ON THE USE OF CFD AS A TOOL IN THE LICENSING OF NUCLEAR INSTALLATIONS[1]

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ABSTRACT

This paper considers the present role of computational fluid dynamics (CFD) used as a tool in the licensing of nuclear installations. The discussion covers present issues on this subject, dealing with necessary definitions in the field, user effects and best practice guidelines, scope of accepted applications and suggestions for future developments. It is asserted and justified that CFD may be a support to well-established methodologies when based on validation experiments. In the case of CFD such experiments have not been performed and systemized in a general way, being the subject of intense activity in the nuclear field. Some examples show how the particular regulatory context may define the scope of the studies, but without recommending procedural "recipes".

RESUMEN

En éste trabajo se define cual puede ser hoy ser el papel de la fluidodinámica computacional (denominada usualmente CFD por su acrónimo en inglés) como herramienta, para su consideración en el proceso de licenciamiento de instalaciones nucleares. La discusión cubre cuestiones actuales en el tema, definiciones necesarias, lineamientos para el uso apropiado de la CFD, el rango actualmente aceptado de aplicaciones y sugerencias para desarrollos futuros. Se afirma y se justifica que la CFD puede ser un soporte de técnicas ya aceptadas y establecidas a partir de experimentos de validación. Para la CFD, estos experimentos todavía no han sido realizados y sistematizados de manera general y son motivo de intenso desarrollo en la actividad nuclear. Se ejemplifica la dependencia del alcance de los estudios como una función del contexto regulatorio en particular, pero ello sin recomendar explícitamente "recetas" de procedimiento.

FOREWORD

The following text is aimed at pointing out the author´s views on the use of CFD as a tool in relation to the licensing of nuclear installations. Moreover, the document is not a review on the subject because the latter implies a huge number of documented activities that started to be formally consolidated around year 2000. Not surprisingly, this is contemporary with the widespread availability of powerful personal computers and industrial computer codes. Obviously, the use of CFD techniques in Nuclear Reactor Safety started before, in the early 70´s. The widespread use triggered the need for verification and validation of codes and made evident to many people the lack of "CFD-grade" experimental data, which is expected to be consistent with the degree of detail that a CFD code may provide. If considered in this restricted way it almost precludes using the huge set of qualified experimental data generated in integral test facilities and separate tests effects (with a cost of billions of dollars) because this people may consider that detailed calculations can be validated only considering such detailed, "CDF-grade" experimental data. Perhaps their thinking is founded in the availability of dependent derived variables that CFD codes provide and not in the real usefulness of this qualified data for relevant aspects of Nuclear Safety like accident analysis. Fortunately, some experiments have been used since a long time ago to validate one-dimensional codes and also –quite recently- to validate models in CFD codes (e.g. subcooled boiling). In the last case CFD predictions have been used to get cross section averages to be compared with the experiments. This seems to be the way to deliver proper consideration to consolidated, "non-CFD-grade" experimental data, despite the error compensations that may affect averaged variables. Global data agreement (e.g. pressure losses) must also be checked, imposing further effort.

Locally, new CFD users contribute new results and it may be verified that sometimes they are not the outcome of sound extrapolations of previous experience in the field. This is a symptom that must be carefully considered. Having pioneered in the field of CFD techniques in the limited context of Argentina, the author believes that this document may help to bring useful information, again in this context, to CFD codes users.

INTRODUCTION

The use of CFD techniques as a tool to perform Nuclear Safety thermal-hydraulics (TH) related analyses of nuclear installations components is almost at its beginning in Argentina. Few studies of restricted scope have been submitted to the Nuclear Regulatory Authority (ARN) supporting the analysis of the TH behavior of components. These cases relate to single phase flow and the results sometimes may be also be obtained by means of standard engineering methods or by using one-dimensional (1D) TH codes.

This paper is aimed at stating constraints that should be considered in the use of CFD analyses when they are related to licensing applications. This type of discussion is not new and has also been considered in appropriate fora dealing with nuclear safety analysis. A particularly valuable series of meetings are the CFD4NRS-xxxx meetings (CFD4NRS-2006; XCFD4NRS, 2008; CFD4NRS-3, 2010; CFD4NRS-4, 2012 and CFD4NRS-5, 2014). However, the explicit consideration of licensing aspects is not too frequent. An example may be found in the presentations by Boyd, 2014 and Boyd, 2015. Perhaps this is not the only author making reference to regulation, but it is not evident who else have addressed these aspects before and explicitly in this particular subject in relation to nuclear energy. Discussion at these fora have promoted the proliferation of papers on the subject of verification and validation (V&V) of codes in general, along with their associated uncertainty quantification, code inter-comparison experiments, uncertainty metrics in particular contexts and, surely more importantly, realizing the need of “CFD grade experimentation". The latter triggered efforts to provide the CFD community with data relevant to safety analysis considering complex, two-phase flow regimes. All these efforts resemble the ones related to the use of systems TH codes for the analysis of transients in nuclear power plants, performed since four decades ago, which permitted the construction of an impressively huge database of experimental information. This consolidated experimental data, collected from experimentation in integral test facilities and separate effect tests have provided the basis for the understanding of the complex phenomena in transients in nuclear power plants, including accidents. The present status of the maturity of CFD in relation to nuclear safety analysis may be corroborated, among many other references to be considered below, in CFD4NRS-4, 2012 and CFD4NRS-5, 2014).

Institutions have also addressed these aspects since some years ago, like AIAA, ASME, US-NAS, OECD/NEA-CSNI, ERCOFTAC and the US-NRC, sometimes in relation to general engineering practices. This information will also be discussed later in this paper.

In Argentina, at least in the author´s knowledge, these aspects have not been considered in a formally documented way; this is the main motivation for issuing this document. It should, hopefully, motivate regulators, licensees, members from the nuclear industry and proponents of nuclear technologies in general, to consider by themselves the subject of verification and validation and uncertainty quantification of the results of codes, regardless of their degree of detail of physical representation. It is essential to ensure the safety by design that will lead to the safe operation of nuclear installations. Obviously, innovative designs should rely on these aspects from their very beginning. The clarification of what should be considered in order to satisfy regulatory constraints will be the subject of the next sections. In what follows a discussion on what regulatory constraints are and an early definition of the present CFD role in the licensing of nuclear installations in the author´s view, will precede its discussion and justification. A brief consideration of trends in the subject is included and exemplified, a proposal for future action is given and conclusions from the previous steps are drawn.

On regulatory constraints

It is important to state some definitions that may be evident in other fields of the engineering practice but having a relatively loose meaning for code users in the nuclear field[3]. The definition of regulatory constraint[4] is firstly considered.

A regulatory-constraint is a particular kind of constraint that specifies a governmental law or regulation that must not be violated by the applicant, licensee or designer. The typical objective of a regulatory constraint is to ensure that the application for licensing does not violate any relevant laws or regulations.

The difference between qualified engineering prediction results using CFD codes and qualified, licensing-compliant, CFD prediction results aimed at licensing acceptance is the satisfaction of regulatory constraints. Please note that this statement also applies to any type of code or even to calculations by hand.

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[3] It must be recalled that some assertions, like this, are not assumed to be "universally" valid, i.e. they hold in Argentina

[4] Constraint: a) something that limits or restricts someone or something; b) control that limits or restricts someone's actions or behavior (Merriam-Webster online dictionary, http://www.merriam-webster.com/)

Licensees and regulators have different roles in the process of licensing, namely: a) Licensees are the natural providers of nuclear safety; b) Regulators are the guarantees of that safety facing society and set the constraints. Licensees must provide (i.e. are responsible for providing) sound safety analyses satisfying licensing constraints. Enforcements (like sanctions or compulsory measures) by the regulator to ensure regulatory safety constraints satisfaction by licensees may be a symptom of regulatory system weakness associated to safety culture[5]. Regulatory requirements to the licensee to provide further evidences for nuclear safety analysis do not necessarily constitute symptoms of weakness.

On the other side, applicants or licensees do not specify the requirements for CFD calculations acceptability in licensing. Regulators should explicitly specify the constraints. The main constraint regarding CFD codes is that they have to be verified and validated for the intended application and that they are used by qualified personnel and in the range of validity of their development and V&V.

The constraints are necessarily technical and procedural. In this case, a new aspect emerges for consideration: the risk of regulations over-specification or over-constraining[6]. This may have a negative effect on the licensee attitude, due to the different actions that may follow: a) the licensee *per se* avoids implementing an optimized solution for the sake of simplifying the presentation and because there is no contradiction with system behavior by considering the regulatory specification, saving time and money; b) the design is submitted and the regulator does not accept the

[5] Partially based on a somewhat old (*circa* 2003) discussions with Ing. Alfredo Biaggio, ARN

[6] From a discussion with Dr. Francisco Spano, ARN, 2014

optimized solution because it is not compliant with the (over-constraining) regulatory constraint; c) the licensee implements the optimized solution at the risk of engaging in a costly technical discussion with the regulator. Obviously this list is not exhaustive and only shows three possible situations from which, (a) and (b) contradict the ALARA principle of Radiological and Nuclear Safety.

In some cases, licensing is based on system global performance evaluation (like the Argentinean regulation AR-3.1.3) rather than on specific system parameter values or figures of merit (like in the NRC´s documents CFR 10 §50.46 and Appendix K to Part 50 - ECCS Evaluation Models) embedded in a global framework. In both cases the licensees and designers have to face by themselves the question of a developing a work program dealing with the qualification of codes and their users for the intended application. Qualification implies codes V&V activities, uncertainties quantification, in a nuclear quality assurance framework. Coming to the case of system global performance evaluation, licensees –not undesirably- may state particular (sometimes called "intermediate") safety goals to be reached in their analyses leading to compliance with global safety criteria and this should be agreed with the regulator[7]. This may save time, particularly when dealing with the evaluation of safety barriers, because figures of merit naturally emerge and must be discussed at different levels of safety analyses during the licensing process, even if they are not explicitly mentioned in a regulation. Early consideration is beneficial. In the case of specified systems parameters, step by step satisfaction of safety goals is accomplished, even when the licensee is free to

[7] From a discussion with Ing. Oscar A. Mazzantini, Nucleoeléctrica Argentina S.A., 2014

make its proposals, and global system performance must be also demonstrated. In the end, satisfaction of Radiological and Nuclear Safety constraints imposed must be demonstrated in both regulatory approaches.

Depending on the particular regulatory context (like country) regulations may establish requirements on the submission of licensing documentation involving nuclear safety calculations to ensure satisfaction of regulatory constraints. Requirements deal, among QA and other procedural aspects, with code verification and validation, uncertainty quantification, user qualification and more. An interesting example may be found in a requirements document NNR (2006) and its associated licensing guide NNR (2006a) that specify about 100 items to be satisfied for the submission of licensing documentation involving code calculations.

Preliminary statements on CFD role

The following statements (Answers A1 and A2) are introduced to fix ideas on which is the rationale that will be followed in the rest of the paper.

Q1. What is today's role of CFD in nuclear safety applications dealing with the licensing of a nuclear installation?
A1. *To provide support to well established, general methods of analysis by means of detailed results*

Q2. What should never be the role of CFD in nuclear safety applications dealing with the licensing of nuclear installation?
A2. *To provide results extending the range of existing experimental data or replacing its lack for validation support in the licensing documentation*

Discussion and justification

This section is aimed at presenting the aspects that should lead to conclusion A1. Background material is also considered and discussed later, focusing on providing further elements for the justification at seek. It is implicitly assumed that CFD *per se* is nowadays not a sufficiently developed methodology to self-sustain as an independent analysis tool in relation to nuclear reactor safety. This implies the necessary V&V of codes results. It must be emphasized that V&V methodologies are, also nowadays, sufficiently established.

There is plenty of literature on CFD applied to nuclear installations and due to different methodologies, non-public scrutiny of proprietary validation data (i.e. the impossibility of reproducing results or using them to enhance expertise in the modelling of a particular subject) and originating schools, it is usually difficult to discern on their validity. Reproducibility of results is almost impossible without detailed access to input data if the same code is to be used (anyway, this is a doubtfully fruitful activity for a regulator). It must be recalled that different codes may produce different results under the same hypotheses and input parameters. It must be recalled that different codes may produce different results under the same hypotheses and input parameters.

Contrary to the conviction of many CFD practitioners, results from their papers do not necessarily constitute an endorsement to the quality of safety analyses. Experimental results databases from integral test facilities (ITFs) and separate effect tests (SETs), on the contrary, are valid references when properly intra/extrapolated. This will be discussed later in this paper. On the other side, CFD provides access to dependent variables (DVs) that are otherwise impossible to check. However, not necessarily all DVs are relevant to safety, although they may be important in R&D. The same applies to flow patterns. It is interesting to point out that the generalization of 1D results by CFD approximations may be costly and time consuming. Obtaining a set of results by CFD for an almost 1D flow in non-isothermal conditions (like in natural circulation) in TH circuits consisting of horizontal and vertical pipes including heat sources and sinks may be difficult if agreement with 1D codes results is at seek. The results obtained must be checked for agreement of macroscopic variables too (i.e. checking the accuracy of distributed and concentrated pressure losses, flow rates, thermodynamic behavior, etc.).

Section 3 of Smith et al. (2015) considers the NRS problems where (single-phase) CFD analysis is expected to bring real benefits. The declared basic objective of the activity is to provide documented evidence on the need to perform CFD simulations, showing benefits and shortcomings of the present status of CFD development. The following problem listing, identified in the quoted reference is: Erosion, Corrosion and Deposition; Core Instability in BWRs; Transition boiling in BWRs – determination of MCPR; Recriticality in BWRs; Lower Plenum Debris Coolability and Melt Distribution; Boron Dilution Mixing, Stratification and Hot-Leg Heterogeneities including: a) Hot Leg Heterogeneities, b) Heterogeneous Flow Distributions, c) BWR/ABWR Lower Plenum Flow, c) Water-Hammer, d) Condensation e) Pressurized Thermal Shock (PTS), f) Pipe Break Induced Break, g) Thermal Fatigue in Stratified Flows, h) Hydrogen Distribution, i) Chemical Reactions /Combustion /Detonation, j) Aerosol Deposition/ Atmospheric Transport (Source Term), k) Atmospheric Transport (Source Term), l) Direct-Contact Condensation, m) Bubble Dynamics in Suppression Pools, n) Behavior of Gas/Liquid Interfaces, o) Special Considerations for Advanced Reactors, p) Flow induced vibration of APWR radial reflector, q) Natural circulation in LMFBRs, r) Natural Circulation in PAHR (Post Accident Heat Removal), s) Gas Flow in the Containment following a Sodium Leak, t) AP600, AP1000 and APR1400, u) SBWR, ESBWR and SWR-1000, v) High Temperature Gas-Cooled Reactor, v) Sump Strainer.

It is almost obvious that this rather long list brings many opportunities to profit from established developments also in other areas than the nuclear. However, as may be clear also from reading the report, it is not a closed issue and many applications need development and V&V so, direct extension of these items to licensing is not yet possible.

Very recently, a forum for activities related to the use of systems thermo-hydraulics best estimate codes has been presented (Ahn et al., 2015) intended also to promote the connection of these codes with CFD codes on a common ground. In relation to BPGs for two-phase flows, Bestion (2012) contributed an enunciation that clearly specify steps to correctly posing the analysis of these flow using CFD codes. The emphasis is on physical aspects rather than on computational aspects.

Summarizing, there is an important *corpus* of information from which it is possible to get guiding principles to consider in the formulation of CFD computer models. Most of them recognize that they are limited in scope (something that is also implicit in the intended field of application). Nevertheless, nothing is enough or closed to assure the appropriateness of a CFD analysis. The user of a code must be certain that its validation database includes the case under analysis in an appropriate way. Otherwise, this work must be undertaken by the user, making this task not easily achievable in a reasonable time. Having basic skills, intuition regarding the solution, knowledge on the model limitations and a very careful examination of the results obtained may be a way to proceed if limited support is at seek, but **A2** above must always be respected.

Further considerations

The following paragraphs are aimed at clarifying several aspects related to the use of CFD in the Nuclear Reactor Safety context. They are part of the present discussions in specialized fora, aimed at improving the usefulness of CFD predictions. Specific items are preceded by some necessary definitions.

V&V, Unavoidable definitions

The errors associated with calculations and measurements can also be characterized with regard to their accuracy and precision.

→ ***Accuracy*** refers to how closely a computed or measured value agrees with the true value.

→ ***Precision*** refers to how closely individual computed or measured values agree with each other.

A graphical illustration and further use may be found in Chapra (2012). These concepts have been key to the development of particular techniques for uncertainty quantification for validation analyses.

To introduce the subject some definitions are unavoidable. Instead of attempting dubiously original, independent definitions it is considered more appropriate including some consolidated definitions, as extracted from (NAS, 2014). The interested reader may also consult (Roache, 2009). Figure 1 shows a way to (clockwise) proceed when dealing with the setup of models to represent the behavior of a physical system.

→ ***Mathematical model (Synonym: conceptual model)*** A model that uses mathematical language (sets of equations, inequalities, etc.) to describe the behavior of a system

→ ***Computational model (Synonym: computer model)*** Computer code that (approximately) solves the equations of the mathematical model.

→ ***Verification*** The process of determining whether a computer program ("code") correctly solves the mathematical-model equations. This includes code verification (determining whether the code correctly implements the intended algorithms) and solution verification (determining the accuracy with which the algorithms solve the mathematical model equations for specified quantities of interest).

→ ***Validation*** The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

→ ***Extra[intra]polative prediction*** The use of a model to make statements about quantities of interest in settings (initial conditions, physical regimes, parameter values, etc.) that are outside [inside] the conditions for which the model validation effort occurred.

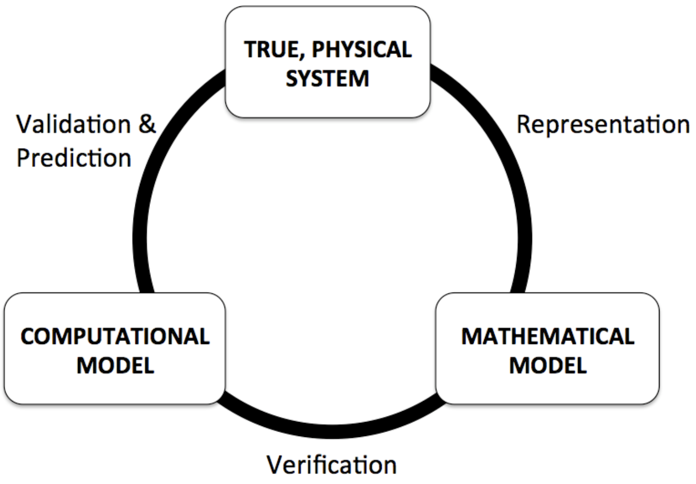

Figure 1 A circular road for models formulation in relation to real world (NAS, 2014)

The previous definitions may be illustrated as shown in Figure 2, which is aimed at putting also in evidence the particularly important aspect of scaling distortions in experiments designed and constructed for validation purposes. This aspect will be discussed later. In passing, it may be noted that it is the computational model that needs verification to a large extent. The verification step location in Figure 1 is somewhat arbitrary.

On the use of codes and its relation with V&V

Figure 3, taken from (Oberkampf and Trucano, 2002), illustrates how models can be used in a usual case in engineering, when the prediction point falls outside the validation domain. This situation may often arise when dealing with substantially new designs. It must be clarified that these authors introduced this flowchart to illustrate the relationship between prediction and validation processes. The link between both aspects is shown in the arrow "Inference from comparisons". However, a cautionary comment must be stated with reference to this procedural flowchart: it is somewhat difficult to accept that the jump from comparisons to sound extrapolative predictions can be performed more precisely than by induction, as one possible way of inference[8] and this imposes some limitations on the validity of conclusions.

Firstly, a digression on the role of induction in science could be worth considering and the reader is referred to the specialized literature, starting from the very classic chapter in Russell´s book of 1912 to the

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[8] INFER: 1- to derive as a conclusion from facts or premises
INDUCE: 3- to determine by induction; specifically : to infer from particulars
DEDUCE: 1- to determine by deduction; specifically: to infer from a general principle
From Merriam-Webster online dictionary, http://www.merriam-webster.com/

specific analysis in Bunge, (1960). The conclusion in the latter reference is herein quoted[9].

This quotation is justified because it may shed some light to the following problem[10]:

Q. suppose you are faced to a *new* (Engineering) thermal-hydraulic design problem, how do you proceed to advance on its best estimate (CFD) solution?

A. the answer is procedural and may be synthetized as follows: a) Setup up of a theoretical model, even of limited scope, with appropriate hypotheses; b) Setup of a preliminary design by application of established engineering practices and "low resolution" codes; c) Detailed flow analysis using a CFD approximation; d) Theoretical optimization of a prototype; e) Setup of an experimental study, implementation of an experimental rig and obtainment of results; f) Final design adjustment and g) finally and more importantly, validation of the simulation by the obtainment of new, hopefully improved, results. These steps establish, in a qualitative way, what is implicit in the quoted reference before.

A fully experimental approach without a theoretical specification frame is almost useless. The proper balance of modeling hypotheses must lead

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[9] **"5. Conclusion. As must have been suspected by many, scientific research seems to follow a via media between the extremes of inductivism and deductivism. In this middle course induction is instrumental both heuristically and methodologically, by taking part in the framing of some hypotheses and in the validation of all kinds of hypotheses. Induction is certainly powerless without the invention of audacious transcendent hypotheses which could not possibly be suggested by the mere examination of experiential data; but the deepest hypotheses are idle speculation unless their lower-level consequents receive instantial confirmation. And induction plays scarcely a role in the design of experiments, which involves theories and creative imagination; but experiment is useless unless it is interpreted in terms of theories that are partly validated by the inductive processing of their empirically testable consequences. To sum up, induction -which is but one of the kinds of plausible reasoning- contributes modestly to the framing of scientific hypotheses, but is in-dispensable for their test, or rather for the empirical stage of their test."**

[10] From a question following the original lecture presentation

experimentation, i.e. inductivism and deductivism should be used to offer a mid-way route to successful approach to useful data collection[11].

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In passing, a naive exemplification on the validity of a pure inductive analysis is illustrated in the side picture for a plausible sequence of facts. There is no behavior explanation without a set of theoretical hypothesis concerning the possible appearance of a discording evidence. They must be previous to the collection of proving evidences, no matter how numerous they can be.

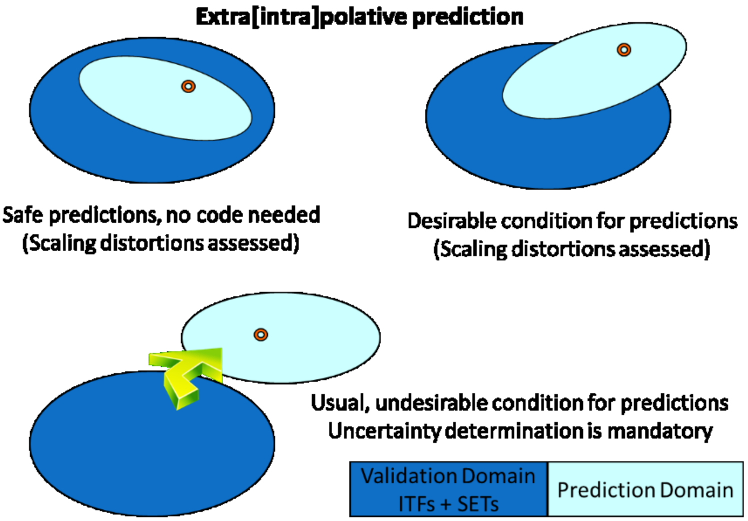

Figure 2 Definition of prediction domains

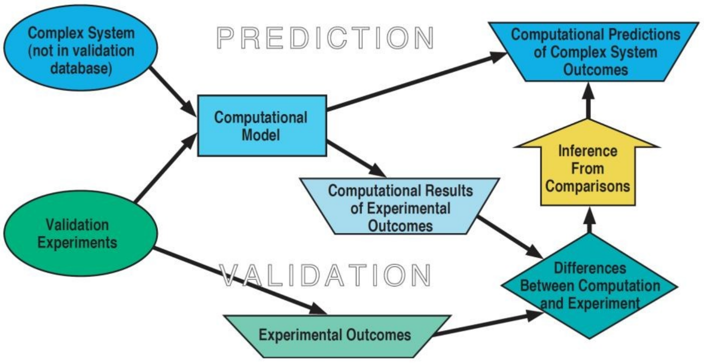

Figure 3 "Relationship of validation to prediction"
(This is Figure 7 and its caption in Oberkampf and
Trucano, 2002)

In particular, scaling aspects are important when dealing with ITFs that reduces a 3D geometry installation to an almost 1D set of components, since the CFD detailed capabilities analysis may be not relevant for a 1D representation that does not reflect the peculiarities of the flow patterns in a (usually) 3D geometry. A somewhat recent discussion on the subject of scaling and the related "scaling issues" have been considered at a workshop on scaling effects (NURETH-15, 2013). Separate effect tests in other than equal height, volume to power scaling may be guiding for validations but it is not clear whether or not they may cover the necessary range of data needed.

Suppose now that a code has passed the stage of verification. Again in Figure 2, the three illustrated prediction scenarios in relation to validation purposes, imply considering a) a domain of (valid, statistically characterized) representative existing quantitative, experimental data for the prediction problem at seek; b) a domain of known predictions (that may provide inductive evidence of code validity) and c) a prediction point, where the solution is to be predicted. The upper-left condition implies intrapolation, a condition that may be considered "safe" provided that the necessary scaling distortions are assessed. This aspect is obviated for one-to-one correspondence between physical model geometry and thermodynamic conditions, e.g. when constructing a mockup or prototype. Really, the use of codes for predictions in these conditions does not seem justified, except for the obtainment of confirmatory DVs not accessible experimentally. Please note that a NPP prototype is not suitable for this analysis because plant conditions cannot be all under the control necessary to get detailed data (this aspect has been discussed since years ago, see e.g., Shotkin, 1996). Nevertheless, the sought DVs cannot be considered an essential part of the licensing process, recall **Q2** and **A2** from a previous Paragraph, again because of the induction process limitations. The upper-right condition is perhaps the desired condition for code predictions, implying "prudent extrapolation" from the experimentation domain. Predicting in these conditions, after having assessed the effects of scaling distortions will be a prudent interpretation of Figure 3, despite the warnings discussed before and the explicit enunciation that it is intended for prediction of complex systems response not in the validation database. Figure 3 should really be considered, according to their authors, for the lower-left illustration of code prediction processes. In these cases, the aforementioned comments must be considered plus a mandatory evaluation of uncertainties which, in this case, includes scaling distortions and codes modeling uncertainty. Anyway, it must be recalled that the evaluation of the prediction uncertainties is nowadays considered essential in all types of code predictions, at least to generate qualified results in the nuclear field.

User effects

The so-called "user effects", well addressed for systems TH codes and consolidated almost two decades ago (IAEA, 1998), are quite important also with CFD codes because codes dials are still present explicitly or implicitly, sometimes in a subtler way (like interaction of grids and sub-models, the introduction of code enhancements by users, user defined functions, codes validity extrapolations, etc.). It is useful to mention here what is implicit in the qualified use of CFD (and also other type of) codes: that user skills must include deep knowledge of Fluid Dynamics. This author contributed to the discussion, pointing out the essential aspects that user qualification meant regarding the finite-difference methods in Fluid Dynamics, a well-known antecessor of present industrial CFD codes, in relation to NPPs. Some particular aspects are excerpted in Appendix I. The evolution of detailed industrial CFD codes lead to complex codes, sometimes constituted by sets of interacting complex codes. This increments complexity and Wulff, (2007) has pointed out these aspects, showing how two-phase flows in practical systems may also be handled without increasing the complexity, while keeping physical aspects in mind.

Best Practice Guidelines (BPGs)

BPGs stands for "Best Practice Guidelines" and is a guiding, non-prescriptive, succession of steps to follow to produce sound predictions by means of computational models, in the particular field of CFD. The denomination BPGs seems to have originated in an initiative by ERCOFTAC Special Interest Group in 1997 that produced a report cited in Menter (2002), under the authorship of Casey and Wintergerste (2000). Without such a name, BPGs have been considered implicitly in CFD codes as a recommendations step in the solution process when the problem setup finishes. Careful consideration of the classic book by Roache (1998), a second edition of its 1972 predecessor, may help to find many hints to deal with the appropriateness of problem setup. In a limited context, this author (Ferreri, 1989) also contributed with a helping system for the selection of numerical schemes to solve advection problems based on the desired properties of the solution. More recently (Mendelhall, 2006), presented an advising expert system called BPX (for Best Practices eXpert) that has been developed to assist in the solution of Fluid Dynamics problems in Aerodynamics. It provides expert knowledge for CFD codes to users, developers, and technology managers to enable high quality solutions with reduced uncertainty and lower cost. This expert system provides,

according to its authors, searchable knowledge databases with guidelines for problem definition, input preparation, grid generation, code selection, results interpretation and V&V. In its original formulation, BPGs have been established as an outcome of a collaborative effort of the OECD/CSNI to a) show to end-users, utilities and regulators to which extent CFD can enhance the accuracy of safety analysis and b) that it implies "addressing the lack of certainty on CFD results". BPGs have been also considered for marine applications (WS Atkins, 2002).
Present efforts deal with the definition of accuracy metrics for CFD calculations in limited Nuclear Safety contexts. The original BPGs are documented in Menter (2002) -consolidated in Scheuerer (2005)- and contain detailed information on: a) the formalized judgment of results obtained with different CFD software packages that includes the definition and quantification of round-off, iteration and discretization errors and the assessment of modeling errors; b) the consistent use of CFD methods for reactor safety problems. These guidelines relate to geometry and grid generation, boundary and initial condition specification, selection of suitable physical models and handling of solution algorithms and c) the judgment of experiments regarding their use for verification and validation of CFD methods.

The guidelines include criteria for checking global mass, momentum, and energy balances, consistency checks for field data and plausibility checks. Experiments are grouped in a hierarchy ranging from laboratory studies to industrial field tests. In 2007 the BPGs have been updated and given a more general scope under the authorship of seventeen specialists led by Mahaffy (2007/2015) and an additional group of experts, whose opinions were considered, either verbally or by e-mail.

The guidelines include (in 164 pages):

a. A historical introduction, based on institutional and country contributions (most activities are reported starting in the 80's)
b. An account of all the aspects to be considered in setting up and application criteria for CFD methods use in Nuclear Reactor Safety, including problem definitions, ranking of phenomena, gridding and V&V of codes. Opinions are stated in many cases and practical advises are given.
c. Appropriate consideration to the fact that "computer simulation is much more than generating an input and observing results"
d. A "check list for a calculation" that is included

As a general advice, it may be stated that BPGs must be carefully considered because they reflect the opinion of a qualified group of experts. However, a senior CFD specialist may be sometimes reluctant to the specification of BPGs, in particular the check list, because non-experienced CFD codes users may be led to feel too confident in the results of a particular case after having solved a set of problems in a more limited prediction domain and precluding discussions, even more if the steps provided by a check list have been followed[12]. The discussion: "On the use of codes and its relation with V&V" before and also the risks imposed by over specification may be worth considering. Also, and surely more importantly, the objectives of the report in

[12] The present author firmly adheres to this position but its enunciation to an audience of senior colleagues produced some rejection. The consensus of non-tight adherence to BPGs check lists but considering them as a non-binding guidance and that they are not enough to assure valid results was finally reached.

Mahaffy (2007/2015) and shown in the excerpt[13], clear up the scope of these BPGs. It must be emphasized that the scope was restricted to single-phase problems. Sometimes, authors of advising documents or systems including BPGs are not so prudent in their assertions.

A comparison of V&V methodologies was presented by Peters et al. (2011). It must also be considered that following all the steps for V&V and UQ, like in Mahaffy (2007/2015) or ASME V&V 20 (2009), implies a hard work, a long time to perform the analyses and very high costs.

Institutionally sponsored approaches to BPGs, V&V, QA and related issues

The following is a non-exhaustive list of reports related to what has been discussed before. Some of them are referenced in full in the REFERENCES section at the end of this document or may be searched in the web.

ASME NQA-1 Certification Program, 2014
AIAA G-077, 1998
ASME V&V 20, 2009
ASME V&V 30 (HTGR specific, compliant ASME NQA-1, to be issued)
ASTM E1355-05a (NUREG-1824, for fire simulation in NPPs), 2005

[13] "Objective of the Work: This document is intended to provide an internally complete set of guidelines for a range of single phase applications of CFD to NRS problems. However, it is not meant to be comprehensive. We recognize that for any specific application a higher level of specificity is possible on questions of nodalization, model selection, and validation. This document should provide direct guidance on the key considerations in known single phase applications, and general directions for resolving remaining details. It is our intent that this will serve as a template for further application specific (e.g. PTS, induced break) BPG documents that will provide much more detailed information and examples."

ERCOFTAC SIG on Dispersed Turbulent Multi-phase Flow, 2007
ITTC 7.5 – 03 02 – 03, 2011
MARNET-CFD Report, 2002
NASA TECHNICAL STANDARD, NASA-STD-7009, 2008
NEA/CSNI/R(2007)5, 2007 and Revised R(2014)11, 2015, Nuclear Eng. specific
NEA/CSNI/R(2014)12, phase 3, 2015
NRC CSAU (Nuclear Eng. specific, TH systems codes), 1988
NUREG 2152, (for CFD in dry casks simulations), 2013

This list is worth considering because it reflects the technical opinion of many people and may give a qualified guiding to CFD practitioners. Even when some topics may seem away of the Nuclear Reactor Safety applications, particular aspects of interest may be found along with their discussion (e.g. CFD with free liquid surfaces, like in the MARNET-CFD Report). In this author´s opinion, such a proliferation of BPGs indirectly confirms that user qualification is at the root of trustiness of CFD applications in all the fields of engineering.

Metrics for CFD codes predictions in particular contexts

Perhaps the most systematic and rigorous analysis on the question of defining and applying metrics in relation to computation and experiment may be found in Oberkampf and Barone (2006). Although general, the analysis is particularly relevant for CFD. Defining a metric implies having quantitative criteria to compare computer code results with reference results. This applies to both V&V processes but more importantly to validation. Also, Trucano et al., (2006) advanced in the definitions of important questions like calibration, validation, and sensitivity analysis differences in order to clarify these, sometimes misused, terms. Some interesting considerations on accuracy quantification metrics have been advanced by Moretti and D'Auria (2014) who base their analysis, in the particular context of CFD simulation of in-vessel flows, on physical aspects of the flow.

1. Related to perturbation appearance: a. location(s) of appearance (and related difference) b. time of appearance (and related difference) c. time of disappearance (and related difference) d. perturbation transit time (and related difference)	**4. Related to accumulated perturbation:** a. value at plateau (and related difference) b. average amplitude from FFTBM application
2. Related to maximum perturbation: a. location of maximum (and related difference) b. time of maximum (and related difference) c. maximum value (and related difference)	**5. Related to perturbation barycentre:** a. time-averaged location b. maximum standard deviation of perturbation spatial distribution (and related difference) c. average standard deviation of perturbation spatial distribution (and related difference)
3. Related to core-averaged perturbation:	**6. Related to FLOMIX deviations:** a. deviation #3, with sign

a. time of maximum (and related difference) b. maximum value (and related difference) c. mean time (and related difference) d. standard deviation (and related difference) e. time gradient of perturbation front (and related difference)	b. deviation #3, without sign c. deviation #3, root mean square **7. Related to spatial gradients:** a. maximum slope (and related difference) **8. Related to 3D Fast Fourier Transform Based Method (FFTBM):** a. average amplitude

Table 1 Set of indicators for code-to-experiment comparison and accuracy quantification

Table and caption from Moretti and D'Auria (2014)

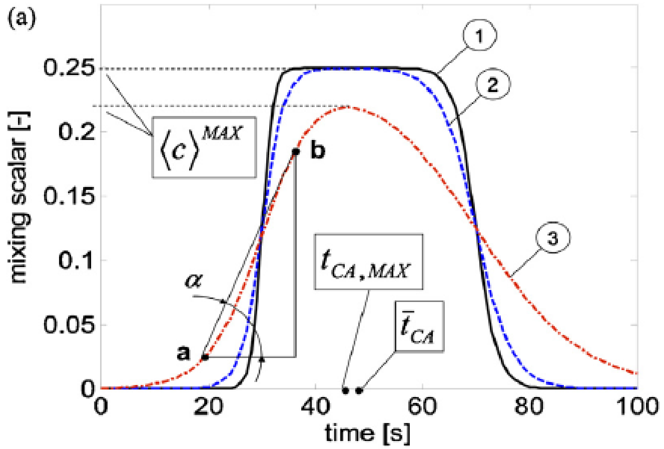

Figure 4 Illustration of core-averaged perturbation trends for the passage of a de-borated slug

Table and caption from Moretti and D'Auria (2014)

The interested reader is referred to the quoted reference for details but some comments are appropriate here. Perhaps, one aspect worth considering of this analysis is that they explicitly take into account the qualitative analysis of results before proceeding to quantitative accuracy determinations. Making reference to Figure 4, which illustrates the transport of a slug of boron concentration (recall that it is scalar transport plus diffusion), it may be stated that diffusion is mainly originating in numerical diffusion for curve (3) with respect to curve (1) that may be supposed near to the original perturbation. What is important to point out is that condition (3) is less conservative if some set point is based on a low value for concentration, because of interaction with neutron kinetics. In the case shown, overestimation of boron concentration, may lead to overconfidence on having reached a safe state. The time appearance of the slug may have strong influence in reactor safety analysis and determine the regulatory constraints for acceptance of a boron injection system installation, although this applies mainly to injection start rather than to transport into the core. The previous comment applies also to this case depending on the position of the injection point.

Trends: cooperative efforts and consortiums and a proposal of local validity for collective progress

Presently, collaborative efforts are widespread, aimed at accomplishing high-tech goals. The collaborative inter-institutional efforts will continue in the decades to come. This originates on the huge amounts of economic resources and person-hours needed. In the USA efforts are leaded by the Consortium for Advanced Simulation of Light water reactors (CASL) that includes academia, DOE National Laboratories and industry. Industry participation comes from software products and provision of problems and to provide a link to affordable computer clusters, instead of "frontline" systems like Titan at ORNL (report CASL-U-2014-0006-000).

In Europe, the OECD/NEA/CSNI organizations have several working groups that provide the reports that have been cited before. It seems that "working isolated" is inappropriate to face the near future. This situation is particularly true when resources are somewhat scarce.

Establishing a local consortium to deal with joint work to promote knowledge on the application of advanced computational techniques in Nuclear Engineering and Technology has been the subject of a recent local meeting[1]. This is an objective to be reached despite of institutional skepticism and selfishness. This author is convinced of its convenience and it was the consensus reached. Establishing a database of existing experimental data in relation to local nuclear installations and some benchmark experiments should be the next step.

Conclusions

Maturity of CFD is still to be reached regarding TH applications for NPP licensing. "Maturity" should be applied in a general way to models, modeling and modelers. This is particularly true in Argentina (just a few applications using CFD). The difference between R&D and licensing applications approaches must be clearly understood by all the people involved. This is particularly true when dealing with Nuclear Safety *plus* Licensing.

Reasons for the above assertions come from the need of unified, more general approaches for physical models (e.g. two-phase flows, turbulence models, etc.) and the need of huge efforts and resources dedicated to V&V and codes uncertainty quantification. User qualification through validation work must be undertaken with care and must be the subject of future work. This applies to licensees and regulators.

It may be verified that even in the leading projects like CASL, systems TH codes (1D) will be used to model out-of-core TH and heat transfer, providing the linking between the whole system TH behavior and the in-core advanced simulations. Specific working groups to deal with this interface are already established. Consequently, developing expertise in the use and development of codes like TRACE, maintenance of RELAP5 and other non-CFD codes is worth considering. Even when the search for simplicity is neither always convenient nor obligatory, it must be remembered that interaction of complex codes increase the complexity of the systems analysis.

In this author's opinion, both questions (Q1 and Q2) and answers (A1 and A2) above should be included conceptually in the regulatory constraints imposed by the regulatory body.

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References

Please note: **CFD4NRS-*xx*** refers to the following Meetings: **CFD4NRS; CFD4NRS-3; CFD4NRS-4; CFD4NRS-5 ; XCFD4NRS**

Ahn, S.H., Aksan, N., Austregesilo, H., Bestion, D., Chung, B.D., D'Auria, F., Emonot, P., Gandrille, J.L, Hanninen, M., Horvatović, I., Kim, K.D., Kovtonyuk, A. and Petruzzi, A., "FONESYS: The FOrum & NEtwork of SYStem Thermal-Hydraulic Codes in Nuclear Reactor Thermal-Hydraulics", Nuclear Engineering and Design, 281, pp. 103-113, 2015

ASME, "ASME V&V 20-2009 Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer", American Society of Mechanical Engineers, 2009

Boyd, C., "Perspectives on CFD analysis in Nuclear Reactor Regulation", CFD4NRS-5, 2014

Boyd, C., "Advancements and Challenges of CFD in Nuclear Reactor Regulation at the USNRC", Invited Lecture, 1st Pan-American Congress of Computational Mechanics, Hilton Hotel, Buenos Aires, April 27-29, 2015

Bestion, D., "Applicability of two-phase CFD to nuclear reactor thermalhydraulics and elaboration of Best Practice Guidelines", Nuclear Engineering and Design, 253, pp. 311- 321, 2012

Bunge, M., "The Place of Induction in Science", Philosophy of Science, Vol. 27, No. 3, pp. 262-270, 1960

Casey, M. and Wintergerste, T. (Eds.), "Special Interest Group on 'Quality and Trust in Industrial CFD' Best PracticeGuidelines, Version 1," ERCOFTAC Report, 2000

Chapra, S.C., "Applied numerical methods with MATLAB for engineers and scientists", 3rd ed., Mc Graw Hill, 2012

Ferreri, J.C. and Grandi, G.M., "On Expert System Assisted, Finite-Difference Schemes Selection in Computational Fluid Dynamics", Proc. of Sixth Int. Conf. on Numerical Methods in Laminar & Turbulent Flows, C. Taylor, P.M. Gresho, J. Thompson, R.L. Sani and J. Hauser (Eds.), Swansea, July 1989, Pineridge Press, 2, pp. 1663-1673, 1989

IAEA, Summary report of the IAEA specialist meeting on user qualification for and user effect on accident analysis for nuclear power plants, Vienna, August 31-September 2, 1998

Mahaffy, J., Lead Author, "Best Practice Guidelines for the use of CFD in Nuclear Reactor Safety Applications", OECD/NEA/CSNI/R(2007)5, 2007; Also see the Revision under the same title in: Nuclear Safety NEA/CSNI/R(2014)11, 2015

Mendenhall, M.R., Stremel, P.M. and Hegedus, M.C., "A Best Practices System for reduced uncertainty in CFD", ICAS 2006 – 25th International Congress of the Aeronautical Sciences, Sep. 3.-8. 2006, Hamburg, Germany

Menter, F., "CFD Best Practice Guidelines for CFD Code Validation for Reactor-Safety Applications", ECORA Project, CONTRACT N° FIKS-CT-2001-00154, Report EVOL– ECORA – D 01, February, 2002

Moretti, F., D'Auria, F., "Accuracy quantification metrics for CFD simulation of in-vessel flows, Nuclear Engineering and Design, Vol. 279, pp. 200–209, 2014

National Academy of Sciences (NAS), "Assessing the Reliability of Complex Models: Mathematical and Statistical Foundations of Verification, Validation, and Uncertainty Quantification", Committee on Mathematical Foundations of Verification, Validation, and Uncertainty Quantification, NAS, 2012

NURETH-15, The 15th International Topical Meeting on Nuclear Reactor Thermal-hydraulics, Pisa, Italy, Conference Workshop W19, Relevance and Purpose of Scaling Analysis for the development of Better Simulation Thermal-Hydraulic Tools, May 12-15, 2013

Oberkampf, W.L. and Trucano, T.G., "Verification and Validation in CFD", Progress in Aerospace Sciences, vol. 38, pp. 209-272, 2002; for this figure see also SANDIA REPORT SAND2002-0529, March 2002

Oberkampf, W.L., Barone, M.F., "Measures of agreement between computation and experiment: Validation metrics", Journal of Computational Physics, Vol. 217, pp. 5-36, 2006

OECD, "Benchmarking of CFD Codes for Application to Nuclear Reactor Safety (CFD4NRS)", Workshop Proceedings, Garching (Munich), Germany, 5-7 September 2006, © OECD 2007

OECD/NEA & IAEA Workshop, "Experiments and CFD Code Applications to Nuclear Reactor Safety (XCFD4NRS)", Commissariat à l'Energie Atomique, Grenoble, France, 10-12 September, 2008

OECD/NEA & IAEA Workshop, "CFD for Nuclear Reactor Safety Applications (CFD4NRS-3)", Bethesda (Washington), USA, September 14 -16, 2010

OECD/NEA & IAEA Workshop, "CFD for Nuclear Reactor Safety Applications (CFD4NRS-4), September 10 – 12, Daejeon, Korea, 2012

OECD/NEA & IAEA Workshop, "Application of CFD/CMFD to Nuclear Reactor Safety and Design and their Experimental Validation (CFD4NRS-5)", September 9-11, Zurich, Switzerland, 2014

Peters, S., Tschaepe, L., Zhang, B. and Ruggles, A., "V&V Methodology Comparisons: AIAA G-077(1998), ASME V&V 20 (2009), ASTM E1355-05a (2005), NEA/CSNI/R (2007), and NRC CSAU (1988)", The 14th International Topical Meeting on Nuclear Reactor Thermalhydraulics, NURETH-14 Log Number: 586, Toronto, Ontario, Canada, September 25-30, 2011

Roache, P.J., "Fundamentals of Computational Fluid Dynamics", Hermosa Publishers, USA, 1998

Roache, P.J., "Fundamentals of Verification and Verification", Hermosa Publishers, New Mexico, USA, 2009

Russell, B., "The Problems of Philosophy", London: Williams and Norgate; New York: Henry Holt and Company, 1912. This book may be found in various formats version as a Project Gutenberg's file, http://www.gutenberg.org/files/5827/5827-h/5827-h.htm, updated in February 2013, among many other source formats

Scheuerer, M., Heitsch, M., Menter, F., Egorov, Y., Toth, I., Bestion, D., Pigny, S., Paillere, H., Martin, A., Boucker, M., Krepper, E., Willemsen, S., Muhlbauer, P., Andreani, M., Smith, B., Karlsson, R., Henriksson, M., Hemstrom, B., Karppinen, I. and Kimber, G., "Evaluation of computational fluid dynamic methods for reactor safety analysis (ECORA)", Nuclear Engineering and Design, 235, pp. 359–368, 2005

Shotkin, L. M., "Development and Assessment of U.S. Nuclear Regulatory Commission Thermal-hydraulic System Computer Codes", Nuclear Technology, 116, pp. 231-244, 1996

Smith, B.L. et al., "Assessment of CFD for Nuclear Reactor Pafety problems", NEA/CSNI/R(2014)12, phase 3, 2015

South Africa NNR, "Requirements for Licensing Submissions Involving Computer Software and Evaluation Models for Safety Calculations", National Nuclear Regulator, License Document RD-0016 Rev. 0, 2006

South Africa NNR, LG-1045 Guidance for Licensing Submissions Involving Computer Software and Evaluation Models for Safety Calculations, National Nuclear Regulator, License Document LG-1045, Rev. 0, 2006

Trucano, T.G., Swiler, L.P., Igusa, T., Oberkampf, W.L. and Pilch, M., "Calibration, validation, and sensitivity analysis: What's what", Reliability Engineering and System Safety, Vol. 91, pp. 1331-1357, 2006

WS Atkins Consultants, "Best Practices Guidelines for Marine Applications of CFD," MARNET-CFD Report, 2002

Wulff, W., “Simulation of Two-Phase Flow in Complex Systems”, Nuclear Technology, Vol. 159, pp. 292-309, 2007

APPENDIX

Excerpted from the presentation: "User Qualification and NPP Safety Analysis: A Case Dependent Issue or a Discipline of Learning?" by J.C. Ferreri (IAEA, 1998).

A REGULATOR'S SMALL DILEMMA

- Suppose you usually perform safety analyses using a standard[14], thermal-hydraulic systems code
- Suppose you setup a usual, computer-wizard assisted nodalization for a standard NPP
- Suppose you perform a series of standard, smooth code runs and you get results that look standard
- Suppose you write a report according to standards
- Suppose you report to a (standard) boss / manager who expects (hopes for) such standard results

Then,

- Who's going to ask you non-usual questions?
- Or, equivalently, who will be able to detect some possible flaw in the data/results or unforeseen aspects in system's behavior?
- From the point of view of Engineering Judgement: may things be worse?
- Some snappy possibilities for yes:
- What if the regulatory body analysts are not skilled on discretization effects?
- What if instead of a regulator you are a designer?

[14] Standard: a level of quality, achievement, etc., that is considered acceptable or desirable, from Merriam-Webster online dictionary.

- What if you do not realize that in the design/licensing stage all full-plant analyses are pre-test? (in the sense that analyses apply to postulated scenarios)
- Did you realize that consequences are post-test (i.e. they occur to the plant)?

PRESENTATION'S GOALS

- Showing some results coming from well-known aspects of numerical methods and their application to the analysis of systems code results
- Discussing about the basic skills needed for proper nodalization setup from the numerical point of view

ITEMS COVERED

- Emphasis on stability analysis using finite-difference methods
- The effects of:
    1. Dependent variables definition
    2. Variable coupling
    3. Nodalization: variable centering
    4. Nodalization: node number

ANALYSIS SKIPPED…

CONCLUSIONS

BASIC USER SKILLS (Should have appropriate credits in)

- Fluid dynamics (1-p / 2-p)
- Computational modeling
- Uncertainty evaluation
- Data structure QA
- Plant layout and related systems

- Full awareness of systems code models and capabilities (*added:* Being aware of error compensation effects)

BASIC USER ATTITUDES

- Continuous disposition to check his/her ability as a modeler against benchmark analytical and experimental scenarios
- Being non-confident of standard rules as applying to every situation
- Keeping confident on the necessary steps to perform a qualified analysis, disregarding non-affordable deadlines

BASIC USER NEEDS (Should deserve)

- Being defined as a developer and qualifier of nodalizations or/and the person in charge of the analysis of scenarios
- Respect for his/her patient, time consuming work for data preparation and qualification (a typical NPP nodalization implies nearly 3000 lines of 12 items each)
- Time to seek for convergence of results in a given scenario
- Enough time and collaboration for unforeseen aspects of his/her results
- Collaboration for nodalization QA and exploitation regarding plant scenarios
- Respect for his/her interest to check standard modeling criteria for new scenarios leading the code to its boundaries of validity (these will be of obvious help to understand "strange" results)
- Interacting with colleagues in appropriate forums (users' clubs, code developer meetings and so on)
- Reporting to skilled officers