. Davis, G. Martinez, K. Washington and J. Tills (1997), *Code Manual for CONTAIN 2.0: A Computer Code for Nuclear Reactor Containment Analysis*, NUREG/CR-6533, SAND97-1735, Sandia National Laboratories.

[36] Hong, S., Y. Choo, S. Hwang, B. Lee and S. Ha (2015), *Development of CAP Code for Nuclear Power Plant Containment: Lumped Model*, NED, 291(2015), pp. 47-63.

[37] NEA (1987), "Code Validation Matrix of Thermo-Hydraulic Codes for LWR LOCA and Transients", CSNI Report 132, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_15784.

[38] NEA (1987), "Code Validation Matrix of Thermo-Hydraulic Codes for LWR LOCA and Transients", CSNI Report 132, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_15784.

[39] Aksan, N. (2008), "International standard problems and small break loss-of-coolant accident (SBLOCA)", *Proceedings of "THICKET 2008: Seminar on Transfer of Competence, Knowledge and Experience Gained through CSNI Activities in the field of Thermalhydraulics",* CSNI OECD/NEA, INSTN and IRSN, Pisa (Italy) 5-9 May 2008.

[40] IAEA (2001), *Validation of Accident and Safety Analysis Methodology*, International Atomic Energy Agency, Internal Technical Report, Vienna.

[41] Zuber, N. et al. (1998), "An integrated structure and scaling methodology for severe accident technical issue resolution: Development of methodology", *Nuclear Engineering and Design*, Vol. 186, Issues 1-2, 1, pp. 1-21.

[42] D'Auria, F., G. Galassi and P. Gatta (1997), "Scaling in nuclear system thermal hydraulics: A way to utilise the available database", *ASME 32nd National Heat Transfer Conference*, vol. 350, pp. 35, Baltimore, MD, United States.

[43] Ivanov, K., E. Sartori, E. Royer, S. Langenbuch and K. Velkov (2007), "Validation of coupled thermal-hydraulic and neutronic codes for safety analysis by international cooperation", *Nuclear Technology*, Vol. 157, No. 2, pp. 177-195.

[44] Avramova, M. and K. Ivanov (2010), "Verification and validation and uncertainty quantification in multi-physics modeling for nuclear reactor design", *Progress in Nuclear Energy*, 52 (2010) 601-614.

[45] Avramova, M., K. Ivanov, T. Kozlowski, I. Pasichnyk, W. Zwermann, K. Velkov, E. Royer, A. Yamaji and J. Gulliford (2015), "Multi-physics and multi-scale benchmarking and uncertainty quantification within OECD/NEA framework", *Annals of Nuclear Energy*, Invited paper, Vol. 84, pp. 178-196.

[46] Finnemann, H. and A. Galati (1991), *Final Specifications: NEACRP 3-D LWR Core Transient Benchmark*, NEACRP-L-335.

[47] NEA (1993), "NEA-NSC 3-D/1-D PWR Core Transient Benchmark Uncontrolled Withdrawal of Control Rods at Zero Power", NEA/NSC(93)9, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_16310.

[48] Kozlowski, T. and T. Downar (2006), *PWR MOX/UO2 Core Transient Benchmark*, Final Report, , NEA/NSC/DOC(2006)20, www.oecd-nea.org/jcms/pl_14074.

[49] Toptan, A., R., Salko and M. Avramova (2017), "Review of CTF's fuel rod modeling using FRAPCON-4.0's centerline temperature predictions", *Proceedings: 2017 ANS Annual Meeting*, San Francisco, CA, US, 11-15 June 2017.

[50] Magedanz, J., M. Avramova, Y. Perin and A. Velkov (2015), "High-fidelity multi-physics system TORT-TD/CTF/FRAPTRAN for light water reactor analysis", *Annals of Nuclear Energy*, Invited paper, Vol. 84, pp. 234-143.

[51] NEA (2004), *CRISSUE-S – WP2 Neutronics/Thermal-hydraulics Coupling in LWR Technology: State-of-the-art Report* (REAC-SOAR), Technical Report, www.oecd-nea.org/jcms/pl_13968.

[52] Grandi, G. and D. Hagrman (2007), *Improvements to the INTERPIN Code for High Burnup and MOX Fuel*, Vol. 97, TANSAO 97, pp. 614-615.

[53] Grandi, G. and K. Smith (2007), *SIMULATE-3K Explicit Fuel Pin Modeling in RIAs*, Vol. 96, TANSAO 96, pp. 627-629.

[54] Turner, J., K. Clarno, M. Sieger, R. Bartlett, B. Collins, R. Pawlowski, R. Schmidt and R. Summers (2016), "The virtual environment for reactor applications (VERA): Design and architecture", *Journal of Computational Physics* 326 (2016), 544-568.

[55] Avramova, M., K. Ivanov (2017), "Multi-physics modeling of nuclear reactors", *Access Science*, McGraw-Hill Global Education Holdings, LLC.

[56] Ziabletsev, D., M. Avramova, K. Ivanov (2004), "Development of PWR integrated safety analysis methodology using multi-level coupling algorithm", *Nuclear Science and Engineering*, Vol. 148, No. 3, pp.414-425.

[57] Solis, J., M. Avramova, K. Ivanov (2004), "Multi-level methodology in parallel computing environment for evaluating BWR safety parameters", *Nuclear Technology*, Vol. 146, No. 3, pp. 267-278.

[58] Schneidesch, C. and J. Zhang (2004), "Qualification of the coupled RELAP5/PANTHER/COBRA code package for licensing applications", *Proceedings of International Meeting on Updates in Best-Estimate Methods in Nuclear Installation Safety Analysis (BE-2004)*, Washington, DC, 14-18 November 2004.

[59] IAEA (2008), "Best estimate safety analysis for nuclear power plants: Uncertainty evaluation", *IAEA Safety Reports Series* No. 52, IAEA, Vienna.

[60] Cacuci, D. (2003), "Sensitivity and uncertainty analysis Volume 1 Theory", *Chapman & Hall/CRC*.

[61] Glaeser, H. (2008), "GRS method for uncertainty and sensitivity evaluation of code results and applications", *Science and Technology of Nuclear Installations*, Vol. 2008, Article ID: 798901.

[62] Petruzzi, A. and F. D'Auria (2008), "Approaches, relevant topics and internal method for uncertainty evaluation in predictions of thermal-hydraulic system codes", *Science and Technology of Nuclear Installations*, Vol. 2008, Article ID 325071.

[63] Triola, M. (2007), *Elementary Statistics Using Excel*, 3rd edition, Pearson Education, Boston 2007.

[64] Hofer, E., M. Kloos, B. Krykacz-Hausmann, J. Peschke and M. Woltereck (2002), "An approximate epistemic uncertainty analysis approach in the presence of epistemic and aleatory uncertainties", *Reliability Engineering and System Safety* 77 (2002), 229-238.

[65] Helton, J. and F. Davis (2002), "Illustration of sampling-based methods for uncertainty and sensitivity analysis", *Risk Analysis*, Vol. 22, No. 3.

[66] USNRC (1988), *Emergency Core Cooling Systems, Revisions to Acceptance Criteria*, Federal Register 53, 180.

[67] Boyack, B. et al. (1989), *Quantifying Reactor Safety Margins*, NUREG/CR-5249, R4.

[68] Rohatgi, U., J. Jo, L.Y. Neymotin and W. Wulff (1989), *Bias in Peak Clad Temperature Predictions Due to Uncertainties in Modeling of ECC Bypass and Dissolved Non-Condensable Gas Phenomena*, NUREG/CR-5254, BNL-NUREG-52168.

[69] Weiss, P., R. Emmerling, R. Hertlein and J. Liebert (1994), "UPTF experiment refined PWR LOCA thermal-hydraulic scenarios: Conclusions from a full-scale experimental program", *Journal of Nuclear Engineering and Design*, Vol. 149, Issues 1–3, 1 September 1994, pp. 335-347.

[70] Nalezny, C.L. (1983), *Summary of Nuclear Regulatory Commission's LOFT Program Experiments*, NUREG/CR-3214, EGG-2248.

[71] Murao, Y., T. Iguchi, H. Akimoto and T. Iwamura (1993), "Large-scale multi-dimensional phenomena found in CCTF and SCTF experiments", *Nuclear Engineering and Design*, Vol. 145, Issues 1-2, 2 November 1993, pp. 85-95.

[72] Umminger, K. (2012), "Integral test facility PKL: Experimental PWR accident investigation", Review Article, Hindawi Publishing Corporation, *Science and Technology of Nuclear Installations*, Vol. 2012, Article ID 891056, 16 pages, DOI:10.1155/2012/891056.

[73] Hofer, E. (1993), *Probabilistische Unsicherheitsanalyse von Ergebnissen umfangreicher Rechenmodelle*, GRS-A-2002.

[74] Wilks, S. (1941), "Determination of sample sizes for setting tolerance limits", *Ann. Math. Statist.*, 12, pp. 91-96.

[75] Guba, M., M. Makai and L. Pai (2003), "Statistical aspects of best estimate methods", *Reliability Engineering and System Safety*, Vol. 80, No 3, pp. 217-232.

[76] Zwermann, W., B. Krzykacz-Hausmann, L. Gallner and A. Pautz (2009), "Influence of nuclear covariance data on reactor core calculations", *Proc. WONDER 2009*, Saint-Paul-Lez-Durance, France, 29 September – 2 October 2009.

[77] Williams, M., G. Ilas, M.A. Jessee, B.T. Rearden, D. Wiarda, W. Zwermann, L. Gallner, M. Klein, B. Krzykacz-Hausmann and A. Pautz (2013), "A statistical sampling method for uncertainty analysis with SCALE and XSUSA", *Nucl. Techn*. 183, pp. 515-526.

[78] Krzykacz, B., E. Hofer and M. Kloos (1994), "A software system for probabilistic uncertainty and sensitivity analysis of results from computer models", *Proceedings of International Conference on Probabilistic Safety Assessment and Management (PSAM-II)*, San Diego, CA, US.

[79] ORNL (2011), *SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design*, ORNL/TM-2005/39, Version 6.1.

[80] Bostelmann, F., F.-P. Weiss, A. Aures, K. Velkov, W. Zwermann, B. Rearden, M.A. Jessee, M. Williams, D. Wiarda and W. Wieselquist (2015), "Uncertainty and sensitivity analysis in criticality calculations with perturbation theory and sampling", *Proceedings of Joint International Conference and Mathematics and Computation (M&C), Supercomputing in Nuclear Applications (SNA) and the Monte Carlo (MC) Method*, Nashville, TN, US, 19-23 April 2015, on CD-ROM.

[81] Bostelmann, F., W. Zwermann, B. Krzykacz-Hausmann, L. Gallner, A. Aures and K. Velkov (2015), "Sampling-based nuclear data uncertainty analysis in criticality and depletion calculations", *Proc. ANS MC2015*, Nashville, TN, US, 19-23 April 2015.

[82] Hofer, E., M. Kloos, B. Krzykacz-Hausmann, J. Peschke and M. Woltereck (2002), "An approximate epistemic uncertainty analysis approach in the presence of epistemic and aleatory uncertainties", *Reliability Engineering and System Safety* 77 (2002), 229-238.

[83] Glaeser, H. (2008), "GRS method for uncertainty and sensitivity evaluation of code results and applications", *Science and Technology of Nuclear Installations*, Vol. 2008, Article ID: 798901.

[84] Kloos, M. (2015), "Main features of the tool SUSA 4.0 for uncertainty and sensitivity analyses", *ESREL 2015, European Safety and Reliability Conference*, Zürich, Switzerland, 7-10 September 2015.

[85] Frepoli, C. (2007), *A Review of Westinghouse Realistic Large Break LOCA Evaluation Model*, Hindawi Publication, August 2007.

[86] Martin, R., L. O'Dell (2007), *Development Considerations of AREVA NP Inc's Realistic LBLOCA Analysis Methodology*, Hindawi Publication, December 2007.

[87] D'Auria, F., G. Giorgio and N. Debrecin (1995), "Outline of the uncertainty methodology based on accuracy extrapolation (UMAE)", *J. Nuclear Technology*, 109, No 1, pp. 21-38.

[88] Ambrosini, W., R. Bovalini and F. D'Auria (1990), "Evaluation of accuracy of thermal-hydraulic codes calculations", *J. Energia Nucleare*, **7**, No. 2.

[89] Petruzzi, A., F. D'Auria (2005), *Accuracy Quantification: Description of the Fast Fourier Transform Based Method (FFTBM)*, DIMNP NT 556(05).

[90] NEA (1997), *Proceedings of the OECD/CSNI Workshop on Transient Thermal-hydraulic and Neutronic Codes Requirements*, Annapolis NEA/CSNI R(97)4, Washington, DC, US, www.oecd-nea.org/jcms/pl_16162.

[91] D'Auria, F., W. Giannotti (2000), "Development of code with capability of internal assessment of uncertainty", *J. Nuclear Technology*, 131, No. 1, pp. 159-196.

[92] Petruzzi, A., F. D'Auria, W. Giannotti and K. Ivanov (2005), "Methodology of internal assessment of uncertainty and extension to neutron-kinetics/thermal-hydraulics coupled codes", *Nuclear Science and Engineering*, 149, pp. 1-26.

[93] Petruzzi, A., F. D'Auria (2008), "Thermal-hydraulic system codes in nuclear reactor safety and qualification procedures", Hindawi Publishing Corporation, *Science and Technology of Nuclear Installations*, Vol. 2008, Article ID 460795.

[94] Petruzzi, A., F. D'Auria, W. Giannotti and K. Ivanov (2004), "Enlargement of the uncertainty database of the CIAU methodology", *PHYSOR 2004*, Chicago, Illinois, US.

[95] Petruzzi, A., W. Giannotti, F. D'Auria (2004), "Development, qualification and use of a code with the capability of internal assessment of uncertainty", *CNS, Sixth International Conference on Simulation Methods in Nuclear Engineering*, Montreal, Canada.

[96] Petruzzi, A., F. D'Auria (2016), "Standardized consolidated calculated and reference experimental database (SCCRED): A supporting tool for V&V and uncertainty evaluation of best-estimate system codes for licensing applications", *Nuclear Science and Engineering*, 15-79.

[97] Bovalini, R., F. D'Auria, M. Leonardi (1992), *Qualification of the Fast Fourier Transform based Methodology for the Quantification of Thermal-hydraulic System Code Accuracy*, DCMN NT 194(92), Pisa.

[98] D'Auria F., G.M. Galassi (1998), "Code validation and uncertainties in system thermal-hydraulics", *J. Progress in Nuclear Energy*, 33, No. 1 and 2, pp. 175-216.

[99] NEA (1989), *Thermo-hydraulics of Emergency Core Cooling in Light Water Reactors-A State of the Art Report*, NEA/CSNI 161, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_15836.

[100] D'Auria, F., V. Faluomi, N. Aksan (1995), *A Proposed Methodology for the Analysis of a Phenomenon in Separate Effects and Integral Test Facilities*, Kerntechnik, 60, 4, 166.

[101] D'Auria, F., V. Pellicoro (1995), "Scaling and uncertainty in BWR instability problem", *2nd Regional Meeting*, Nuclear Energy in Central Europe, Portoroz, Slovenia, 11-14 September 1995.

[102] Groeneveld, D.C., L.K.H. Leung, P.L. Kirillov, V.P. Bobkov, I.P. Smogalev, V.N. Vinogradov, X.C. Huang and E. Royer (1996), "The 1995 look-up tables for critical heat flux in tubes", *J. Nuclear Engineering and Design*, 163, 1,1.

[103] Cacuci, D.G., M. Ionescu-Bujor (2010), "Sensitivity and uncertainty analysis, data assimilation and predictive best-estimate model calibration", Chapter 17 in Vol.3, pp. 1913-2051, *Handbook of Nuclear Engineering*, D.G. Cacuci, Editor, ISBN: 978-0-387-98150-5, Springer New York/Berlin.

[104] Cacuci, D.G., M. Ionescu-Bujor (2010), "Model calibration and best-estimate prediction through experimental data assimilation: I. Mathematical framework", *Nucl. Sci. Eng*., 165, 18-44.

[105] Cacuci, D.G. (2003), "Sensitivity and uncertainty analysis", Theory, Vol. I, *Chapman & Hall/CRC*, Boca Raton (Fl, US), ISBN 1-58488-115-1.

[106] Cacuci, D.G., M. Ionescu-Bujor, I.M. Navon (2005), "Sensitivity and uncertainty analysis, application to large scale systems", Vol. II, *Chapman & Hall/CRC*, Boca Raton (Fl, US), ISBN-10 1-58488-116-X.

[107] Petruzzi, A. (2008), *Development and Application of Methodologies for Sensitivity Analysis and Uncertainty Evaluation of the Results of the Best Estimate System Codes Applied in Nuclear Technology*, PhD Thesis, University of Pisa.

[108] Petruzzi, A., D.G. Cacuci, F. D'Auria (2010), "Model calibration and best-estimate prediction through experimental data assimilation: II. Application to a blowdown benchmark experiment", *Nucl. Sci. Eng*., 165, 45-100.

[109] Petruzzi, A., F. D'Auria (2014), "Uncertainties in predictions by system thermal-hydraulic codes: The CASUALIDAD method", *10th International Topical meeting on Nuclear*

Thermal-Hydraulics, Operation and Safety (NUTHOS-10), 14-18 December 2014 Okinawa, Japan.

[110] Petruzzi, A., F. D'Auria (2005), "Development, qualification and use of the CIAU method for internal assessment of uncertainty in system codes", *Nureth-11*, Avignon, (F).

[111] Bovalini, R., F. D'Auria (1993), "Scaling of the accuracy of Relap5/mod2 code", *J. Nucl. Eng. & Des.* 139, pp. 187-204.

[112] Cacuci, D.G. (2006), "On the use of adjoint operators for global optimization and data assimilation", Lectures Notes, *Workshop on Predictability, Observations, and Uncertainties in Geosciences*, Tallahassee (Fl, US), 13-15 March 2006.

[113] Pourgol-Mohammad, M., A. Mosleh, M. Modarres (2007), *Integrated Methodology for Thermal-Hydraulics Code Uncertainty Analysis*, A. James Clark School of Engineering, University of Maryland at College Park, March 2007.

[114] SEC NRS (2016), *General Safety Provisions for Nuclear Power Plants*, OPB-88/97; NP-001-15, approved by Rostechnadzor on 17 December 2015.

[115] Gosatomnadzor (2000), *Requirements to Composition and Contents of Report on Verification and Justification of Software Applied for Nuclear Facilities Safety Analysis*, RD-03-34-2000, approved by Gosatomnadzor of Russia on 28 December 2000.

[116] Bogdan, S.N. et al. (2016), "Updating of regulatory requirements to software applied at nuclear facilities safety analysis", *Rostechnadzor Council on software certification: 25 years on safety service*, Collection of publications, Works of SEC NRS. – M.: SEC NRS.

[117] Bogdan, S., O. Kovalevich, N. Kozlova, S. Shevchenko and D. Yashnikov (2017), "About the calculation error evaluation in the framework of the nuclear facilities safety analysis", *Nuclear and Radiation Safety*, No. 2 (84)-2017, Moscow.

[118] Moiseenko, E.V., A.S. Filippov (2011), "A methodology for multivariate simulation with massively parallel computing systems for NPP safety assessment: VARIA code", *Journal of Engineering Thermophysics*, 2011, Vol. 20, No. 3, pp. 249-259.

[119] Moiseenko, E.V., A. Filippov, N. Drobyshevsky, V. Strizhov and A.E. Kisselev (2011), "VARIA − An application for mass computing and statistical analysis of the simulation results in BEPU safety assessment", *Proceedings of ICONE-19*, 24-25 October 2011, Osaka, Japan, ICONE-43435.

[120] Petruzzi, A., F. D'Auria, J. Micaelli, A. De Crecy and J. Royen (2004), "The BEMUSE programme (Best-Estimate Methods – Uncertainty and Sensitivity Evaluation)", *International Meeting on Best-Estimate Methods in Nuclear Installation Safety Analysis* (BE-2004) IX, Washington D.C. (US), 14-18 November 2004.

[121] NEA (2006), *BEMUSE Phase II Report: Re-Analysis of the ISP-13 Exercise, Post Test Analysis of the LOFT L2-5 Test Calculation*, Report NEA/CSNI/R(2006)2, www.oecd-nea.org/jcms/pl_18346/.

[122] NEA (2007), *BEMUSE Phase III Report, Uncertainty and Sensitivity Analysis of the LOFT L2-5 Test*, NEA/CSNI/R(2007)4, 11 October 2007, www.oecd-nea.org/jcms/pl_18442 .

[123] NEA (2011), *BEMUSE Phase VI Report, Status Report on the Area, Classification of the Methods, Conclusions and Recommendations*, NEA/CSNI/R(2011)4, 28 March 2011, www.oecd-nea.org/jcms/pl_19020.

[124] NEA (1998), *Report of the Uncertainty Method Study for Advanced Best Estimate Thermal-hydraulic Code Applications*, OECD/NEA/CSNI R (97) 35, I and II.

[125] NEA (2016), "PREMIUM, a Benchmark on the quantification of the uncertainty of the physical models in the system thermal-hydraulic codes: methodologies and data review", NEA/CSNI/R(2016)9, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_19720.

[126] Bratton, R., M. Avramova, K. Ivanov (2014), "Benchmark for uncertainty analysis in modeling (UAM) for LWRs − Summary and discussion of neutronics cases (Phase I)", *Nuclear Engineering and Technology (NET)*, Vol. 46 No. 3, pp. 313-349, Special Issue on Neutronics Sensitivity and Uncertainty Analysis, Invited paper.

[127] NEA (1996), *Integral Test Facility Validation Matrix for the Assessment of Thermal-Hydraulic Codes for LWR LOCA and Transients*, OCDE/GD(97)12, NEA/CSNI/R(96)17, www.oecd-nea.org/jcms/pl_16134.

[128] NEA (1994), *Separate Effects Test Matrix for Thermal-Hydraulic Code Validation Volume I, Phenomena Characterization and Selection of Facilities and Tests*, OECD/GD(94)82, OECD publishing, Paris, www.oecd-nea.org/jcms/pl_15968.

[129] NEA (1994), *Separate Effects Test Matrix for Thermal-Hydraulic Code Validation Volume II, Facilities and Experiment Characteristics*; OECD/GD(94)83, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_15968.

[130] Petruzzi, A., F. D'Auria (2016), "Standardized consolidated calculated and reference experimental database (SCCRED): A supporting tool for V&V and uncertainty evaluation of best-estimate system codes for licensing applications", *Nuclear Science and Engineering*, 182.

[131] NEA (2006), *BEMUSE Phase II Report: Re-Analysis of the ISP-13 Exercise, Post Test Analysis of the LOFT L2-5 Test Calculation*, NEA/CSNI/R(2006)2, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_18346.

[132] Wang, C., S. Schunert, P. Talbot, B. Baker, Y. Wang, J. Ortensi, F. Gleicher, M. DeHart and C. Rabiti (2017), "Uncertainty and sensitivity analysis of TREAT transient test #15", *Proceedings of the 2017 American Nuclear Society Annual meeting*, San Francisco.

[133] Talbot, P., C. Wang, C. Rabiti and A. Prinja (2016), "Multistep input reduction for high dimensional uncertainty quantification in RAVEN code", *Proceeding of PHYSOR 2016*.

[134] Schunert, S., C. Wang, Y. Wang, F. Kong, J. Ortensi, B. Baker, F. Gleicher, M. DeHart and R. Martineau (2017), "A generalized perturbation theory solver in Rattlesnake based on PETs with application to TREAT steady state uncertainty quantification", submitted to *M&C 2017*.

[135] NEA (2016), *Benchmark for Uncertainty Analysis in Modelling (UAM) for Design, Operation, and Safety Analysis of LWRs, Volume 2: Specification and Support Data for the Core Cases (Phase II)* − Version 2, NEA/NSC/DOC(2012)11, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_71109.

[136] Porter, N. (2015), *Sensitivity and Uncertainty Study of CTF Using the Uncertainty Analysis in Modeling Benchmark*, MS Thesis, Pennsylvania State University.

[137] Porter, N., M. Avramova, K. Ivanov (2015), "Uncertainty and sensitivity analysis of COBRA-TF for the OECD LWR UAM benchmark using Dakota", *Proc. Int. Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH)*, Chicago, IL, 30 August − 4 September 2015, American Nuclear Society.

[138] Morris, M. (1991), "Factorial sampling plans for preliminary computational experiments", *Technometrics*, 33, 161.

[139] Porter, N., M. Avramova (2016), "Uncertainty analysis of CTF for the uncertainty analysis in modeling benchmark", *Proc. Winter Meeting and Nuc. Tech. Expo*., Las Vegas, NV, 6-10 November 2016, American Nuclear Society.

[140] Porter, N., M. Avramova, V. Mousseau (2017), *Uncertainty Quantification Study of CTF for the Uncertainty Analysis in Modeling Benchmark*, NCSU.

[141] Avramova, M., K. Ivanov (2017), "Approach for testing multi-physics uncertainty propagation in reactor core calculations within the framework of OECD/NEA LWR UAM benchmark", *Proceedings: 48th Annual Meeting on Nuclear Technology (AMNT 2017*), 16-17 May 2017, Berlin, Germany.

[142] Petruzzi, A., M. Cherubini, F. D'Auria, M. Lanfredini and O. Mazzantini (2016), "The BEPU evaluation model with RELAP5-3D for the licensing of the Atucha-II NPP", *Nuclear Technology* Vol. 193, 2016 − Issue 1, pp. 113-160.

[143] Wilson, G., B. Boyack (1998), "The role of PIRT process in experiments, code development and code applications associated with reactor safety analyses", *Nuclear Engineering and Design*, Vol. 186.

[144] Wulff, W., N. Zuber, U. Rohatgi, I. Catton (2009), "Application of Fractional Scaling Analysis (FSA) to loss of coolant accidents (LOCA); system level scaling for system depressurization", *ASME Journal Fluids Engineering*, August 2009, Vol. 131.

[145] Luo, H. (2012), *Quantified PIRT and Uncertainty Quantification for Computer Code Validation*, Ph.D thesis, Oregon State University.

[146] Shaw, R.A., S.Z. Rouhani, T.K. Larson and R.A. Dimenna (1988), *Development of a Phenomena Identification and Ranking Table (PIRT) for Thermal-Hydraulic Phenomena during a PWR Large-Break LOCA*, NUREG/CR-5074, USNRC, August 1988.

[147] NRC (1989), *Best-Estimate Calculations of Emergency Core Cooling System Performance*, Regulatory Guide 1.157.

[148] NRC (2005), *Transient and Accident Analysis Methods*, Regulatory Guide 1.203.

[149] Boyack, B. et al. (1991), *An Integrated Structure and Scaling Methodology for Severe Accident Technical Issue Resolution*, Draft NUREG/CR-5809, USNRC, November 1991.

[150] Zuber, N. et al. (1998), "An integrated structure and scaling methodology for severe accident technical issue resolution: Development of methodology", *Nuclear Engineering and Design*, 186 (pp. 1-21).

[151] Wilson, G., B.E. Boyack (1998), "The role of the PIRT process in experiments, code development and code applications associated with reactor safety analysis", *Nuclear Engineering and Design*, 186 (pp. 23-37).

[152] Wulff, W. (1994), *Uncertainty Analysis of Suppression Pool Heating during an ATWS in a BWR-5 Plant*, NUREG/CR-6200, USNRC, March 1994.

[153] Watkins, J.C., L.S. Ghan (1992), *AHP Version 5.1, User's Manual*, EGG-ERTP-10585, Idaho National Engineering Laboratory, October 1992.

[154] Holmström, H., H. Glaeser, A. Wickett and G. Wilson (1994), "Status of code uncertainty evaluation methodologies", *Proceedings of the International Conference on New Trends in*

Nuclear System Thermohydraulics, Dipartimento di Costruzioni Meccaniche Nucleari, Pisa, Italy.

[155] Reyes, J., L. Hochreiter (1998), "Scaling analysis for the OSU AP600 test facility (APEX)", *Nuclear Engineering and Design*, 186 (pp. 53-109), 1 November 1998.

[156] Banerjee, S., M. Ortiz, T. Larson and D. Reeder (1998), "Scaling in the safety of next generation reactors", *Nuclear Engineering and Design*, 186 (pp. 111-133), 1 November 1998.

[157] Ransom, V., W. Wang and M. Ishii (1998), "Use of an ideal scaled model for scaling evaluation", *Nuclear Engineering and Design*, 186 (pp. 135-148), 1 November 1998.

[158] Ishii, M. et al. (1998), "The three-level scaling approach with application to the Purdue University Multi-Dimensional Integral Test Assembly (PUMA)", *Nuclear Engineering and Design*, 186 (pp. 177-211), 1 November 1998.

[159] Fletcher, C.D. et al. (1997), *Adequacy Evaluation of RELAP5/MOD3, Version 3.2.1.2 for Simulating AP600 Small Break Loss-of-Coolant Accidents*, INEL-96/0400 (nonproprietary version), April 1997.