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APPROACH AND METHODS TO EVALUATE THE UNCERTAINTY IN SYSTEM THERMALHYDRAULIC CALCULATIONS

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Abstract: The evaluation of uncertainty constitutes the necessary supplement of Best Estimate (BE) calculations performed to understand accident scenarios in water cooled nuclear reactors. The needs come from the imperfection of computational tools on the one side and from the interest in using such tool to get more precise evaluation of safety margins. In the present paper the approaches to uncertainty are outlined and the CIAU (Code with capability of Internal Assessment of Uncertainty) method proposed by the University of Pisa is described including ideas at the basis and results from applications. An activity in progress at the International Atomic Energy Agency (IAEA) is considered.

Two approaches are distinguished that are characterized as "propagation of code input uncertainty" and "propagation of code output errors". For both methods, the thermal-hydraulic code is at the centre of the process of uncertainty evaluation: in the former case the code itself is adopted to compute the error bands and to propagate the input errors, in the latter case the errors in code application to relevant measurements are used to derive the error bands.

The CIAU method exploits the idea of the "status approach" for identifying the thermal-hydraulic conditions of an accident in any Nuclear Power Plant (NPP). Errors in predicting such status are derived from the comparison between predicted and measured quantities and, in the stage of the application of the method, are used to compute the uncertainty.

1. INTRODUCTION

Deterministic safety analysis frequently referred to as accident analysis is an important tool for confirming the adequacy and efficiency of provisions within the defense in depth concept for the safety of Nuclear Power Plants.

Typical upgraded international licensing environments offer two acceptable options for demonstrating that the safety is ensured with sufficient margin: use of best estimate computer codes either combined with conservative input data or with realistic input data but associated with evaluation of uncertainty of results. The second option is particularly attractive because it allows for more precise specification of safety margins and their potential use for higher operational flexibility. This constitutes the framework for the present paper.

Thermal-hydraulic system codes are needed to perform deterministic safety analyses and are suitable to calculate complex accident scenarios expected in water cooled nuclear reactors. The outputs of those codes are affected by unavoidable errors that are referred as uncertainties, notwithstanding extensive qualification programs carried out in the last three or four decades. In the current situation it can be said that the experimental programs have not been capable to prevent those errors but to identify and to characterize them.

The present paper, based on an activity still in progress at the IAEA, ref. [1], aims at discussing the major source of errors or uncertainties, at characterizing approaches for performing uncertainty studies and at presenting one successful uncertainty method proposed by the University of Pisa.

2. BACKGROUND

Prior to having the capability to calculate the uncertainty of key values that define a NPP operational envelope, conservative calculations were performed instead. For the present operational plants, the most important limiting parameter is arguably the Peak Cladding Temperature (PCT) since this parameter defines the threshold where fuel damage will likely occur. To the degree the fuel cladding temperature exceeds the specified limiting value, the probability and extend of core damage, including cladding rupture and fission product release, increases.

The absolute requirement to ensure the NPP core integrity for all events, both abnormal and normal, dictated the regulatory requirement that an acceptable safety margin be formulated and imposed on the operation of NPP.

In the USA prior to the existence of Appendix K of the Title 10 Part 50.46 section of the Code of Federal Regulations (10 CFR50.46), Interim Acceptance Criteria was the vehicle used to define the plant operational requirements and also the calculation requirements for ensuring that the safety limits were not exceeded. Some of these criteria were plant-specific. After that, the regulatory bodies required that all calculations of the limiting parameters such as PCT be performed using specified conservative procedures. For example, fuel linear power is bounded by conservatively estimated power rating factors or the critical coolant outflow in case of Loss of Coolant Accident (LOCA) is calculated using a model that is known to overestimate the flow at given boundary condition with an additional multiplication factor higher than 1.0 imposed on the calculated value.

In 1976 the first formulation of 10 CFR50 with applicable sections specific to NPP licensing requirements was released. Over a decade later 10 CFR 50.46 (1996) allowed the use of best estimate codes instead of conservative code models but uncertainties have to be identified and quantified. Guidelines were released that described interpretations developed over the intervening years that are applicable. Other countries established similar "conservative" procedures and acceptance criteria. Because 'conservative' methods were used to calculate the peak values of key parameters, such as PCT, it was always acknowledged that a large margin, between the 'conservative' calculated value and the 'true' value, existed.

While the licensing regulations were being codified, a parallel, international effort was initiated to:

- develop "best-estimate" systems codes with the capability to calculate accurate values of the key phenomena that restrict plant operational limits,
- obtain data to enable Validation & Verification (V&V) of the system codes to be accomplished, and then
- perform code V&V to ensure the quality of the code is known and acceptable.

The effort to generate relevant data was subdivided into experiments defined to study entire transients, including the various interactions between them (integral test facilities - ITF), and experiments designed to study important phenomena in relative isolation from other phenomena (separate effects test facilities - SETF).

The effort to produce comprehensive data sets for the V&V of systems codes resulted in the rigorous study and subdivision of plant systems transients into phases that differed by the governing phenomena and dominant plant behavioral characteristics. For example, the earliest phase of the Large Break Loss of Coolant Accident (LBLOCA) is characterized by a rapid depressurization, large loss of primary system inventory, loss of cooling to the core fuel rods, and core heat-up. The next phase differs as a function of many phenomena characteristic of Emergency Core Cooling System intervention; inventory begins to accumulate and refill the primary system. Consequently, a clear boundary exists between the two early LB LOCA phases. Using this reasoning process, the entire transient, and in fact all relevant transients, are partitioned into phases that contain 'phenomenological windows' which in turn leads to the construction of a convenient phenomena-based system code validation matrix. A number of validation matrices have been developed for various code applications by OECD Nuclear Energy Agency, Committee of the Safety of Nuclear Installations (CSNI).

With the completion of the CSNI code validation matrices, in 1989, the enormous experimental database was categorized according to transient phase and dominant phenomena to both correlate the available data to the code validation needs and to highlight the areas that required further experimental investigation.

With the creation of a data base that includes experimental results from a multitude of experiments and the creation of best-estimate systems analysis codes such as ATHLET, CATHARE, RELAP5, and TRAC, the components necessary to develop a methodology for calculating the uncertainty of parameters calculated using the BE codes became available.

The first uncertainty framework was proposed by US NRC and denominated Code Scaling, Applicability, and Uncertainty (CSAU, ref. [2]). The application of the CSAU methodology resulted in the calculation of the PCT during a LBLOCA Design Basis Accident (DBA) event for a Westinghouse 4-loop pressurized water reactor (PWR) with the uncertainty to a 95% confidence level. The PCT was calculated using the TRAC thermal-hydraulic analysis code and was given as a single-valued number with uncertainty bands.

In the meantime, a number of uncertainty methodologies have been created in other countries, including the GRS, the UMAE and the AEA Technology methods, as summarized in refs. [3] and [4]. These methods, although sharing a common goal with CSAU, use different techniques and procedures to obtain the uncertainties on key calculated quantities. More importantly, these methods have progressed far beyond the capabilities of the early CSAU analysis. Presently, uncertainty bands can be derived (both upper and lower) for any desired quantity throughout the transient of interest, not only point values like peak cladding temperature. For one case, the uncertainty method is coupled with the thermal-hydraulic code and is denominated CIAU (Code with capability of Internal Assessment of Uncertainty, ref. [5]) and discussed below in more detail.

3. THE ORIGIN OF UNCERTAINTY

Application of best-estimate (realistic) computer codes to the safety analysis of nuclear power plants implies the evaluation of uncertainties. This is connected with the (imperfect) nature of the codes and of the process of codes application. In other words, 'sources of uncertainty' affect the predictions by best-estimate codes and must be taken into account. Three major sources of uncertainty are mentioned in the Annex II of the IAEA guidance Accident Analyses for Nuclear Power Plants, ref. [6]:

- Code or model uncertainty.
- Representation or 'simulation uncertainty'.
- Plant uncertainty.

A more detailed list of uncertainty sources can be found in ref. [4], where an attempt has been made to distinguish 'independent' sources of 'basic' uncertainty. The list includes the following items:

A) Balance (or conservation) equations are approximate:
   - not all the interactions between steam and liquid are included,
   - the equations are solved within cylindrical pipes: no consideration of geometric discontinuities, situation not common for code applications to the analysis of Nuclear Power Plants transient scenarios

B) Presence of different fields of the same phase: e.g. liquid droplets and film. Only one velocity per phase considered by codes, thus causing another source or uncertainty.

C) Geometry averaging at a cross section scale: the need "to average" the fluid conditions at the geometry level makes necessary the '*porous media approach'*. Velocity profiles happen in the reality: These correspond to the '*open media approach'*. The lack of consideration of the velocity profile, i.e. cross-section averaging, constitutes an uncertainty source of 'geometric origin'.

D) Geometry averaging at a volume scale: only one velocity vector (each phase) is associated with a hydraulic mesh along its axis. Different velocity vectors may occur in the reality (e.g. inside lower plenum of a typical reactor pressure vessel, at the connection between cold leg and down-comer, etc.). The volume-averaging constitutes a further uncertainty source of ‘geometric origin’.

E) Presence of large and small vortex or eddy. Energy and momentum dissipation associated with vortices are not directly accounted for in the equations at the basis of the codes, thus introducing a specific uncertainty source. In addition, a large vortex may determine the overall system behaviour (e.g. two-phase natural circulation between hot and cold fuel bundles), not necessarily consistent with the prediction of a code-discretized model.

F) The 2nd principle of thermodynamics is not necessarily fulfilled by codes. Irreversible processes occur as a consequence of accident in nuclear reactor systems. This causes ‘energy’ degradation, i.e. transformation of kinetic energy into heat. The amount of the transformation of energy is not necessarily within the capabilities of current codes, thus constituting a further specific energy source.

G) Models of current interest for thermal-hydraulic system codes are constituted by a set of partial derivatives equations. The numerical solution is approximate, therefore, approximate equations are solved by approximate numerical methods. The ‘amount’ of approximation is not documented and constitutes a specific source of uncertainty.

H) Extensive and unavoidable use is made of empirical correlations. These are needed ‘to close’ the balance equations and are also reported as ‘constitutive equations’ or ‘closure relationships’. Typical situations are:

- The ranges of validity are not fully specified. For instance, pressure and flowrate ranges are assigned, but void fraction, or velocity (or slip ratio) ranges may not be specified.
- Relationships are used outside their range of validation. Once implemented into the code, the correlations are applied to situations, where, for instance, geometric dimensions are different from the dimensions of the test facilities at the basis of the derivation of the correlation. One example is given by the wall-to-fluid friction in the piping connected with reactor pressure vessel: no facility has been used to derive (or to qualify) friction factors in two phase conditions when pipe diameters are of the order of one meter. In addition, once the correlations are implemented into the code, no (automatic) action is taken to check whether the boundaries of validity, i.e. the assigned ones, are over-passed during a specific application.
- Correlations are implemented approximately into the code. The correlation, apart from special cases, are derived by scientists or in laboratories that are not necessarily aware of the characteristics or of the structure of the system code where the correlations are implemented. Furthermore, unacceptable numeric discontinuities may be part of the original correlation structure. Thus, correlations are ‘manipulated’ (e.g. extrapolated in some cases) by code developers with consequences not always ascertained.
- Reference database is affected by scatter and errors. Correlations are derived from ensembles of experimental data that unavoidably show ‘scatter’ and are affected by

errors or uncertainties. The experimentalist must interpret those data and achieve an ‘average-satisfactory’ formulation.

I) A paradox: shall be noted: ‘Steady State’ & ‘Fully Developed’ (SS & FD) flow condition is a necessary prerequisite or condition adopted when deriving correlations. In other terms, all qualified correlations must be derived under SS & FD flow conditions. However, almost in no region of the Nuclear Power Plant those conditions apply during the course of an accident.

J) The state and the material properties are approximate. Various materials used in a NPP are considered in the input deck, including liquids, gases and solids. Thermo-physical properties are part of the codes or constitute specific code user input data. These are of empirical nature and typically subjected to the limitations discussed under item H). A specific problem within the current context can be associated with the derivatives of the water properties.

K) Code User Effect (UE) exists. Different groups of users having available the same code and the same information for modelling a Nuclear Power Plant <u>do not</u> achieve the same results. UE (see also below) is originated by:
- Nodalisation development, see also item N), below.
- Interpreting the supplied (or the available) information, usually incomplete, see also item M) below.
- Accepting the steady state performance of the nodalisation.
- Interpreting transient results, planning and performing sensitivity studies, modifying the nodalisation and finally achieving “a reference” or “an acceptable” solution.

The UE might result in the largest contribution to the uncertainty and is connected with user expertise, quality and comprehensiveness of the code-user manual and of the database available for performing the analysis.

L) Computer/compiler effect exists. A computer code is developed making use of the hardware selected by the code developers and available at the time when the code development starts. A code development process may last a dozen years during which period profound code hardware changes occur. Furthermore, the code is used on different computational platforms and the current experience is that the same code with the same input deck applied within two computational platforms produces different results. Differences are typically small in ‘smoothly running transients’, but may become noticeable in the case of threshold- or bifurcation-driven transients.

M) Nodalisation (N) effect exists. The N is the result of a wide range brainstorming process where user expertise, computer power and code manual play a role. There is a number of required code input values that cannot be covered by logical recommendations: the user expertise needed to fix those input values may reveal inadequate and constitutes the origin of a specific source of uncertainty.

N) Imperfect knowledge of Boundary and Initial Conditions (BIC). Some BIC values are unknown or known with approximation: the code user must add information. This process unavoidably causes an impact on the results that is not easily traceable and constitutes a specific source of uncertainty.

O) Code/model deficiencies cannot be excluded. The system code development started toward the end of the sixties and systematic assessment procedures were available since the eighties. A number of modelling errors and inadequacies have been corrected or dealt with and substantial progress has been made in improving the overall code capabilities. Nevertheless, deficiencies or lack of capabilities cannot be excluded nowadays. Examples, not applicable to all thermal-hydraulic system codes, are connected with the modelling of:

- the heat transfer between the free liquid surface and the upper gas-steam space,
- the heat transfer between a hotter wall and the cold liquid down-flowing inside a steam-gas filled region.

Those deficiencies are expected to have an importance only in special transient situations.

4. THE APPROACHES TO CALCULATE THE UNCERTAINTY

An uncertainty analysis consists of identification and characterization of relevant input parameters (input uncertainty) as well as of the methodology to quantify the global influence of the combination of these uncertainties on selected output parameters (output uncertainty). These two main items are treated in different ways by the various methods.

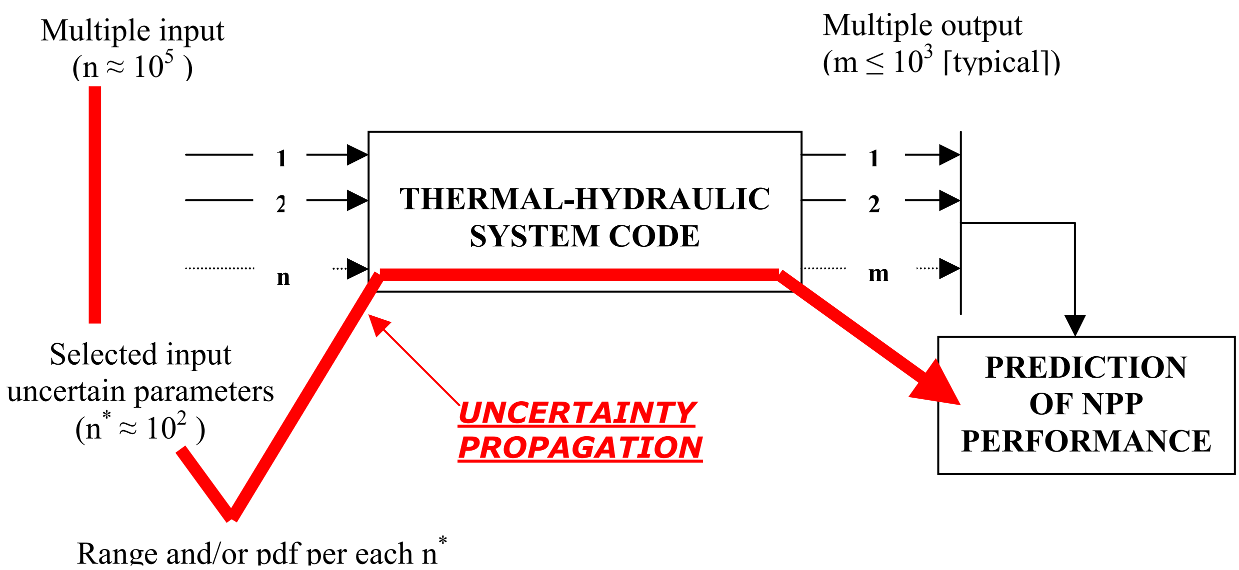

Fig. 1 – Uncertainty approach: propagation of code input uncertainty.

One approach is to evaluate the 'propagation of input uncertainties', Fig. 1: uncertainty is derived following the identification of 'uncertain' input parameters with specified ranges or/and probability distributions of these parameters, and performing calculations varying these parameters. The propagation of input uncertainties can be performed either by deterministic or by probabilistic methods.

The other approach, Fig. 2, is the 'extrapolation of output uncertainty': uncertainty is derived from the (output) uncertainty based on the comparison between calculation results and significant experimental data.

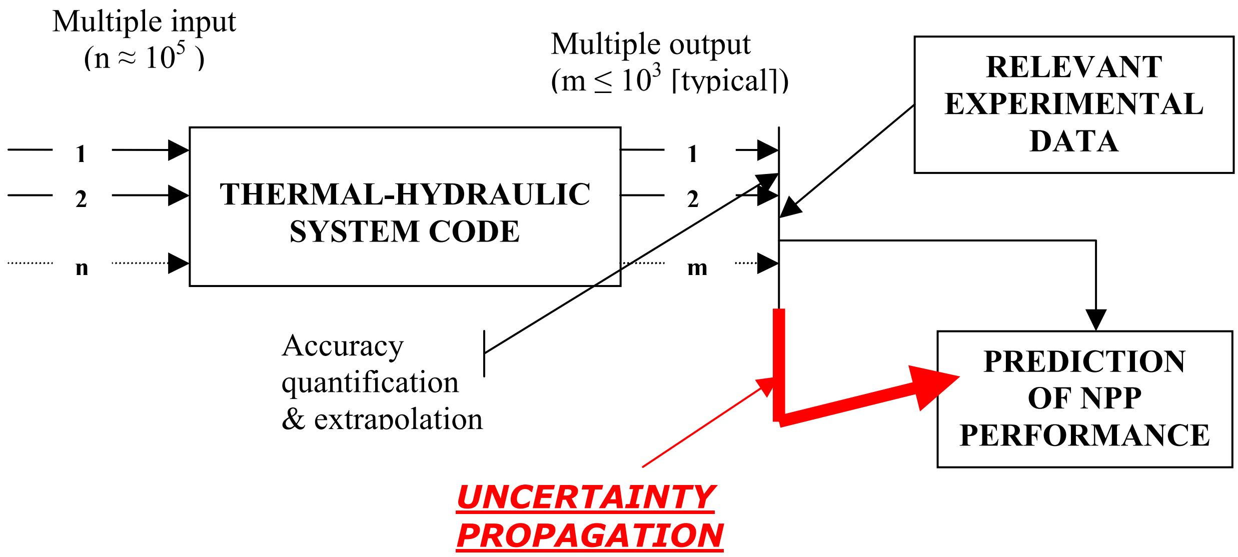

Fig. 2 – Uncertainty approach: propagation of code output errors.

The propagation of code input uncertainty

The GRS is selected as the prototype method, ref. [7], for the description of the *"propagation of code input uncertainty"* approach. In these methods, the state of knowledge of each uncertain input parameter within its range is expressed by a subjective probability distribution. The word "subjective" expresses the state of knowledge rather than stochastic variability. Dependencies between uncertain input parameters should be identified and quantified.

Peculiarities 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 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.

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 has to be modified.

Experts identify significant uncertainties to be considered in the analysis, including the modeling uncertainties, and the related parameters, and identify and quantify dependencies between uncertain parameters. Subjective Probability Density Functions (PDF) 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 has to be quantified as model uncertainty. Additional uncertain model parameters can be included or PDF can be modified, accounting for results from the analysis of Separate Effects Tests.

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. α = 95% means that PCT is below the tolerance limit with at least α = 95% probability). One can be β % confident that at least α% of the combined influence of all the characterized 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 due to the fact that 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

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

and is representing the size of a random sample (a number of calculations) such that the maximum calculated value in the sample is an upper statistical tolerance limit. The required number n of code runs for the upper 95% fractile is: 59 at 95% confidence level, 45 at 90% confidence level, 32 at 80% confidence level. Two-sided statistical tolerance intervals can be adopted.

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.

The propagation of code output errors

The UMAE is the prototype method, ref. [8], 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 NPP.

Considering integral test facilities of a 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.

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 minimized 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 utilizes a database from similar tests and counterpart tests performed in integral test facilities, that are representative of plant conditions. The quantification of code accuracy is carried out by using a procedure based on the Fast Fourier Transform characterizing the discrepancies between code calculations and experimental data in the frequency domain, and defining figures of merit for the accuracy of each calculation. Different requirements have to be fulfilled in order to extrapolate the accuracy. Calculations of both Integral Test Facility experiments and NPP 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. The demonstration of the similarity of the phenomena exhibited in test facilities and in plant calculations, accounting for scaling laws considerations, leads to the Analytical Simulation Model (ASM), i.e. a qualified nodalisation of the NPP.

The flow diagram of UMAE is given in Fig. 3. The bases of the methods and the conditions to be fulfilled for its application, including the use of the FFTBM can be found in refs. [9] to [13].

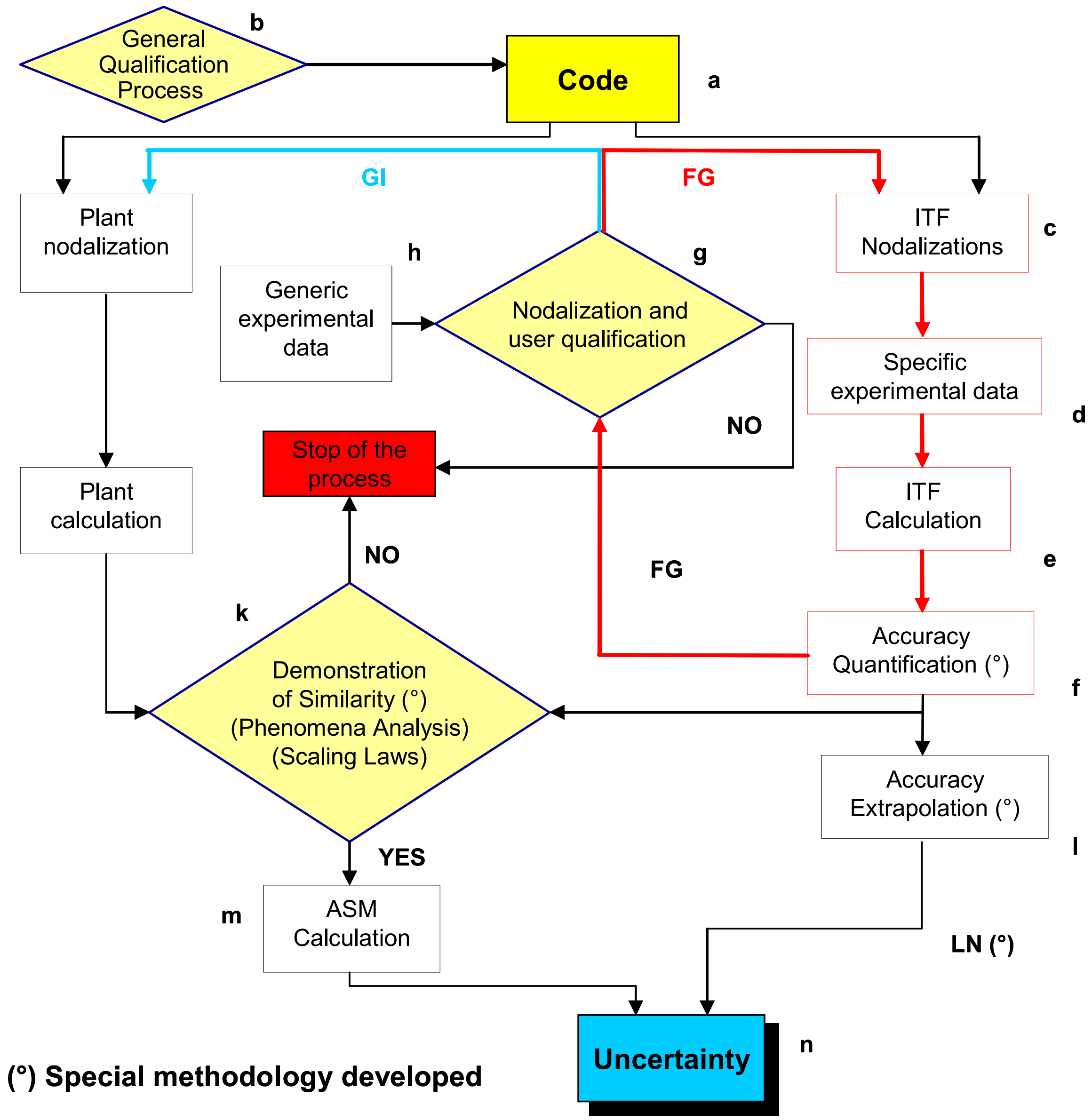

Fig. 3 – UMAE flow diagram (also adopted within the process of application of CIAU).

5. THE CIAU METHOD

All of the uncertainty evaluation methods are affected by two main limitations:

- The resources needed for their application may be very demanding, ranging to up to several man-years;
- The achieved results may be strongly method/user dependent.

The last item should be considered together with the code-user effect, widely studied in the past, e.g. ref. [9], 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 an international conference jointly organized by OECD and US NRC and held in Annapolis in 1996. The CIAU method, ref. [5], has been developed with the objective of reducing the above limitations.

The basic idea of the CIAU can be summarized in two parts, Fig. 4:

- Consideration of plant status: each status is characterized by the value of six relevant quantities (i.e. a hypercube) and by the value of the time since the transient start.
- Association of an uncertainty to each plant status.

In the case of a PWR the six quantities are: 1) the upper plenum pressure, 2) the primary loop mass inventory, 3) the steam generator pressure, 4) the cladding surface temperature at 2/3 of core active length, 5) the core power, 6) the steam generator downcomer collapsed liquid level.

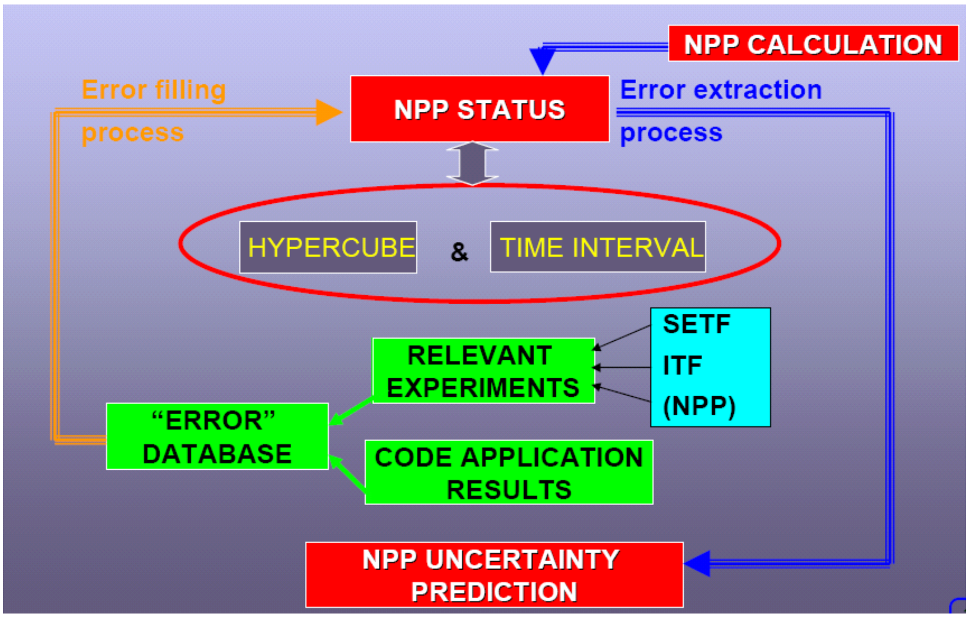

Fig. 4 – Outline of the idea at the basis of the CIAU method.

A hypercube and a time interval characterize a unique plant status to the aim of uncertainty evaluation. All plant statuses are characterized by a matrix of hypercubes and by a vector of time intervals. Let us define Y as a generic thermal-hydraulic code output plotted versus time.

Each point of the curve is affected by a quantity uncertainty (Uq) and by a time uncertainty (Ut). Owing to the uncertainty, each point may take any value within the rectangle identified by the quantity and the time uncertainty. The value of uncertainty, corresponding to each edge of the rectangle, can be defined in probabilistic terms. This satisfies the requirement of a 95% probability level to be acceptable to the NRC staff for comparison of best estimate predictions of postulated transients to the licensing limits in 10 CFR (Code of Federal Regulation) Part 50.

The idea at the basis of CIAU can be made more specific as follows: the uncertainty in code prediction is the same for each plant status. A Quantity Uncertainty Matrix (QUM) and a Time Uncertainty Vector (TUV) can be set up including values of Uq and Ut derived by an uncertainty methodology, Fig. 5. At the moment the UMAE constitutes the 'engine ' for the rotation of the CIAU shaft. The QAM and TAV, respectively Quantity Accuracy Matrix and Time Accuracy Vector in Fig. 5, are derived from an UMAE like process and are the precursor of QUM and TUV. However, within the CIAU framework, any uncertainty method can be used to derive directly QUM and TUV.

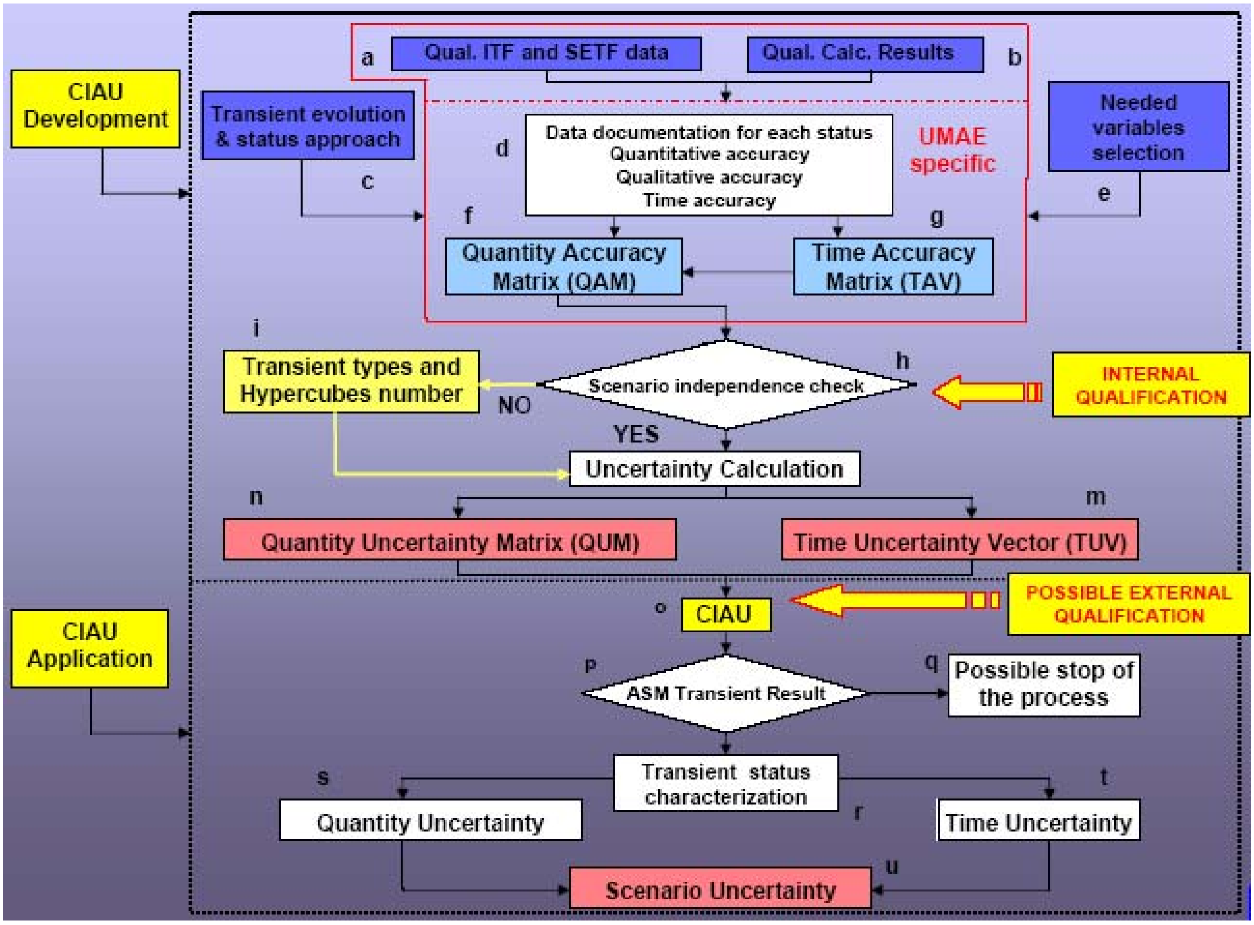

Fig. 5 – Flow diagram at the basis of the CIAU methodology.

6. CONCLUSIONS

The start of the development of uncertainty method in thermal-hydraulic system code calculations can be dated as in the early 80's. Much before (even in the 60's) similar activities were in progress in different technological areas like meteorology and neutron kinetics. A pioneering effort in the area of thermal-hydraulics was made by the US NRC with the publication of the CSAU method at the beginning of 90's. However, background activities were carried out in the previous decade within the umbrella of OECD/CSNI.

Mature methods exist nowadays that are capable 'of fixing the boundaries' for the error of thermal-hydraulic system codes. Two main approaches, characterized as "propagation of code input uncertainty" and "propagation of code output errors", have been discussed in the paper. These approaches are pursued by two reference methods ready for applications, i.e. the GRS method and the CIAU. The last method has been described with more detail.

All the working methods to estimate the uncertainty derive from complex pictures of a complex reality that is constituted by the transient scenarios of water cooled NPP. Even though extensive documentation exist and (in most cases) is available, the level of common understanding about the capabilities and the drawbacks of the methods is not sufficient for achieving a full acceptability of the method. Therefore, rather than additional qualification of the methods, training and communication are needed for spreading the application of coupled best-estimate calculation and uncertainty evaluation.

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