Panel discussion role of a phenomenological validation and integral experiments for maturing the predictive simulations

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PANEL DISCUSSION: ROLE OF A PHENOMENOLOGICAL VALIDATION AND INTEGRAL EXPERIMENTS FOR MATURING THE PREDICTIVE SIMULATIONS

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ABSTRACT

Best Estimate Plus Uncertainty (BEPU) in its basis pretends on an exact use of high-fidelity simulations in a process of safety assessment. Despite on shared definition of BEPU has not been yet presented it seems to be a Decision Making (DM) support tool. BEPU needs, of course, in a consistent experiment-based UQ otherwise it could make a little sense for characterization of safety margins and, in its order, in safety assessment. Panel discussion stresses the needs to provide consistent system of criteria intended to prioritize existing IEs with respect to their impacts on V&UQ process. Given that IEs bring unique objective information inaccessible via differential experimentation one can see that to make this information useful IEs should be evaluated quantifying total uncertainties of each single IE and correlations between IE cases.

1. INTRODUCTION

Best Estimate Plus Uncertainty (BEPU) might be considered as an approach which presume reliance on simulation in a safety assessment process. In other words, assessor using BEPU complements of even replaces subjective experts' elicitations by modelling. These modelling, in its order, must have a solid basis in evidence, e.g. all tools to be accepted for safety assessment shall be thoroughly validated against representative sets of Integral Experiments (IEs). Scientific community subtracts [1] s an importance of consistent evaluation of IEs including benchmark experiments, experimental mock-ups or Plant Measurements and Observation (PMO).

2. BEPU SWOT ANALYSIS

Since BEPU means wide use of simulations its advantages and disadvantages are close to ones of simulations. Simply talking BEPU advantages are in predictive capabilities of modelling while disadvantages are in limited opportunity to prove a credibility of such prediction (see below).

2.1 Strength and weakness of BEPU

Any mechanistic tool going deeply in the detail matters helps to better understand essential items and to programming dedicated Researches and Developments (R&Ds).

In other words an approach like BEPU has a rationale in progressive objectivization of assessment minimising human-errors.

Unfortunately such objective seems unachievable due to many reasons. One of them is a kind of unity of opposites where all potential IEs form a countable set while decision should be taken in a continuous universe. BEPU does not eliminate experts' judgments but turns them from assessment to planning of V&UQ and to selection of IEs using expert-based PIRT and QPIRT[1].

In addition there is non-formalized part of knowledge associated with unique expert competences. So BEPU requires new level of competence of experts not ignoring expertise at all.

2.2 Opportunities and threats related to BEPU

Reliance on simulation, first of all, will be attractive for newcomers since they have a limited access to an excellence of expertise. Using BEPU it would be possible to compensate lack of expertise by comprehensive and predictive simulation. Reliance on simulation could help experienced assessors as well to examine mistaken believe.

It requires, as it was mentioned above, deployment of comprehensively validated tools as far as the only validated one might be a tool for user while non-validated one should be considered as a tool for developers/researches.

At the same time "safety leadership" (being essential for regulation) presumes understanding in detail matters as phenomena as rationale behind the judgments. BEPU doesn't provide such information by default – it should be extracted and learned separately. Of course, assessor should be aware of the V&UQ basis (methodology and list of IEs) otherwise assessor could face a risk to miss essential factors that would be invisible on the basis of existing experiments and simulations.

In addition there is a domain where all of us are newcomers. It is domain of innovations and advanced technologies. Absence of experts' background shall be replaced by imitative modelling and mechanistic simulation where BEPU would remain for long term the only way to support assessment. However its overuse leads to stimulated degradation of consistency and excellence of expertise.

2.3 Table of preliminary analysis of SWOT of BEPU approach to safety assessment

Summarising the reasoning presented above we can propose one synthetic diagram on SWOT analysis relatively to the BEPU approach implementation in practice of safety assessment (see Figure 1).

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[1] PIRT and QPIRT are expert panel studies that mean Phenomena Identification and Ranking Table (PIRT) and Quantified PIRT respectively.

Strength	**Weakness**
Prediction of consequences and system behaviour using mechanistic high-fidelity modelling	All statements shall be validated against representative objective observations while the term of representativity is not clear yet
An opportunity to go more deeply in details better identifying the sources of threats as well as the parameters needed to risk management	The limited resolution of high-fidelity tools resulted from complexity of extrapolation relevant to Best estimate modelling
Objectivization of judgement minimising human-error in a preparatory phase of Decision making process	Requires specific knowledge management (new competences are needed); has limits using non-formalized experts' elicitations
Opportunities	**Threats**
Objectivization of assessment facilitate new-comers to perform consistent safety assessment	Near term: risk of missing essential factors that are not visible on the basis of existing experiments and simulations
Allows assessing in a conformable way such concepts where past-experience might be in-effective like innovative and advanced ones	Long term: BEPU application could result in accelerated degradation of expertise consistency

Figure 1 – Brief SWOT analysis of BEPU.

On the basis of SWOT we can see that the major issues relay in certain extent to experimental validation, to selection or design of representative experiments and to methodology in a wide sense of uncertainty quantification and extrapolation.

3. KNOWLEDGE MANAGEMENT IN SAFETY ASSESSMENT

The idea to combine the best estimate values with their uncertainties is not only a nuclear engineering prerogative. Bibliography on BEPU provides with numerous references mainly relied to financial or actuary mathematics, or to decision making process. They all agree on predictive capabilities of best estimate tools presuming at the same time that quality of prediction can be characterized by precisely quantified uncertainties.

Since BEPU is a decision making support tool its outlines should be pragmatic ones, i.e. no ambiguity might be allowable in safety margins characterization using BEPU

Decision making process (using BEPU) should have a solid basis on reality, i.e. it should be phenomenologically validated involving representative sets of integral experiments. Thus a metrics for BEPU analysis could be based on the following main axes:

- Availability of a best estimate tool, a correct set of input data and a suitable algorithm for best estimate modelling process,
- Existence and affordability of representative high-fidelity experiments suitable for comprehensive testing of the best estimate tool in a given application domain,

- Multi-lateral and / or international consensus of specific validation methodology for a given application domain.

For BEPU the major challenges stand alongside with the major advantages. Objectivization of simulation and uncertainty quantification require confirmation on the basis of observations and experiments.

We are talking over here about the latest bullet focusing on experimental support of V&UQ. We would tackle various issues on how numerous and of what quality experiments should be and how far they should be evaluated in order to provide solid basis for experimental validation of complex best estimate tools.

4. EXPERIMENTAL DATA FOR VALIDATION

V&UQ (and BEPU in its order) has heavily reliance to availability of representative experimental data, while the degree of representativity should be based (multi-physics case) on panel studies (PIRT and QPIRT).

There would be one unresolved issue over there if an assessor will ignore experiments because they are in-affordable ore are under proprietary constraints or assessor will use a proprietary data unavailable for cross-check. So the question is whether or not such ignorance would compromise credibility of a V&UQ process.

Although normally Validation and Uncertainty Quantification (V&UQ) process should accepts all kinds of experiments if they are consistently evaluated, it would be better to include in V&UQ only representative ones reducing computational efforts and duration of testing. In this field, it is necessary first a critical review of existing experimental databases in each area and, successively, to establish/ agree criteria for use of available experiments (availability of documentation, robustness of experimental uncertainty assessment; relevance; similarity/‘‘representativity’’ etc.).

5. ADDING VALUE THROUGH MUTUALISATION OF EFFORTS

It is also a consensual statement that collaborations within international frameworks add credibility of V&UQ merging different visions and mentalities as well as engineering cultures. There are numerous examples of such collaboration while Panel Discussion touches some of them [1], [5], [6], [11], [12].

5.1 Reactor physics and criticality studies

First topic to be discussed is a status of V&UQ for neutronics and reactor physics tools. Domain of neutronics has been more deeply elaborated than others because only in neutronics there are available high-fidelity and precise codes like Monte-Carlo continuous energy [1] etc. It should be noted that nowadays users are provided with all kinds of precise modelling including perturbation theory ones. One should distinguish two aspects of modelling: 1) stand-alone computations, and 2) modelling within a multi-physics tool.

There is no, therefore, methodological issues except for computational time and credibility of a nuclear data (ND). The first one - the problem of lapsed time - can be solved with progressive growing of computational capabilities and the second one – ND uncertainties - by systematic theoretical and experimental researches.

5.1.1 Criticality and stand-alone reactor physics modules

Bottle neck in V&UQ is existence of a robust theoretical model [1] that fully available for such linear-physics domains as criticality safety and stand-alone reactor physics. The decades of persistent efforts have been completed by fully physics-based V&UQ Bayesian methodology (scientifically-driven one [1])[2]. The methodology can include as deterministic - like Generalized Linear Least Square Method (GLLSM) [1], [3] - as probabilistic algorithms.

Deterministic – GLLSM - [1], [2], [5] uses ND covariance matrices (C_{ND}) as a first guess, observations - Calculation-to-Experiment ratio (C/E) – uncertainties of calculations and experimental data, experimental data covariance matrices (C_{IE}) and sensitivity coefficients (S_C) computed using precise tools. DA[3] translates initial C_{ND} (Figure 2a) onto posterior one reducing uncertainties and generating cross-covariance terms in C_{ND} (Figure 2b) . DA outlines expected bias, uncertainties and matrix of similarities between IEs cases and applications (Figure 2c).

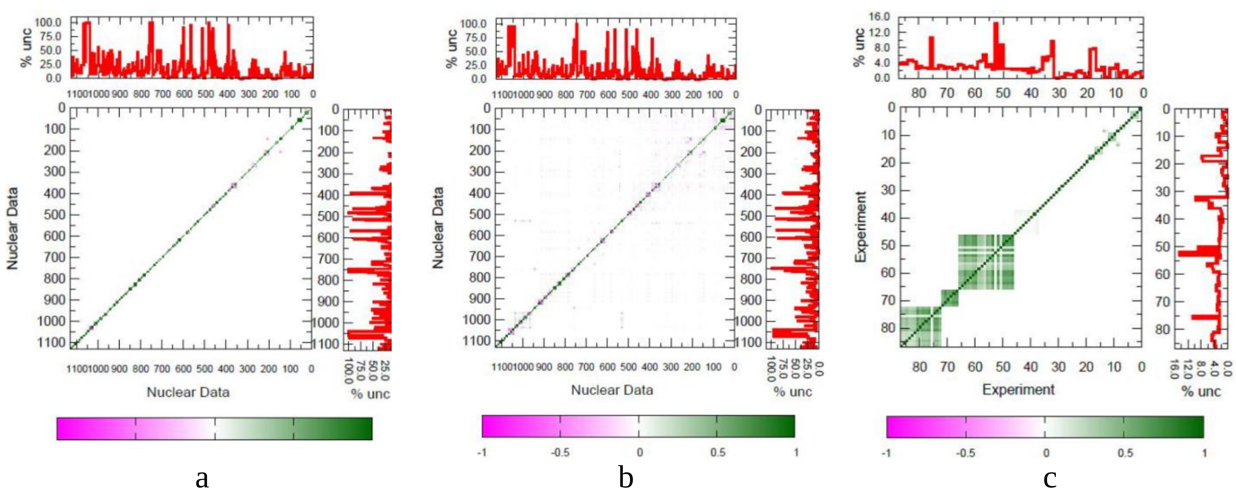

Figure 2 ND covariance matrices before (a) and after calibration (b), and posterior C_{IE} (c) [1]

Typically outlined uncertainties become of the same order as of IEs, i.e. tenfold cut in comparison with the first guess. Mentioned above cross-covariance terms are appearing exactly due to this reduction [1].

One should note that (GLLSM) and (DA) techniques have been included in SCALE code system [2] and practically deployed in the US and Canada.

5.1.2 Progressive validation of multi-physics simulations

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[2] It should be noted that modern status of computational models and tools confirms disappearance of all sources of uncertainties to be associated with tools except for ones due to nuclear data (ND). Indeed uncertainties of nuclear data in reactivity and reaction rates computations are factor of ten higher than ones of measurements and of factor of hundred higher than residual in high-fidelity computations.

[3] GLLSM as well as any Bayesian approach is a partial case of a Data Assimilation

Albeit the theory of V&UQ for stand-alone neutronics and reactor physics is practically completed there is not yet clarity concerning validation of neutronic models incorporated in a multi-physics environment.

First of all multi-physics tools are not precise since coupling brings approximations. Then boundary conditions for single-physics model are different for stand-alone tool and for ones incorporated in another complex tool. It evident, also, that optimized V&UQ depends on how modules will be merged – whether it would be explicit or implicit coupling.

If coupling is explicit ones (like in the most popular multi-physics projects - CASL and NEAMS [3], Figure 3) each modules are pre-validated for stand-alone applications. The only needed is to test the emerging phenomena of coupling.

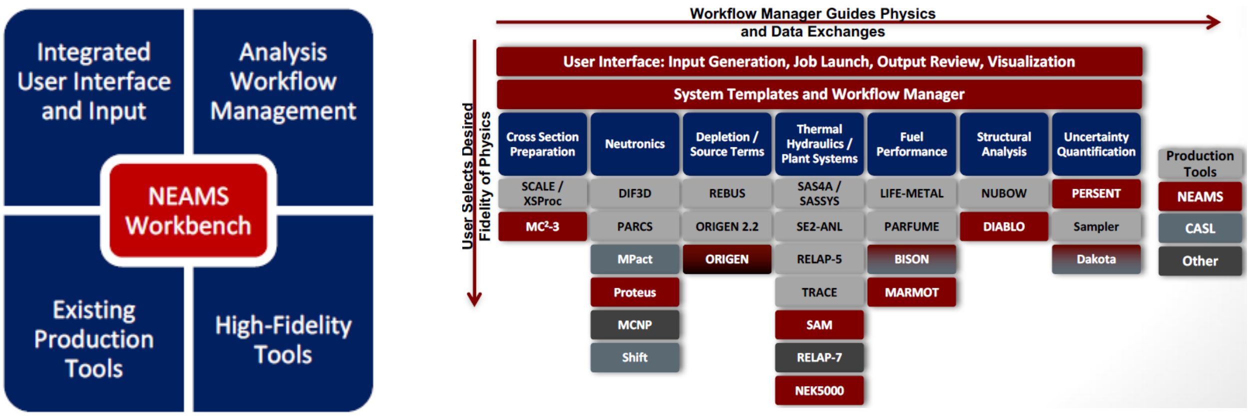

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Figure 3 – NEAMS workbench environment to use modules pre-validated for stand-alone applications [3]

So validation for single-physics modules of coupled codes needs in another methodology that one accepted for stand-alone ones. At the same time it does not preclude the needs in statistically significant, i.e. numerous, sets of representative multi-physics experiments while the latest ones might be much costly in comparison with what exists [1], [2] for single physics.

5.2 Major challenges in system thermal hydraulics

Uncertainty assessment associated with Best-Estimate (BE) calculations has become of prime importance in nuclear safety studies. If uncertainty propagation methods are now considered as mature for industrial applications, several open issues need to be tackled when dealing with input uncertainty quantification (IUQ). In order to progress on this topic, the OECD/NEA PREMIUM [6] ("Post-BEMUSE Reflood Models Input Uncertainty Methods") benchmark (2012-2015) was organized as a first step towards the development and the application of model IUQ methods. However, the analysis of PREMIUM Phases III and IV has shown a large dispersion of participants' results (Figure 4). Moreover, the results were not satisfactory when moving from the FEBA tests to PERICLES tests that were used respectively to quantify and validate input uncertainties.

One main reason could be attributed to the lack of common consensus and practices in the followed process and method (Figure 5).

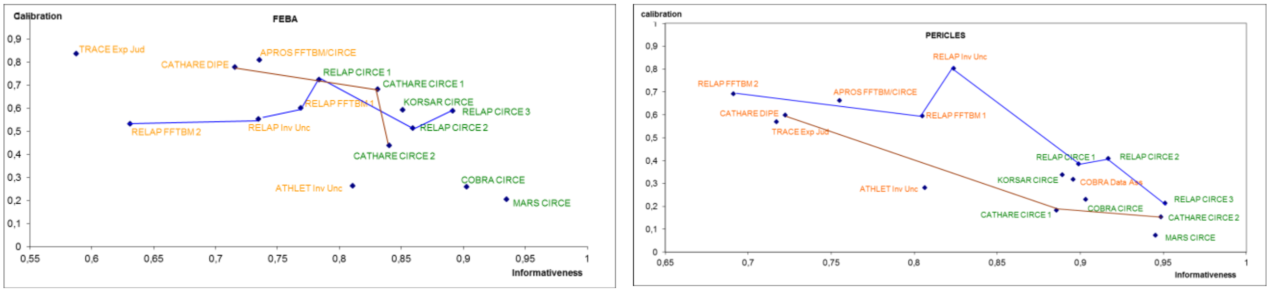

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Figure 4 – PREMUM: spread of results associated to the verification (a) and the validation (b) of quantified input uncertainties. The colored solid line connects the users of a same code [6]

A main lesson learned from the project was that a systematic approach devoted to model input uncertainty quantification and validation should be developed to improve the reliability of the analysis and to ensure the extrapolation of its results to the Nuclear Power Plant (NPP) case.

Participant	Code	Method	Tests used	Responses used
BelV	CATHARE	CIRC É	all 6 FEBA tests	T_{clad} , quench times
CEA	CATHARE		all 6 FEBA tests	T_{clad} , quench times
CVRez	RELAP		FEBA tests 223, 216, 220, 218 and 222	T_{clad} , quench times, DP
KAERI-CIRC É	COBRA		FEBA tests 223, 216, 218 and 214	T_{clad}
KINS	MARS-KS		all 6 FEBA tests	T_{clad}
OKBM-KORSAR	KORSAR		all 6 FEBA tests	T_{clad} , quench times
OKBM-RELAP	RELAP		FEBA tests 223, 216, 220, 218 and 214	T_{clad} , quench times
UPC	RELAP		all 6 FEBA tests	T_{clad} , quench times, water carried over
KAERI-MCDA	COBRA	MCDA	FEBA tests 223, 216, 218 and 214	T_{clad}
KIT	TRACE	FFTBM	FEBA test 216	T_{clad} , quench times
SJTU	RELAP		FEBA test 216	T_{clad} , quench times, DP
UNIPI	RELAP		FEBA test 216	T_{clad} , quench times
VTT	APROS	CIRC É+FFTBM	all 6 FEBA tests	T_{clad} , quench times, T housing
GRS	ATHLET	IUQ	all 6 FEBA tests	T_{clad} , water carried over, DP
IRSN	CATHARE	DIPE	all 6 FEBA tests	T_{clad} , quench times
Tractebel	RELAP	IUQ	all 6 FEBA tests	T_{clad}

Figure 5 – PREMUM: codes, uncertainty treatment methodology, experiments and SRQs used to quantify input uncertainties [6]

From a methodological point of view, a systematic approach has the advantage of providing a common and generic framework to facilitate both discussions between participants and applications to several industrial problems. Therefore, a first investigation has led to the identification of five key generic elements that should be considered in the construction of a systematic approach (Figure 6).

This five-element structure is currently discussed in the frame of the SAPIUM project (2017-2019). The objectives of this project are first to share a common understanding about "good" practices for input uncertainty quantification and validation, and also to resolve the open issues identified in the PREMIUM benchmark. The SAPIUM project will lead to the development of a systematic approach in order to improve the reliability of the analysis and to progress on the validity of extrapolation of its results to the NPP case. The final report will be a first "good practices" document that can be used for safety study in order to reduce user effect and to increase the agreement among experts on appropriate practices as well as on remaining open issues for further developments. End users are research institutes and universities, manufacturers, utilities and safety authorities.

In other words, they are the developers and the users of BEPU approaches, as well as the organizations in charge of evaluating these approaches.

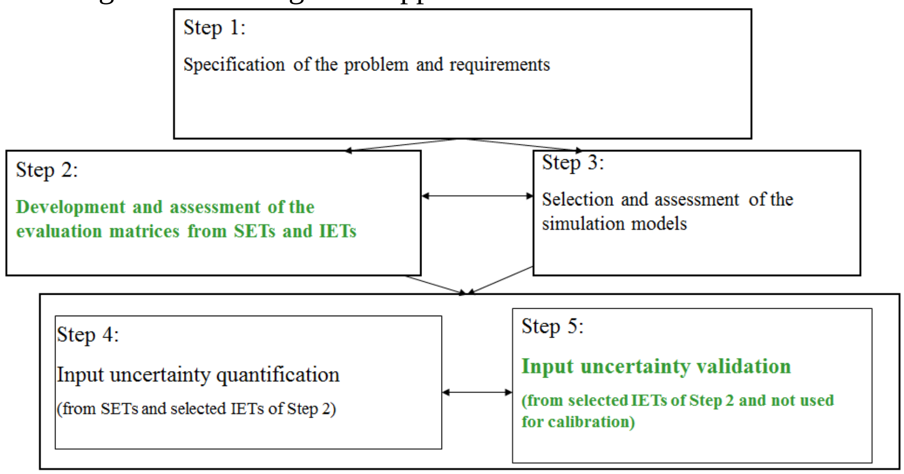

Figure 6 – SAPIUM: the five-element structure of an IUQ systematic approach [7]

Experimental validation plays a key role among the different issues that should be handled to go through the five-element structure. More precisely, it concerns the construction of an experimental database (Element 2) for the problem under study as well as the definition of relevant validation indicators to validate quantified input uncertainties (Element 5).

The first task is based on available Separate Effect Tests (SETs) and Integral Effect Tests (IETs), considering different aspects such as the covered phenomena, the geometry, the scaling effect of the experimental facility or the available measurements with the associated uncertainties. It leads to the separation of the experimental database in two parts, one for input quantification and the other for input validation. A methodological key question is related to the construction of formal methods to objectively and automatically rank experiments according to their adequacy and to evaluate the completeness of a database.

Multi-Criteria Decision Analysis (MCDA) approaches can be efficient tools to exhibit most adequate experiments. Their efficiency first relies on the introduction of a set of criteria to characterize the adequacy of an experiment that obviously depends on the analyst's objectives. Then, the application of MCDA methods encompasses two main steps. The first one is the construction of a decision matrix where each experiment is characterized on the set of criteria and an importance weight is given to each criterion. The second one consists in defining a decision rule to aggregate the information of the decision matrix and order the set of experiments. Among popular MCDA tools, one can mention for example the so-called AHP approach [8] which is based on the computation of a unique synthesis indicator or outranking methods (ELECTRE , PROMETHEE) that requires evaluating concordance and discordance criteria to pairwise compare experiments.

Once input uncertainties have been quantified, their validation is usually performed in the System Response Quantity space after input uncertainty propagation through the simulation model. This task includes [6]: (a) the comparison between the simulation model output uncertainty and experimental data not used in the quantification, and (b) a prediction exploiting the previous comparison and including additional uncertainty estimation resulting from interpolation and extrapolation beyond the existing experimental database to satisfy the intended use, and (c) a checking whether the input uncertainties are acceptable for the intended use.

The second and third topics are related to predictive capability that should integrate the geometrical and thermal-hydraulic scaling of uncertainty results. They still remain open issues in many applications. Concerning the first one, it exploits experiments taken from the experimental database and not used for the quantification. However, traditional experiments are usually performed to improve the understanding of physical phenomena or the models implemented in the computer code. Therefore, they could not be fully appropriate for validation and we refer to the V&V literature for guidelines to design new experiments providing high-quality data. The first step then requires introducing a set of validation indicators whose construction depends on: (a) the chosen Target Quantity for Validation (TQV) (e.g. CDF, uncertainty interval) that will be compared with the experimental results; and (b) the properties of the uncertainty results to capture (e.g. position of the experimental value within an uncertainty band, relative discrepancy between experiment and simulation values, uncertainty band width).

There exist several validation indicators that were established with assumptions (on TQV or properties to capture) that should be carefully taken into account to ensure a reliable validation process.

5.3 Fuel behaviour simulation and uncertainty quantification

The typical structure of a fuel performance code is made of different models, each one representing one particular area of the fuel physics (Figure 7). In material science simulation, and in fuel physics simulation especially, all these models are coupled, as the outputs of one model are the inputs of others. Nowadays, more and more mechanistic models are being developed to simulate the behaviour of materials at different scales (microscopic to macroscopic). But in general, all models depend on internal physical parameters, some of them being measurable, but not all of them.

In the validation phase of a fuel performance code, the first step is a calibration phase of these un-measurable parameters. It also includes a calibration of the measurable parameters, which are generally experimentally determined with an uncertainty related to the specific technique applied.

In most cases, the experimental data used for this calibration/validation phase are uncertain also, due to the experimental technique. For example, puncturing technique used to measure fission gas release in PWR fuel rods leads to an estimated uncertainty on the fission gas release measured of about 6%. This uncertainty has to be considered in the validation phase.

Recently, in the fuel performance code area, inverse methods are being used to quantify the modelling uncertainty due to the experimental data uncertainties [10].

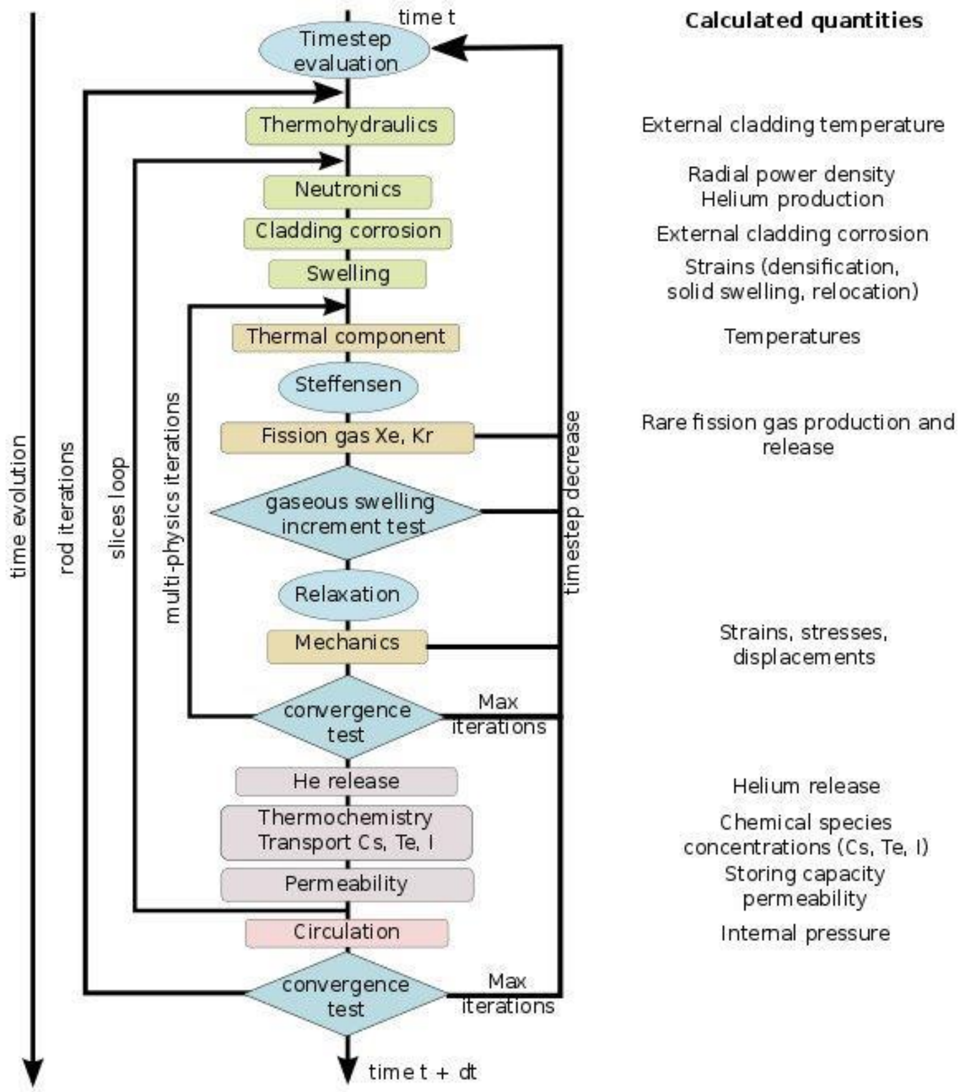

Figure 7 –Typical structure of a fuel performance code (ALCYONE, CEA) [9]

IEs and their uncertainty are key data in the frame of fuel modelling and simulation as they condition part of the uncertainty of the calculations, and the propagation of their uncertainties becomes a conventional procedure in fuel modelling and in fuel modelling tools [11]. Typical chain of uncertainty propagation (see Figure 8) looks like the same for other applications.

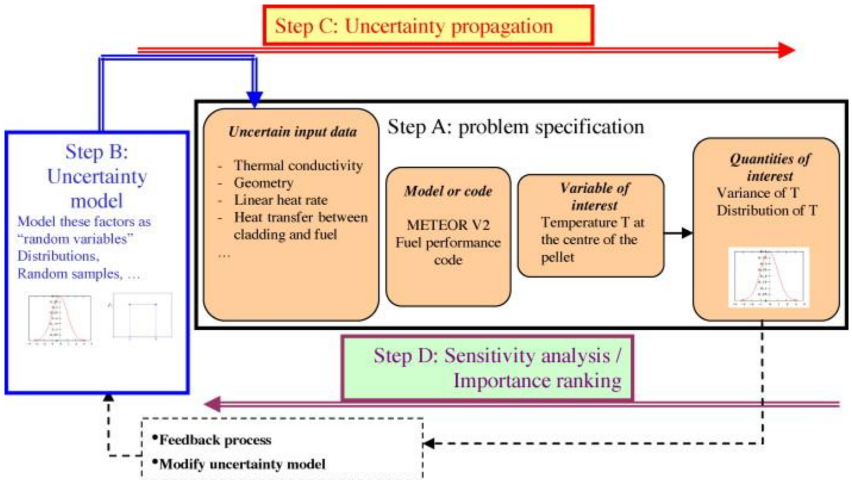

Figure 8 – Scheme of sampling to uncertainty propagation in a fuel behavior modeling [11]

One of the key output quantity of a fuel performance code is the fuel temperature as it affects all the other physical models which describe the behavior of fuel in irradiation conditions. Considering all possible sources of uncertainty that affect the calculation of the fuel maximum temperature [11], the Probability Density Function (PDF) of calculated temperature can be assessed. In the validation process, the experimental temperature measurements are compared to this PDF (Figure 9).

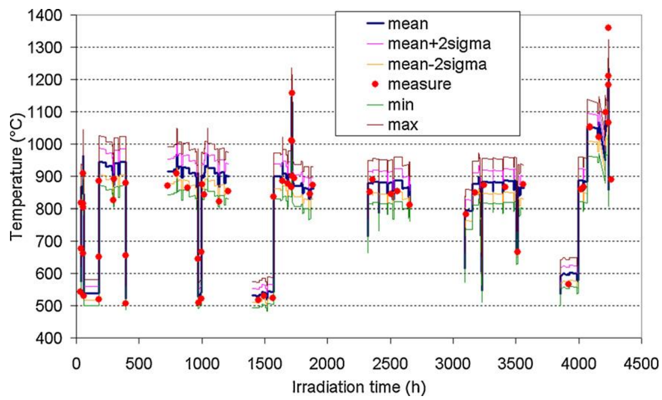

Figure 9 – Comparison of experimental temperature measurements with calculated confidence interval [11]

As several physics are represented in a typical fuel performance code (thermal behaviour, mechanics, diffusion, microstructure modification, corrosion, chemistry, …), different scales of validation are necessary to validate each model at its scale of modelling. The example of temperature is typical of the macroscopic validation.

For fission gas release for example, there is also a microscopic scale for validation, as it is very important to validate the localization of fission gas (intergranular or Intragranular) as it is essential to predict the fission gas release in transient situations (Figure 10).

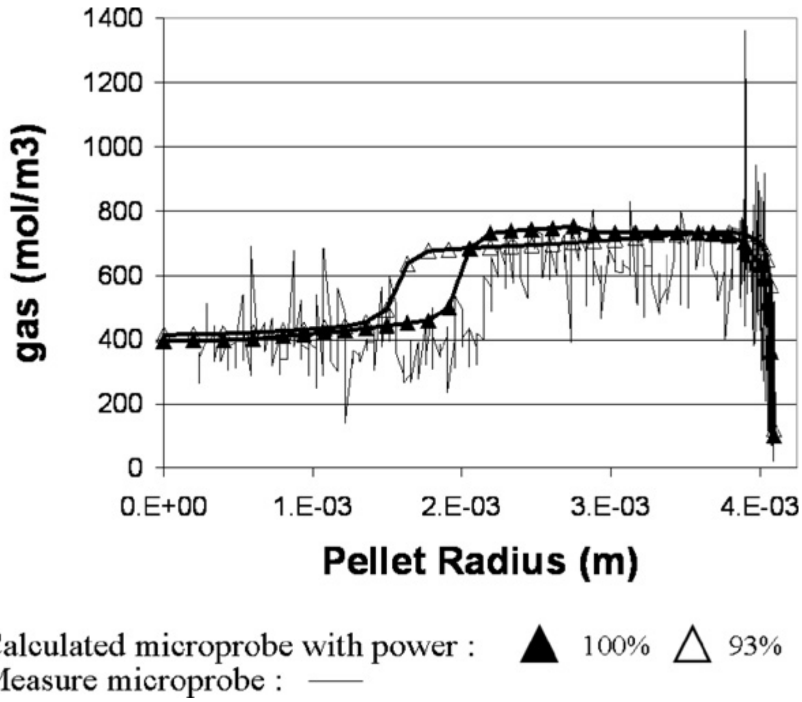

Figure 10 – Comparison of experimental EPMA profile of fission gas concentration with calculated retention profile

The probabilistic description of the uncertain inputs and parameters of the fuel performance code can also be used for safety risk assessment [13]. To do so, reliability methods can be used. Such approaches are denoted in [15] as First-Order Reliability Method (FORM) and Second Order (SORM) ones where both realize a semi-probabilistic reliability analysis which is dedicated to quantification of system's reliability (or failure possibility) basing on randomized experiment-based inputs. The example of fuel melting probability is illustrated in [15] (Figure 11): (a) determine the surface that limits the space where $T_{fuel}<T_{melting}$ → "failure surface", and (b) definition of the point with the highest probability density in the normalized space. The idea is to quantify the probability of failure taking into account all the sources of uncertainty of the thermal chain (conductivity, linear heat rate …).

Nowadays these methods are applied together either directly on the original code if a reasonable number of runs are required, of on surrogate models if computation time is a key issue.

The validation of the fuel performance code is a key issue for this type of application, as the uncertainty determined for each model and parameter of the code condition the assessment of the probability of failure. This is very important for safety analysis.

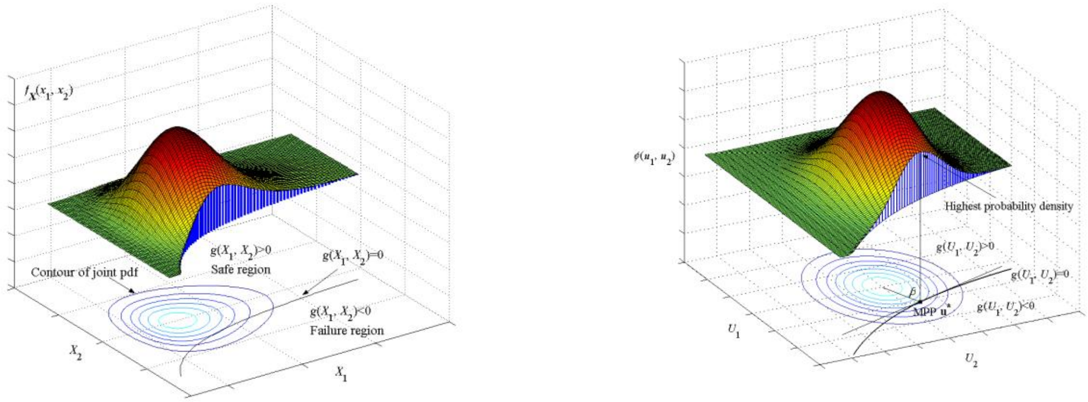

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Figure 11 – The surface that limits the space where $T_{fuel}<T_{melting}$ → "failure surface" (a); the point with the highest probability density in the normalized space (b) [15]

This example also demonstrates that all the most popular approaches developed for other industrial and scientific applications equally form assessors' toolbox in UQ for fuel behaviour.

5.4 PMO in existing reactor cores behaviour

One of the best sources of experimental data is Plant Measurements and Observations (PMO). PMOs are always available as long as plant is under operation.

Despite PMO are difficult to adopt for validation recently developed tools allows developing sophisticated high-fidelity inputs in reasonable time with accepted efforts [12] (see Figure 12) facilitating V&UQ for coupled complex models.

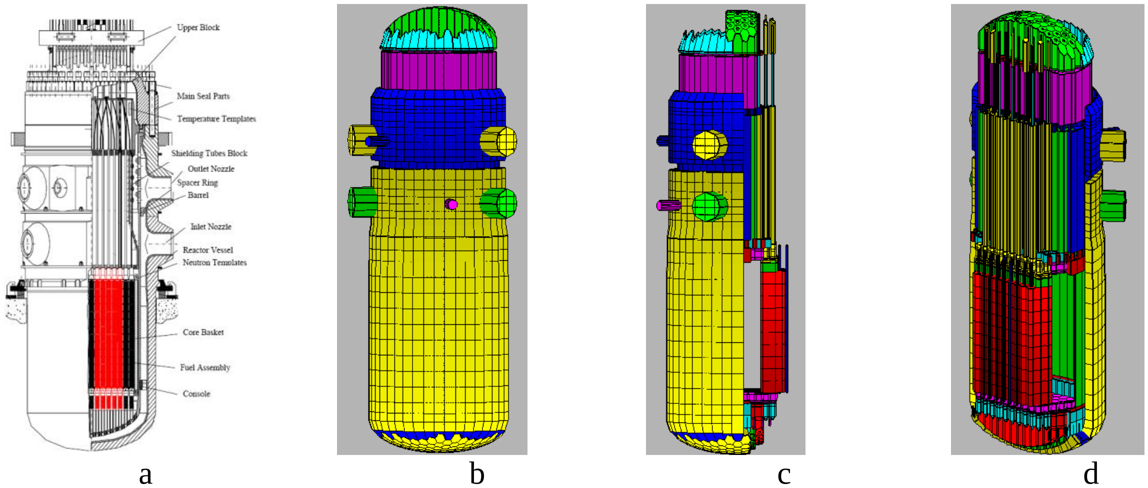

Figure 12 - Common view of reactor and in-vessel structure (left – drawing, right – nodalisation of the RPV and its cuts (only thermo-hydraulic objects are shown) [13]

Although the normal operation and weak transients demonstrated on the basis of this benchmark [14]cannot cover all field of interest for safety these results should be mentioned because the findings and drawbacks minded from the uncertainties studies might be useful in setting and conducting of further research works.

Combing the multi-physics IEs and high-fidelity tools research team provides excellent benchmark (see Figure 13a and b) and orientation on further improvement of ND (see Figure 13c and d).

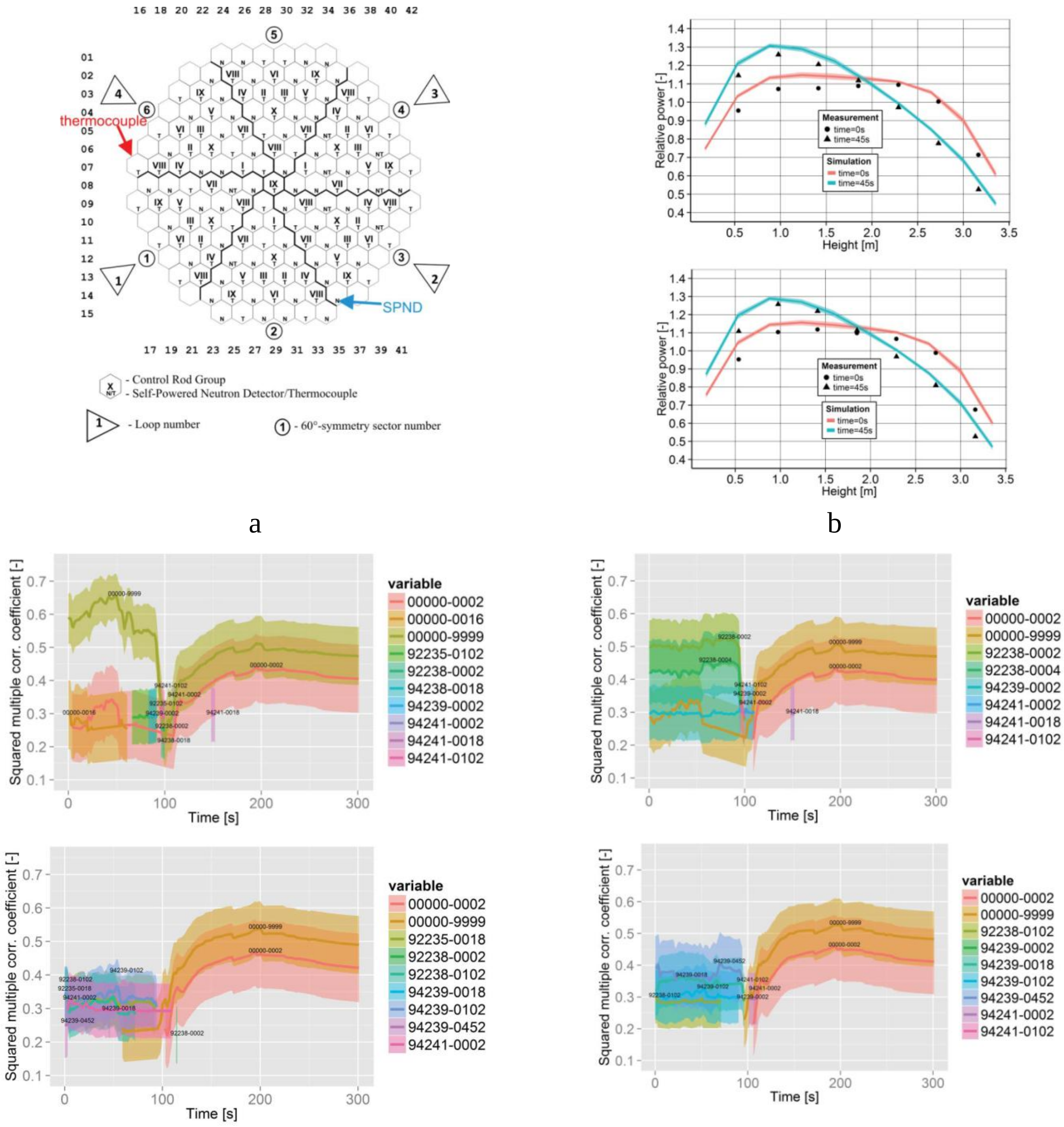

Figure 13 – Benchmark specification details (a), calculated and measured axial profiles (b), and contribution of different nuclear data in final uncertainties (c and d) [12]

6. CONCLUSION

Best Estimate Plus Uncertainty approach being a kind of Decision Making support heavily relies on an availability and affordability of representative sets of experimental-based benchmarks.

Moreover, an experimental validation of Best estimate (mainly multi-physics) simulations is crucial if we want to recommend it as an element of practical safety assessment.

It is almost of consensus that safety assessment must have clear, robust and consistent basis on physical reality, i.e. on evidence. The latest ones might be originated from different sources like benchmark-experiments, mock-ups and objective observation on operational plants, they the only should be experimentally correct and representative to given application.

One should admit that nowadays there are not yet spread and internationally recognized methodology or metrics on quantification of factor of representativity. The only criteria we are all agree is that a set of benchmarks should cover an imposed application domain.

In addition it should be stressed the role of IEs in a calibration, these IEs should be excluded or carefully used in validation process minimizing risks to bias the results of testing.

Finally, IEs bring unique objective information inaccessible via differential experimentation.

To mind and to use this information one should evaluate IEs quantifying the uncertainties of measurements and correlations between different experimental cases.

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