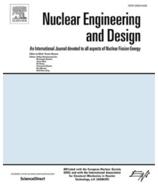
Nuclear Engineering and Design 387 (2022) 111608

Contents lists available at ScienceDirect

Nuclear Engineering and Design

journal homepage: www.elsevier.com/locate/nucengdes



Methodology for phenomenological code assessment with integral test data

Marina Perez-Ferragut [a,b], Víctor Martinez-Quiroga [a,b], Max Casamor [a], Jordi Freixa [a,*]

[a] Department of Physics, Universitat Politécnica de Catalunya (UPC), Spain
[b] Energy Software S.L (ENSO), Spain

ARTICLE INFO

Keywords:
thermal-hydraulic codes
experiment simulation
code validation
uncertainty analysis
BEPU

ABSTRACT

The use of codes in the licensing process requires a rigorous validation process that can be accomplished by means of qualitative and quantitative assessment. In thermal hydraulics, this validation has to be performed at different levels, from separate effects to the integral response of a plant design. Even though the quantitative assessment is preferred, for complex phenomenology involving the behaviour of the whole plant system this approach is difficult and the assessment is usually performed through qualitative expert judgement. In the present article, a methodology is proposed that combines the use of qualitative and quantitative adequacy assessment for the simulation of experiments at integral test facilities. The method makes use of statistical quantification by means of Best Estimate Plus Uncertainty calculations.

1. Introduction

Thermal-hydraulic (TH) system codes are used for deterministic safety analysis to demonstrate that the plant response under operational transient and accident conditions complies with the acceptance criteria with sufficient safety margin. Confidence on the safety analysis results not only relies on the capability of the TH system code to simulate the physical processes but also on the quality of the nodalization in terms of geometrical and discretization aspects, and any other judgment required during the generation of the input model. Therefore, in order to carry out a licensing calculation for a given system it is mandatory to:

- prove the adequacy and accuracy of the TH system code in representing the behavior of the particular system under analysis; and
- assure the quality of the system nodalization and the selection of correlations and special process models.

Regarding the qualification requirement of a system code, the five stages of the process are described by (D'Auria et al., 2017) and consist in: definition of the operational, transient and accidental scenarios; identification of the phenomena involved in each case; verification and validation (V&V) of the system code to assess whether the code is capable of calculating the critical phenomenology; correction or enhancement of the code in case deficiencies are observed; and evaluation of the V&V results using key metrics and conclusions. According to the International Atomic Energy Agency (IAEA) guidelines on deterministic safety analysis (IAEA, 2019), the validation calculations should ideally cover the entire range of postulated conditions and should include four types of test calculations, namely basic tests, separate effects tests (SETs), integral effects tests (IETs), and nuclear power plant (NPP) level tests and operational transients.

On the quality requirement of the input model, the user must consider several choices regarding the space discretization for the different parts of the system, and regarding the selection of code special process models and correlations. Indeed, TH system codes were developed with a high level of flexibility so that they could be applied to very diverse engineering problems. The cooperation between countries in the development and validation of system codes has been crucial to achieve a high maturity of current codes, and in this sense a major effort has been the realization of comparative exercises and benchmarks such as the International Standard Problems (ISPs), in which the participant organizations simulate the postulated experiments and compare their results with each other and with the experimental data (CSNI, 2000).

One relevant outcome from ISPs is the large spread of code results even from participants using the same code (D'Auria, 2017). These differences arise from the well-known issue of "user effect", an inherent source of uncertainty of system code calculations (CSNI, 2006; CSNI, 2007). Namely, "user effect" refers to the variability introduced to calculation results of the same problem, same code, but performed by different users: interpretation of the available documentation; quality of

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* Corresponding authors at: Universitat Politécnica de Catalunya, Spain.

E-mail addresses: marina.pf@ensobcn.com (M. Perez-Ferragut), victor.martinez-quiroga@upc.edu (V. Martinez-Quiroga), max.casamor@upc.edu (M. Casamor), jordi.freixa-terradas@upc.edu (J. Freixa).

https://doi.org/10.1016/j.nucengdes.2021.111608
Received 29 July 2021; Received in revised form 25 November 2021; Accepted 3 December 2021

the documentation describing the code, facility and/or scenario; user expertise; and possible random errors building the input deck can lead to differences in the results. Despite the development of TH advanced codes was expected to reduce this user dependency, the last ISP has shown that it still has a significant impact on the code results (Choi et al., 2012). Recommendations to mitigate the “user effect” mostly rely on user training by performing validation, mentoring, and instruction. Code users need to have a good knowledge of the physical modeling, the limitations of the codes, and the facility to be described, as well as a clear understanding of the major phenomena expected to occur during the transient (D’Auria, 2017). It is also important to bear in mind that, even though there are some similarities, the nodalization approaches and user guidelines are specific for each code. Another important aspect that has been deemed to be crucial is the consistency in the modeling of several experiments (Freixa and Manera, 2012), and hence the confidence in both the system code and the nodalization can be built upon a successful simulations of a range of tests. The large number of available experiments from worldwide facilities offers the possibility to qualify the nodalization of each facility for its entire range of experiments and to develop guidelines and strategies that can be later on applied to the modelling of NPPs. The bottom line is that expertise and consistency are the key to perform robust and reliable TH calculations.

In this paper we introduce a novel methodology for the assessment of system codes against experimental data at IET and SET facilities.

The Advanced Nuclear Technologies (ANT) research group in the Polytechnic University of Catalonia (UPC) has gained extensive experience in accident analysis with thermal-hydraulic system codes such as RELAP and TRACE through the long-term cooperation with the CSN (the Spanish nuclear regulatory authority) and the Spanish NPPs Asco and Vandellos II. These cooperations have allowed the research group to take part in several international projects promoted by the OECD related to the simulation at integral test facilities (PKL, LSTF, ATLAS, LOFT, BETHSY, LOBI) and to the Best Estimate Plus Uncertainties (BEPU) methodologies (BEMUSE (CSNI, 2009), PREMIUM (Skorek and de Crecy, 2011). Through these activities ANT has developed a procedure for building up and maintaining TH nodalizations and the methodology presented in this paper devoted to the validation of system code calculations. These two methodologies have a quite different objective but are linked together in the sense that the code validation requires a consistent generation and maintenance of qualified nodalizations to minimize the “user effect”.

The article describes in detail the ANT assessment methodology for validation calculations (Section 3), with the focus on the accuracy evaluation, along with application examples for each step. The last section provides with an example of the phenomenological assessment (Section 4).

2. Background

The IAEA recommends a combined use of both qualitative and quantitative methods to demonstrate the capabilities of a code to reproduce, or otherwise, the phenomena occurring during transient and accidental conditions in the NPPs (IAEA, 2003). However, the generalized approach to validate codes at IET level relies solely on qualitative methods and expert judgement, see for instance the assessment manuals of RELAP and TRACE (Trace, 2007; Laboratories, 2005).

The ANT methodology for validation of system code calculations is developed specifically for independent assessment against experimental tests (IET, SET). It integrates qualitative and quantitative evaluation steps in compliance with the recommendations provided by IAEA (IAEA, 2003). The methodology aims at measuring the accuracy of code results by means of statistically likely regions for each key-variable.

A number of uncertainty methodologies have been developed since in 1989 the revised 10 CFR 50 rule (USNRC, 1989) allowed the use of best estimate codes instead of the conservative code models, provided that uncertainties are identified and quantified. The Code Scaling, Applicability, and Uncertainty (CSAU) guidelines for uncertainty methodologies were developed by the USNRC to support the amended regulation requirements, and were published in that same year along with an application example to a large break loss-of-coolant accident (LBLOCA) using TRAC code (Boyack et al., 1989). The ANT validation methodology conforms to CSAU guidelines and makes use of the statistical approach based on the Wilks’ formula proposed by GRS (Glaeser, 2008). The novelty of the proposed procedure is that the focus has been shifted from the traditional safety margin evaluation to a phenomenological code assessment. Now the uncertainty evaluation is used to provide a quantification of the code accuracy, and this has an impact on both the selection step of the input uncertain parameters, and on the output representation: the input parameters are selected according to the phenomena described in the experimental report and in the corresponding matrix from the Commitee on the Safety of Nuclear Installations (CSNI); and regarding the output uncertainty, it is estimated from the two-sided tolerance interval to statistically define a data region instead of looking for the typical one-sided tolerance limit, a single value, from which the safety margin is estimated.

Other approaches to quantify the code accuracy at the IET level can be found in the literature. One that stands out is the use of fast Fourier transform-based methods (FFTBM) to quantify the accuracy of a calculation of an IET experiment (Prošek et al., 2002; D’Auria and Lanfredini, 2019). In this method, the transients are split in time regions where the accuracy for different parameters is quantified. Thresholds have been proposed for each region in order to decide the validity of the calculation. This method is not purely quantitative because it makes use of user defined thresholds and parameters that rely heavily on expert judgement. Other researchers have pointed out the use of BEPU methods in the validation process (Zhang, 2019; Ivanov et al., 2020). The main goal of this line of research is to validate both the selection of input parameters and the generation of probabilistic density functions that might have been derived at more specific experimental facilities (separate effect tests). In contrast, the ANT methodology only goal is to determine whether a calculation successfully simulated a phenomenon or not.

3. ANT assessment methodology for validation calculations

The scope of the ANT assessment methodology is the validation of thermal-hydraulic system codes for safety analysis, with the particular objective of evaluating the simulation results against experimental data from SETs and IETs. The method is based on the conventional qualitative comparison but includes the use of a BEPU method to support the assessment with the quantification of the code calculations’ uncertainty. The two steps have its specific goals and procedures. On the one hand, the qualitative validation makes use of a qualified system nodalization to demonstrate that the code is capable of reproducing the phenomena associated to each test, or otherwise to identify the phenomena that cannot be simulated. On the other hand, the quantitative validation generates statistically defined data regions for each key-variable to estimate the uncertainty of the code calculated results.

The structure of the method conforms to CSAU guidelines described by (Boyack, 1990; Wilson, 1990; Wulff, 1990; Lellouche and Levy, 1990; Zuber and Wilson, 1990; Catton et al., 1990). However, there are some logical differences arising from the focus of the analysis: while the object of the method here described is to assess the accuracy of code validation calculations, the primary object of CSAU-type methodologies is the estimation of safety margins for licensing accident analysis. Indeed, the code validation is one of the requirements for such applications.

The methodology is intended for the assessment of a single code validation calculation, i.e. for a specific test selected to validate the code. It is organized into four elements, consistently with CSAU guidelines, but adapted for the code validation analysis:

Element 1 “Code and data Identification, Documentation and Provision (IDP)” establishes the a priori requirements to proceed with the code accuracy assessment.

Element 2 “Input model and base case calculation” refers to the development of the code input model of the facility to generate the code results for the experiment. During this step the relevant phenomena are identified and categorized with the aim of identifying key modelling issues and the figures of merit relevant to the scenario that will determine the quality of the code simulation.

Element 3 “Uncertainty Analysis” relates to the quantification of the uncertainties. It makes use of the validation matrix to generate a list of code parameters to be included in the uncertainty analysis (UA), and it carries out the uncertainty code runs to estimate the tolerance intervals.

Element 4 “Qualitative and quantitative assessment of the base case calculation” consists of the qualitative and quantitative assessment for each particular phenomena identified in Element 2.

The elements and steps contained in the ANT Assessment Methodology are outlined in Fig. 1, and the detailed description of the four elements is presented next.

3.1. *Element 1: Code and data IDP*

The a priori requirements for a code assessment are the provision of the documentation for the code version and for the facility and experiment under analysis. Specifically:

- Identification of the code frozen version: the frozen version used during the validation process cannot be changed, and any detected malfunction would require the generation of a new code version and the starting of the verification and validation process. The frozen version at this point, before the validation with experimental data, has to have gone through exhaustive verification and through some sort of validation with at least SETs. The code version and the executable have to be identified with an alphanumeric tag to univoquely relate the code to the build date, to the compiler version, the operating system, …which will make the code results replicable in the future.
- Provision of the proper code documentation: a proper use of the code requires the reading of the code manuals, which must include the description of the physical models, empirical correlations, numerical techniques, code capabilities, detected limitations, modelling recommendations, results from previous verification and validation calculations and any other fundamental information that characterizes the frozen code version such as the list of modifications from the previous version.
- Provision of the facility documentation: the Facility Description Document should ideally include qualified and referenced data of the reactor system such as the plant design drawings, geometrical data and material properties. For a proper modelling, it is necessary to have either the volume versus elevation curves for the relevant components or the CAD files. In addition, the detailed description of the measurement location, methods and their associated uncertainty ranges is required.
- Provision of the experiment description: quick look reports and final experiment reports with the information on the specific facility configuration, timing of the events, phenomena observed. The necessary data to perform the phenomenological assessment is required. Each phenomenon may require different experimental data. In the case that there is not sufficient data to evaluate a phenomenon, this can be labeled as lack of data and the code will not be assessed for this particular event.

3.2. *Element 2: Input model and base case calculation*

The object of this element is to generate the code results for the experiment, the so-called base case calculation. The process consists in three consecutive steps: (1) identification and characterization of the relevent physical phenomena; (2) development of the input model of the facility; and (3) simulation of the experiment. The generation of an input model requires dealing with a large amount of data as well as making assumptions when there is no other information available or the modelling approaches to simulate complex systems. The data and reasoning followed to generate the nodalization should be reported in the Engineering Handbook (EH), which shall include the input values along with their references, the modelling assumptions, the nodalization sketches and control logic diagrams, and the qualification results.

The first step consists in the identification and categorization of the physical processes to indicate their suitability for the code assessment. The process is based on the description of the observed thermal-hydraulic phenomena, available in the experiment report, and additional phenomena may be included in the case a phenomenon only appears in the simulation (but not in the experiment). This situation is not common but it may emerge in thermal-hydraulics where cliff edge phenomena are not rare. The cliff edge effects refer to the large variability of an outcome given small changes in the conditions. An example is provided in the paper by (Freixa et al., 2021) on the PKL Intermediate Break Loss Of Coolant Accident (IBLOCA) Test i2.2 benchmark, in which the results of the participants show the effect of the Counter Current Flow Limitation (CCFL) at the core exit on the core level evolution. The final list is cross-checked with the CSNI matrix (Annunziato et al., 1996) corresponding to the transient conditions of the experiment. With this information, each phenomenon in the list is ranked according to the relevance and the validity of the experimental data for the code assessment of the particular phenomenon. Firstly, the phenomenon must be well characterized by the experimentally measured data, thence the phenomenon is ranked by its relevance in the experiment. The four possible labels are:

H Well defined – High relevance
M Well defined – Medium relevance
L Well defined – Low relevance
– Lack of data or not applicable

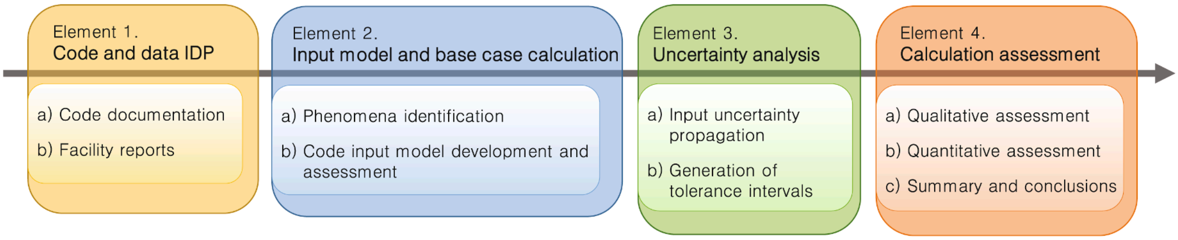

Fig. 1. ANT assessment methodology for code validation calculations.

An example of such list is shown in Table 1 which also includes a second label referring to the code assessment (this label is provided in Element 4 of the methodology, Section 3.4) The phenomenological list will provide a basis for subsequent tasks, specifically: determination of the input model requirements; selection of the input code parameters that will be perturbed in the uncertainty evaluation; and identification of the figures of merit (FOMs) to conclude on the code capabilities. As an example, the list in Table 1 identifies the CCFL phenomenon, for a system code such as RELAP5 the flooding correlation has to be activated in the designated junctions and the available correlations are Wallis, Kutateladze or an in-between form using the Bankoff weighting, then for the selected form the code requires the definition of correlation parameters, which are the Bankoff weighting (Wallis is 0. and Kutateladze is 1.), the slope, and the gas intercept, and finally the appropriate FOM will depend on the location of the CCFL, i.e. an appropriate FOM for the CCFL in the core exit could be the core level.

Eventually, the phenomonological lists from the full range of experiments used in the code assessment are organized into code validation matrices according to “transient”, “facility” and “reactor” criteria. The arrangement and categorization of the phenomena into matrices is a convenient structure for accessing and reviewing the data used for the code assessment.

Table 1
Example of the application of the methodology to different tests of an integral test facility. For each phenomenon first a relevance tag is assigned (Element 1) and later an assessment of the code is provided in Element 4.

Phenomena[1]	Rank and characterization[2]				
	Test 1	Test 2	Test 3	Test 4	Test 5
Break flow	HO	–	–	HO	HO
SGTR break flow	–	HO	HP	–	–
MSLB break flow	–	–	HO	–	–
Core-wide void and flow distribution	HO	–	–	HO	–
Mixture level and entrainment in the core	HO	–	–	HO	–
Core mixture level	HO	–	–	HO	–
Heat transfer in covered core	LO	L-	L-	HO	HO
Heat transfer in uncovered core	HO	–	–	HO	–
Forced 1-phase circulation	–	HO	HO	L-	HO
Forced 2-phase circulation	HO	–	HO	HO	HO
Natural 1-phase circulation	–	HO	HP	–	HO
Natural 2-phase circulation	HO	–	HP	HO	HO
Reflux & Condensation	L-	–	–	HO	L-
Loop seal clearing	HO	–	–	HO	–
CCFL core outlet/ pool formation	HP	–	–	–	–
CCFL U-tube entrance	HO	–	–	HO	–
CCFL hot leg	HP	–	–	–	–
ECC bypass	HO	–	–	–	–
ACC mixing and condensation	HO	–	–	HO	MO
ACC interruption	HP	–	–	MO	MO
LPIS injection	H-	–	L-	–	–
HPIS injection	MO	HP	HO	–	–
Primary to secondary heat transfer	L-	HO	HO	HO	HO
Secondary to primary heat transfer	L-	–	L-	L-	–
Pressurizer thermal-hydraulics	L-	MO	HO	L-	L-
Asymmetric loop behavior	MO	MO	MO	MO	–
RCP shutdown effects	HO	HO	MO	HO	HO
Supercritical flow	–	–	–	HO	–
Mixture level and entrainment on SG	–	L-	HO	L-	HO
Phase sep. without mixture level formation	L-	–	–	L-	–
Stratification in horizontal pipes	L-	–	–	HO	HO
Phase sep. and T-junc. & effect on break flow	L-	–	–	HO	HO
Non condensable gas effect	L-	–	–	–	HO

[1] SGTR (Steam Generator Tube Rupture), MSLB (Main Steam Line Break), ECC (Emergeny Core Cooling), ACC (accumulator), L/HPSI (Low/High Pressure Injection System), RCP (Reactor Coolant Pump).

[2] H (High), M (Medium), L (Low), O (Simulated as in the experiment), X (Not simulated as in the experiment), P (Partially simulated as in the experiment), - (Lack of data or not applicable).

The second and third steps are, respectively, the development of a qualified input model of the facility and the generation of the code results for the specific test. Building an input model requires a high level of expertise in both the understanding of the thermal-hydraulic physical behavior and the application of the code to represent them. Moreover, the accuracy of the code results is not only constrained by the code capabilities and limitations, but by the quality of the nodalization and the input modelling approaches. Having this in mind, the input model is generated following the in–house developed “ANT methodology for building and maintenance of TH nodalizations”, which is conceived to guarantee the quality and traceability of the nodalizations by relying on the principles of expertise and modelling consistency. A lesson learned from the ANT participation in benchmark activities at IETs is that even though a given code version and input model are able to correctly capture the phenomena occurring in one test, it might not be the case in successive tests with different boundary conditions. In order to overcome this problem, ANT has devised a methodology that considers the complexity of developing system nodalizations with the goal of simulating several diverse transients. This is referred to as consistency and is achieved by generating a unique plant model to simulate all tests. The extend of expertise and guidelines obtained by a nodalization that is able to reproduce several tests at the same time is far larger than what one can obtain with few tests, because the performance of the models and correlations is tested in different conditions (Freixa and Manera, 2012; Llopis et al., 2007; Reventós et al., 2007). Likewise, the ANT procedure to generate a qualified system nodalization relies on the concept of robustness by applying the generally accepted recommendations to mitigate the “user effect”, that is having a qualified staff in thermal-hydraulics, using proper code documentation, staff training, experienced supervision and data cross-checking (D’Auria et al., 2017).

In the present paper only the outline of the methodology is presented, full details of applications are only described in confidential internal documents due to proprietary information of the facilities and plants:

- The process begins with the development of the facility input model, which essentially involves geometric and physical models considerations taking into account the modeling considerations of the previous step. The generation of the input model should take into consideration the code modelling guidelines, and will rely on the team experience. Moreover, the recommendation is that an internal document containing information on the recommended modelling approches be produced, and be as experience is gained. Examples of critical modelling issues are the discretization level for the different parts of the reactor system, the activation of special code models to reproduce local phenomena, or the suitability of pseudo-three dimensional modelling (Martínez-Quiroga et al., 2014). The ANT group have produced different guidelines articles for different phenomena or families of scenarios that have to be followed in this step. One example is the guidelines in the modelling of the core exit thermocouples given by (Freixa et al., 2015) or the guidelines in the modelling of SBO scenarios (Freixa et al., 2020).
- The verification of the facility input model is performed first on the gross geometric quantities such as the total volume of the fluid, and second on the boundary and initial conditions (BIC) such as the primary and secondary pressures. This procedure is based on the steady state qualification level of the Bonuccelli methology(Bonuccelli et al., 1993). These two steps must conform to certain acceptance criteria as shown in Table 2 for the geometrical data, and for the BIC values in Table 3. The selected parameters and acceptable errors are derived from both the Bonuccelli methodology and previous NPP nodalization qualifications works performed at the UPC (Berthon, 2005; Reventós et al., 2007). It is worth mentioning that some of the NPP acceptable errors values can not be directly extrapolated to integral test faicilty (ITF) experiments (depending on

Table 2
Criteria for the qualification of the geometric aspects of a nodalization.

Parameters	Acceptable error
Volume of a circuit	2%
Total surface of passive heat structures	10%
Total surface of active heat structures	2%
Total volume of passive heat structures	14%
Total volume of active heat structures	2%
Relative elevation of relevant components	0.05 m
Flow area of relevant components	1%

Table 3
Criteria for the qualification of the steady state parameters.

Parameters	Acceptable error
Pressure	0.1%
Fluid temperature	3 K
Pump speed	2%
Pressure loss	10%
Mass flow	2%
Collapsed liquid level in Pressurizer components	0.05 m

the experiment, system pressures cannot be clearly stable before the start of the transient; or the deviation associated to the instrumentation can be higher than the suggested acceptable error, (Freixa et al., 2021). Hence, acceptable errors must be adapted to the ITF depending on the experiment. Otherwise, as the development and assessment of the nodalization is based on the concept of consistency, final values must be therefore common, as much as possible, for the series of tests carried out in the same facility layout.

- The assessment of the experiment input model is evaluated from the calculated values of the most representative variables looking at the acceptance error. The final list of variables used depends on the experimental set up or the nuclear power plant design, and the acceptance values are set for each type of variable as shown in Table 3. There might be some cases where it is difficult to compare the real measurements with the calculated values due to the lack of detailed information, for instance the exact location of the thermocouple or the measurement technique for a pressure difference ΔP. In these cases, the signal might be discarded for the validation of the steady state. When all parameters are within the acceptable error or the deviations can be justified in terms of the actual uncertainty of the measurements or unsuitable measurement methods, the steady-state calculation has been achieved
- Next follows the development of the particular experiment configuration: the generic input model is adapted by adding and modifying any relevant component and/or thermodynamic condition.
- Once the input model is assessed successfully, the code is executed to generate the base case, that is to say, the calculation with the best-estimate input values and code default coefficients. The generation of the base case may still require some input model decisions such as time step and re-nodalization of components. In addition to consider the modelling requirements identified from the phenomenological list, it is recommended to research on the modelling approaches of similar experiments that may indicate the use of special process models and provide nodalization recommendations. For instance, for an IBLOCA scenario this reference may be of use (Freixa et al., 2013). The calculated results should be organized in plots of the selected FOMs, tables with the timing of the main events, as well as tables with the most representative scalar output values. The approval of the transient calculation should be based on acceptability criteria such as the ones shown in Table 4 that considers two situations: experimental data available or not available. In the case of participation to blind benchmark activities, experimental data is not available or partially available (semi-blind simulation).

At the completion of Element 2 the input model for the experiment configuration has been qualified and the results of the base case have been generated.

3.3. Element 3: Uncertainty analysis

The objective of the uncertainty analysis is to evaluate the impact of having an imprecise knowledge of the input, code data but also from the facility description and experimental data. The imprecise knowledge arises from the uncertainty associated to the measuring devices of pressure, thermal conductivity, …and from the empirical nature of the code correlations to simulate friction, heat transfer, …The values input in the nodalization or hardwired in the code are defined as "best-estimate", but still uncertainty exists and should be evaluated. In most of the UA methods the uncertainty is propagated from the input throughout the code calculations, and the calculated results, either scalar or time evolving, are no longer analyzed as single values but as likely data regions. The successful outcome of an UA requires the experimental data to at least be enclosed by the uncertainty region.

The method adopted for the UA is a statistical type of BEPU, and its basic features are:

- based on CSAU framework (Boyack, 1990; Wilson, 1990; Wulff, 1990; Lellouche and Levy, 1990; Zuber and Wilson, 1990; Catton et al., 1990);
- propagates input uncertainties;
- uses a statistics theory to evaluate the uncertainty of the calculated FOM; and
- follows the method proposed by GRS (Glaeser, 2008).

Element 3 is organized into the three typical steps of statistically-based BEPU methodologies: (1) identification of code parameters and determination of their uncertainty; (2) random sampling and code execution; and (3) generation of the tolerance interval.

The first step consists in determining the input model data and source code correlations governing the processes identified in the phenomenological list from Element 2. For instance, looking at the time the pressurizer empties during a primary system depressurization, we may need to consider the uncertainty in the drag and friction coefficients, and even in the special processes such as choked flow. Some of these parameters are directly available from the input model, but some may require the perturbation of source code coefficients. In the pressurizer example and for RELAP5 code, the friction could be varied from the input deck by changing the loss energy coefficients requested in the junction components and the choked coefficients are also input from the input deck; the drag coefficients cannot be accessed from the input deck and should be approached directly from the source code. This step is clearly code dependent because the choice and availability of empirical models and numerical methods to simulate the physical phenomena are specific to each computational tool.

There has been a growing interest in the evaluation of the uncertainty in the calculations and the system codes have been updated to make accessible the code correlation coefficients for perturbation, typically only accessible from source code modification, from the input deck. Examples of these developments are the RELAP/SCDAPSIM and its

Table 4
Acceptability criteria for a particular case.

Experimental data available:
Qualitative comparison of the evolution of the most representative variables
Comparison of the chronology of the most important events
Evaluation of the most relevant physical phenomena
Experimental data not available:
Evaluation of the most relevant physical phenomena
Other possible sources depend on each particular case

Integrated Uncertainty Package (Perez-ferragut et al., 2008), in which the run mode for uncertainty evaluation allows the perturbation of the wall-to-fluid heat transfer correlations, fluid heat transfer correlations and other code correlations; the RELAP5-3D has implemented modifications to the input deck to allow the perturbation of the reflood interfacial heat transfer, wall heat transfer and interfacial friction routines (Parisi et al., 2020). The TRACE code developed by the NRC has also recently introduced code parameters that can be used for sensitivity analysis directly from the SNAP interface or with the DAKOTA package (Queral et al., 2015).

The method considers two sources of uncertainty: code correlations and plant uncertainty. The first one accounts for the empirical nature of the correlations used by the code to simulate the physical processes. This uncertainty is applied to coefficients and parameters in the correlations, for instance the wall-to-fluid heat transfer coefficients, the friction parameters or the critical flow coefficients. The second one refers to the uncertainty from the measuring devices in the plant and is related to boundary and initial conditions, including material properties.

The impact of the user and of the plant nodalization is not treated directly as source of uncertainty, but is considered indirectly by applying generally accepted procedures to minimize its effect:

- Regarding “user effect”, the general recommendations are followed within Element 2: qualified staff in thermal-hydraulics, use of proper code documentation, staff training, experienced supervision and data cross-checking (D’Auria et al., 2017).
- The plant nodalization effect refers to the specific input model nodalization built to represent the experimental facility: space discretization, simplification of complex geometry and handling of lack of information. Its uncertainty is not considered and instead a quality assurance strategy is followed to ensure the capability of the nodalization to represent the thermal-hydraulic phenomena and plant system behavior.

The present methodology proposes an additional protection to address these two points, which is the consistent development of the nodalization of the facility.

Following the IAEA guide for deterministic safety analysis, the effect of delays in plant safety systems and of equipment failures are not considered in the methodology because the simulation of an experiment implies a defined timing of the events and operational actions.

The uncertainty of the parameters can be established from facility documentation, manufacturer data, code documentation, and previous studies, and it’s described through probabilistic density functions (pdf’s). Common pdf’s are the uniform distribution, defined by the range of values with equal probability; the normal and log-normal distributions, defined by the mean and the standard deviation; and the trapezoidal (also called polynomial) distribution, which is an extended uniform but with the probability dropping to zero at the edges.

The output of this step is a table with a list of the physical processes and boundary conditions, the associated input code parameters, and the uncertainty description with the pdf type and characteristic parameters. The typical number of uncertain parameters ranges from 20 to 80. Table 5 displays an example of selected physical process and boundary conditions.

Table 5

Example of a list of uncertain input parameters for selected physical processes and boundary conditions. Details about the ranges: U is described with minimum and maximum values in brackets, N is described by either ± 2. times the standard deviation, or with its mean and standard deviation in brackets and LN is described with its mean and standard deviation in brackets.

Phenomena[1]	Parameter[1]	PDF[2]	Range	Ref.
HT in the core	Film boiling HTC wall-to-liquid	U	[0.74;1.29]	Freixa et al. (2016)
	Film boiling HTC wall-to-gas	U	[0.49;3.43]	Freixa et al. (2016)
	Nucleate boiling HTC saturated	P	[0.76,0.86,1.19,1.43]	Wickett et al. (1998)
	Nucleate boiling HTC subcooled	U	[0.35;2.5]	Wickett et al. (1998)
	Core power	N	± 0.07 MW	Experimental
	Local boiling factor	LN[3]	[0.37;0.1804]	Wickett et al. (1998)
Global	Interphase friction	U	[0.75,1.29]	Freixa et al. (2016)
	Interphase HT global	U	[0.27;1.94]	Freixa et al. (2016)
ECCS	ACC pressure	N	± 0.054 MPa	Experimental
	ACC temperature	N	± 2.75 K	Experimental
	ACC liquid level	N	± 0.12 m	Experimental
	ACC line friction from loss	LN	[0.00;0.42]	CSNI (2009)
	L/HPIS pump characteristics	N	± 5. %	CSNI (2009)
	L/HPIS liquid temperature	N	± 2.75 K	Experimental

[1] ECCS (Emergency Core Cooling System), HTC (Heat Transfer Coefficient).

[2] U (uniform), N (normal), P (polynomial), and LN (log normal).

[3] The PDF is as follows: local boiling factor = −ln(y), where y∼N (0.37,0.1804), see Wickett et al. (1998)).

The second step carries out the massive code calculations, the so-called uncertainty runs, using the randomly sampled values for the selected parameters. The required number of code runs, N, to estimate the bounds for a percentile of the output under analysis with a certain confidence level is calculated from the Wilks’ formula (Wilks, 1941). It is worth stressing that from the use of the Wilks’ formula, the number of code runs is independent of the number of input parameters selected for uncertainty association. The form of the output uncertainty is the two-sided tolerance interval to statistically define the region of calculated values. The Wilks’ equation to calculate the minimum code runs to generate the two-sided tolerance interval of the $\gamma\cdot100$ (%) percentile at a $\beta\cdot100$ confidence level (%) is:

$$\beta = 1 - I(\gamma, s-r, N-s+r+1) \tag{1}$$

where N is the number of calculations, $I(i,j,k)$ is the incomplete beta function:

$$I(\gamma,j,k) = \int_0^\gamma \frac{u^{j-1}(1-u)^{k-1}B(j,k)}{d} u \tag{2}$$

$$B(m,n) = \frac{\Gamma(m)\Gamma(n)}{\Gamma(m+n)} = \frac{(m-1)!(n-1)!}{(m+n-1)!} \tag{3}$$

For instance, at first order the two-sided tolerance interval is defined by the lowest $r = 1$ and the highest rank $s = N$:

$$\beta = 1 - I(\gamma, N-1, 2) = 1 - \gamma^N - N(1-\gamma)\gamma^{N-1} \tag{4}$$

Substituting the values for the percentile and confidence level $\beta = \gamma = 0.95$ the number of required calculations is 93.

For each of the N code runs an input deck is built from the base-case nodalization and substituting the best-estimates values of the M input selected parameters by the random sampled values. Each code run will use the same input deck, except for these M input parameters.

The procedure in case of code failures, i.e. execution stops before the end of time steps, will be that proposed for Wilks’ based methods during BEMUSE exercise (see phase V report (CSNI, 2009), and Section 7.5 of exercise summary (NEA-CSNI, 2011). The procedure requires no code failures, with the exception of the code failure occurring after all relevant phenomena have occurred and there is no probability of evolving to non-stable conditions. Under the circumstance of a code failure, the number of code executions should be increased to the next order of application of the Wilks' formula to discard the failure, i.e. to assume the code failure had generated the extremest value (highest/lowest rank).

The third step consists in the generation of the tolerance intervals by applying the ranks theory to the output data from the multiple code executions.

In this methodology study the uncertainty region is estimated from a two-sided tolerance interval. This may be a different output compared to safety margin evaluation applications, in which the one-sided tolerance interval is generally preferred: establishing the statistical region of possible values, rather than estimating an upper/lower limit, seems the correct choice for determining the accuracy of code calculations for validation purposes. The characteristic parameters of the two-sided tolerance internal are the generally accepted 95/95, i.e. 95^{th} percentile and 0.95 confidence level, application at first order of the Wilks formula, then the required number is 93 cases.

3.4. Element 4: Qualitative and quantitative assessment of the base case calculation

The assessment of the code is achieved by comparing the code calculated values against the experimental data. It is a structured procedure that evaluates the accuracy of the code calculations for each of the dominant phenomena in the validation matrix (Element 2). In some occasions, when a number of phenomena are interconnected or taking place at the same time, they may be grouped into one assessment subsection. Therefore the ANT method discretizes the experiments in phenomena and not in time regions as opposed to the FFTBM methods.

Element 4 is organized into three consecutive steps. The first two steps consist in the qualitative and the quantitative assessment, respectively, and are carried out for each of the individual or group of phenomena, and the third one is the summary and conclusions of the whole assessment.

3.4.1. Qualitative assessment of a phenomenon

This step requires the description of the expected phenomenology and the observed code results. Expert judgement is used to evaluate if a phenomenon has been correctly reproduced by categorizing them with one of the following marking:

O Simulated as in the experiment.
P Partially simulated as in the experiment.
X Not simulated as in the experiment.
– Lack of data or not applicable.

3.4.2. Quantitative assessment of a phenomenon

The uncertainty bands will help the analyst in making statements and providing marks for each phenomenon. The results can be evaluated by identifying the data and time regions where the experimental data is bounded by the uncertainty band, and by providing statistical information of the results in relation to the experimental values.

For the scalar FOMs the output values from the uncertainty runs are extracted into an array and then sorted from the maximum to the minimum value. The maximum value represents the 96.8^{th} percentile order meaning that all other results are below this value with a confidence of 95% and the minimum value stands for the 3.2^{th} percentile order, no calculations are below this case. The experimental value is thence assigned to the percentile order that fits the sorted data. An example of this figure will be shown in the following subsection.

3.4.3. Summary and conclusions

This last step summarizes the code assessment work for the experiment under analysis and should contain clear statements on whether the code is capable (or not) of reproducing the assessed phenomena. The concluding remarks can also include recommendations on the modelling of particular phenomena. For instance the noding of the break in a LOCA or the use of particular code options. For this final part, a table is generated with the summary of the assessment for each phenomenon. An example can be seen in Table 1, which contains both the relevance of each phenomenon and the assessment.

4. Example of application of Element 4

This section provides an example of the phenomenological assessment performed in Element 4 covering the 4 possible outcomes detailed in Section 3.4. For this purpose, we have selected one relevant phenomenon extracted from a real case application of the methodology but the data sets have been manipulated to illustrate the different possible tag assignment.

The following plots show results from Test 2 of the OECD/NEA ROSA-2 experimental program. Test 2 represented an IBLOCA in the cold leg with additional system failures (Takeda and Ohtsu, 2017).

Let us consider the accumulator interruption phenomena that may take place during small and intermediate break sequences. This phenomenon is ranked as highly relevant in Loss-of-coolant-accident sequences and thus any system code needs to be capable of reproducing it. When accumulator water is injected into the system, cold water may reach the hot core inducing a high amount of vaporization. The expansion of the steam phase may lead to an increase of the primary pressure if the break is not large enough to absorb this expansion. If the primary pressure increases, the accumulator injection may be interrupted ensuing a reduction of the vaporization and a subsequent pressure reduction will follow. In order to assess this phenomenon the following parameters have been used:

- Time at which accumulators are completely depleted.
- Level of the accumulators.
- Time at which accumulators start to inject water.
- Pressure of the pressurizer.
- Accumulator mass flow.
- Core level.

However, in order to fulfill the purpose of this section and for conciseness, only the first two items will be used.

4.1. Partially simulated as in the experiment (P)

Fig. 2 shows the time evolution of the level in the accumulator of the experiment, the base case and the uncertainty bands. From the experiment time trend it is clear that the level dropped in one single step and thus there was no interruption of the injection. In the base case, the accumulator injection was interrupted at about 280 s and was only emptied some time later. However, the uncertainty bands reveal that in some cases (or at least one case), the accumulator injected without interruption. This is clear because the lower uncertainty band reaches 0.0 in one straight line before the experiment (around 260 s).

At this point, we do not know how many cases reproduced well the studied phenomenon. For this purpose we need to look at Fig. 3 that shows the ending time of the accumulator injection for each of the 93 cases. In this figure, the ending time for each case is ranked from the lowest to the highest and organized in a plot. Every value in the X-axis represents the percentile order and the Y-axis is the value obtained for that percentile order. Both the experiment and the base case results are placed in the plot in accordance to the corresponding percentile order. The base case time was about 500 s which corresponds to the percentile order 60, meaning that 60 percent of cases produced a time lower than the base case and 40 percent higher. In the same manner, the experimental value stands at the 23rd percentile order so it is well covered by

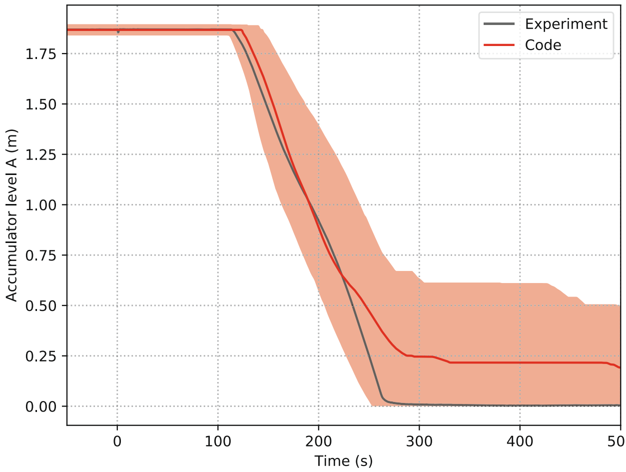

Fig. 2. Accumulator level during an IBLOCA scenario. Example of partially simulated accumulator interruption.

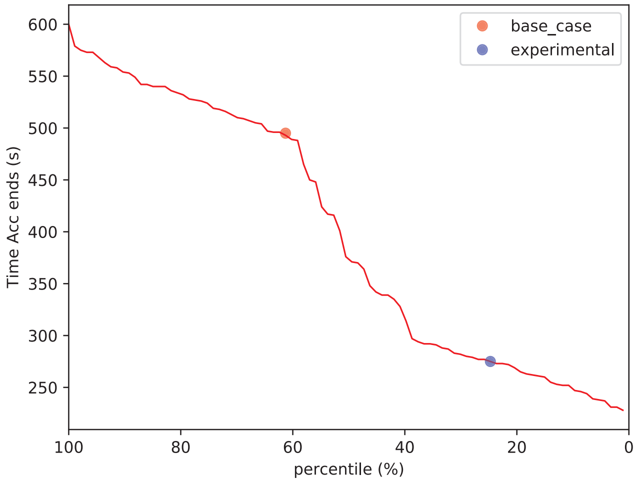

Fig. 3. Quartile plot of the time at which the accumulator is fully depleted during an IBLOCA scenario. Example of partially simulated accumulator interruption.

the spectrum of cases. This plot clearly displays that we have a cliff edge phenomenon and almost half of the cases present an accumulator injection interruption (plateau from percentile order 100 to 60) while in the other half it does not take place.

With these results we can assign the tag “P” for “partially reproduced as in the experiment” since the phenomenon was well reproduced by a percentage of the cases but in another significant bunch of cases the interruption did happen. The bottom line is that the code is capable of representing this phenomenon provided the evaluation of uncertainties will be considered in the application for licensing, and no further action is required. However it may be worth analyzing which parameter triggers or governs the outcome of the calculation, for instance from the measure of correlation between the input parameters and the particular FOM.

4.2. Simulated as in the experiment (O)

Some data manipulation has been performed on the previous set of results to illustrate the “reproduced as in the experiment” case. Basically, we have selected only the cases with no accumulator interruption and excluded the rest to generate new figures. The base case has been selected randomly from the reduced set of cases. In Fig. 4 the accumulator water level is shown, the uncertainty bands still cover well the experimental data. In addition, the upper band tends to 0 indicating that none of the cases had a significant injection interruption. Fig. 5 shows the distribution of times at which the accumulator injection ended. The cliff edge effect seen in Fig. 3 has now disappeared and the experimental case sits well among the spectrum of cases. With these results, it could be concluded that the phenomenon is simulated as in the experiment and the tag “O” would be assigned.

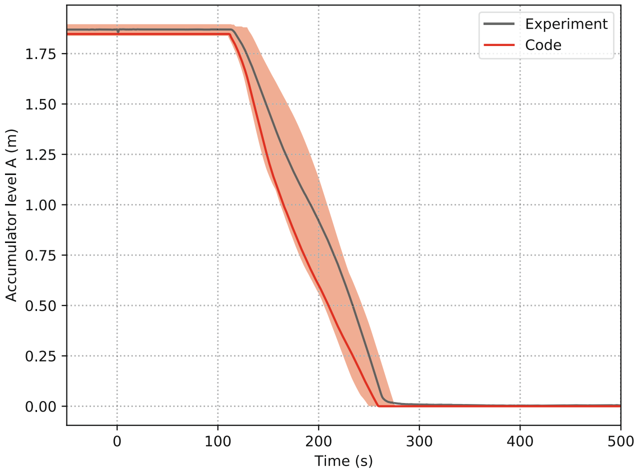

Fig. 4. Accumulator level during an IBLOCA scenario. Example of simulated as in the experiment accumulator interruption.

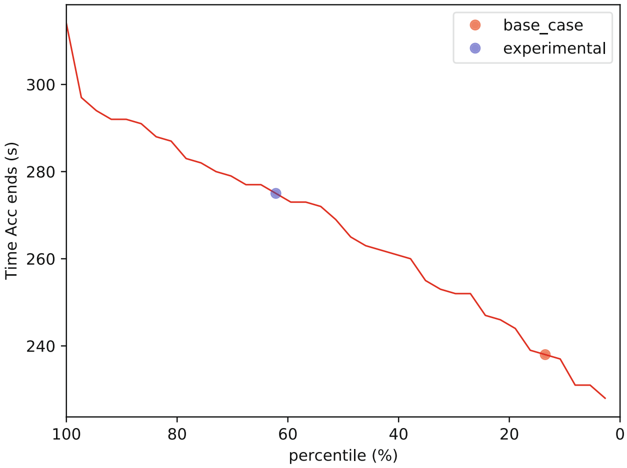

Fig. 5. Quartile plot of the time at which the accumulator is fully depleted during an IBLOCA scenario. Example of partially simulated accumulator interruption.

4.3. Not simulated as in the experiment (X)

For this section, again the data has been manipulated but this time we have selected the cases where the accumulator injection was interrupted. Figs. 6 and 7 display the level in the accumulator and the time of the complete depletion of the accumulator. The uncertainty band shows clearly that interruption occurred in all cases since the lower band does not go linearly to 0 but it halts at around 250 s and only drops to 0 at around 480 s. Again, the cliff edge phenomenon is not present in Fig. 7 and this time, the experimental result is clearly out of the spectrum of cases. With these results, an evaluation of “not reproduced as in the experiment” would be assigned. In this case the conclusion is that the

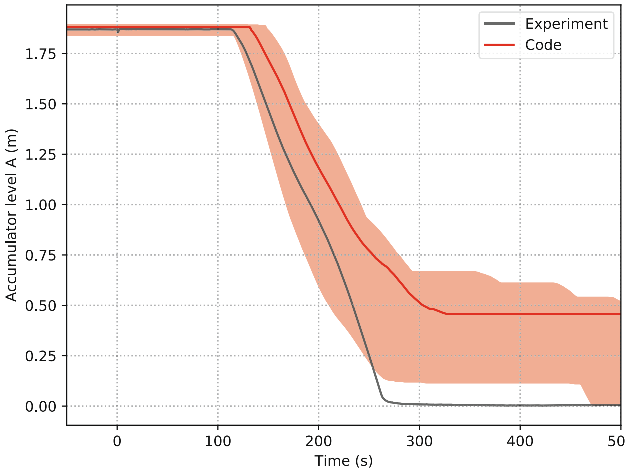

Fig. 6. Accumulator level during an IBLOCA scenario. Example of not simulated as in the experiment accumulator interruption.

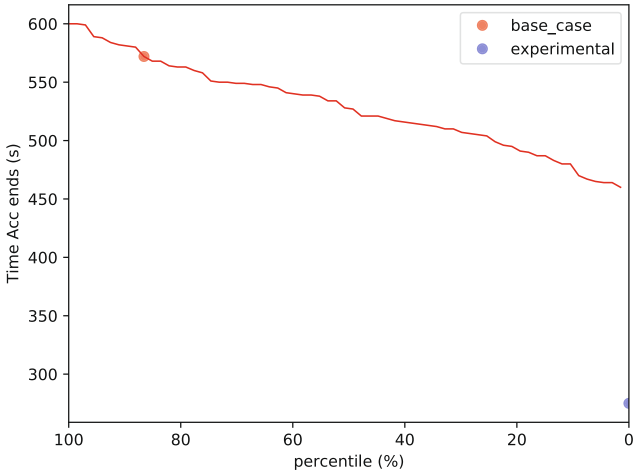

Fig. 7. Quartile plot of the time at which the accumulator is fully depleted during an IBLOCA scenario. Example of partially simulated accumulator interruption.

combination of code and input model is not capable of reproducing the particular phenomenon, and it is therefore required to further assess the modelling approaches or the selected physical models. Any modification of the input model will require the recalculation and revaluation of all tests and phenomena. This was only an example to demonstrate the possibilities of the methodology to better understand and evaluate the performance of the code when we consider the associated uncertainties. However, each phenomenon may require a slightly different approach or the use of a variety of figures of merit.

5. Conclusions

Validation is a compulsory step in the licensing process and for thermal hydraulics involves the simulation of complex phenomenology taking place at integral test facilities. Generally, the validation of codes has been performed through a qualitative assessment. In the present work a new method is presented to combine the qualitative assessment with the quantification of the code accuracy through BEPU calculations. The proposed methodology divides the scenario in different phenomena and defines different figures of merit for each phenomenon. A BEPU calculation is performed and the different FOMs are evaluated. This permits a quantification of the accuracy of the calculation for each FOM. The quantification is combined with the classical thermal hydraulic evaluation of the calculation (qualitative) to provide a final decision on the performance of the code.

The validation of thermal-hydraulic codes against experimental data is a mandatory step for safety analysis and licensing applications. The complexity of the phenomena and their interaction demands the availability of experimental data from integral test facilities to compare and assess the code results. To the knowledge of the authors, the validation of the codes has been traditionally performed through a qualitative assessment. This publication presents a validation methodology in which the qualitative assessment to evaluate and decide on the performance of the code is complemented with the quantification of the code accuracy from a BEPU analysis.

The methodology has been presented along with examples of real applications to facilitate its understanding and illustrate the process of code validation.

CRediT authorship contribution statement

Marina Perez-Ferragut: Conceptualization, Methodology, Formal-analysis, Software, Investigation, Writing-original-draft. **V. Martinez-Quiroga:** Validation, Investigation, Writing-review-editing, Formal-analysis. **M. Casamor:** Software. **J. Freixa:** Conceptualization, Methodology, Formal-analysis, Software, Investigation, Visualization, Writing-original-draft.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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