MODELING APPROACH FOR THE DESIGN OF THE NIST NEUTRON SOURCE

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ABSTRACT

The NIST Neutron Source, or NNS, is a proposed new research reactor at the NIST Center for Neutron Research to replace the currently operational, but aging, National Bureau of Standards Reactor (NBSR). The NNS is currently in the pre-conceptual design stage, which heavily relies on modeling efforts to find an optimal design that fulfills the desired facility goals while ensuring safety and compliance with the United States Nuclear Regulatory Commission (NRC) requirements and other local codes and standards. This work outlines the adopted multi-physics modeling approach for the NNS, which focuses on safety, accuracy, and then simplicity. A paradigm is developed to guide decisions related to any modeling effort, where the safety focus is illustrated via diversified examples. A clear distinction is made between the safety engineering efforts and the regulatory compliance efforts, where the engineering efforts demand higher accuracy while the regulatory efforts favor simplicity and conservatism. This distinction is relevant when preparing the preliminary safety analysis report and provides a level of trust for the engineers proposing the design that goes beyond regulatory concerns. Discussions of the paradigm and the underlying verification & validation processes are the focus of this manuscript, providing a generalized look at the modeling approaches and how they are adopted towards the NNS design.

1. Introduction

An effort to design a future replacement for the National Bureau of Standards Reactor (NBSR) at the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) is currently being pursued by the NBSR engineering staff in collaboration with the Brookhaven National Laboratory (BNL). The proposed replacement, namely the NIST Neutron Source (NNS) [1], is in the pre-conceptual design phase where practically all aspects of the design are not yet finalized. At this point, computational models are primary tools to identify favorable and optimal design characteristics that fulfil the desired goals of the facility while ensuring compliance with regulatory requirements. The NBSR is currently regulated by the United States Nuclear Regulatory Commission (NRC), which means that the NRC is also expected to regulate the NNS; as such, it is vital to consider the NRC's standards and requirements when developing the reactor design, prior to engaging with detailed optimization studies. This paper proposes a framework that may be adopted for the design approach of the NNS with particular emphasis on how modeling activities may be carried out. Specific discussions on how models may be verified and validated are included, with recommendations on potential simplifications. Comparisons and discussions of variations from traditional approaches presented by IAEA TECDOC 2018 [2] and 2010 [3] are also included.

2. Design Approach

Traditionally, a team looking to design a new nuclear reactor (regardless of the technology's novelty) should consider first and foremost the function of the reactor (i.e., reason for building a reactor). The function of the reactor will likely dictate some general core characteristics such as the size, shape, neutron spectrum, etc. Upon dictating these general design characteristics, the team may be tempted to begin their design and optimization activities, which is presently performed using various physics modeling codes and tools. In this design stage, the regulatory pre-engagement is warranted as no real construction or licensing can commence without the regulator's approval. Upon reaching a regulatory compliant design, a preliminary safety analysis report (PSAR) and forthcoming licensing and construction activities may be pursued. This traditional approach is visualized in Figure 1, which agrees with the recommendations provided by IAEA-TECDOC-2010 for integrated risk informed decision making.



Figure 1. A traditional approach to designing a nuclear reactor.

Unfortunately, there are notable flaws with the traditional approach in Figure 1, namely the disconnection between regulatory compliance and the general core characteristics. In this approach, it is assumed that a coolant or fuel choice can be made independent of a regulator's input, which may not be always applicable. Furthermore, another potential flaw is the presence of a design optimization loop that is purely dependent on regulatory compliance; wherein the design is engineered to ensure regulatory compliance. This may be ineffective hence it neglects the facility needs such as performance and cost optimizations, which are not necessarily any importance for the regulator, but it should be of importance to the reactor's stakeholders.

Both the presence of this regulatory compliance optimization loop and the disconnection between general core characteristics and the regulatory compliance can lead to a design that can be stuck in the optimization loop without reaching compliance, simply because the general core characteristics were never compliant with the regulator's expectations and standards. Being stuck in such loop will lead to either (1) restart of the entire design process or (2) the exhaustion of stakeholder's resources/interest, for which many examples are known in the history to the public. A modified design approach is proposed in this paper that places regulatory compliance upstream of the process to make better use of the design optimization stage.

2.1. Proposed Design Approach

The proposed approach is visualized in Figure 2, where the general core characteristics and the design itself are both subject to regulatory compliance checks. Note the replacement of the "Design Engineering" process with the "Safety Engineering" process. This places an emphasis

on safety that is beyond regulatory compliance allowing the design to be more reliable than just its paperwork trail (for lack of better words). Note how the design optimization feeds into the safety engineering, meaning that the optimization is only performed on a design that is already compliant with regulatory standards. This is key to improving the quality of the design, where such approach enables a design optimization for staff and safety engineering standards that meet and potentially exceed the design functions without running the risk of non-compliance with regulatory standards. In other words, all designs in the optimization phase are, by definition, compliant with regulatory standards. Note that optimization is optional, so if no optimization is necessary, the correlations/models used in the design/regulatory compliance stage can be reused as-is for the PSAR stage.



Figure 2. The proposed design approach for the NNS.

In this approach, it is also important to note that the regulatory compliance is ensured via early engagement with the regulator during the selection of the general core characteristics and the design, which does not require detailed descriptions of the system, but instead it requires detailed understanding of the regulator's safety and compliance needs. For example, discussions of the modeling methodologies are not recommended to be detailed in this regulatory compliance stage, but instead, they should be spared for the eventual discussions with the regulator within the PSAR further down the line. At the PSAR stage, the models and/or correlations are justified and adjusted per regulatory feedback.

As such, it is strongly recommended to provide simplified-yet-sufficient results in the PSAR for the regulator to ensure that they receive only the verified and validated results in the most simple form (i.e., algebraic correlations and straightforward plots). Such simplification can help in streamlining the discussions with the regulator during the PSAR stage without burdening them with methodologies that are not particularly relevant to the regulator's safety goals. This of course, still requires transparency on the part of the design team; however, effective communication (simplification) is key to ensuring the success of these discussions. Understanding this design approach will require further discussions on the "Regulatory Compliance" and "Safety Engineering" processes.

3. Proposed Design Processes

Per Figure 2, there are two key processes in the proposed design approach which are the regulatory compliance and the safety engineering, wherein compliance precedes safety engineering.

3.1. Regulatory Compliance

The regulatory compliance process, illustrated in Figure 3, begins by identifying the safety needs of the reactor system proposed to the regulator. This is identified via discussions with the regulator on the general core characteristics and design. For example, a light-water reactor

concept will prompt a boiling concern from the regulator, which will lead to discussions on thermal margins like critical heat flux ratios. A gas-cooled reactor in contrast would not have those same concerns, but it will likely prompt concerns on the operating pressure of the system, which can lead to over-pressurization and malfunction of pressurizer discussions. Such safety needs will dictate required reactor systems, components and scenarios that need to be analyzed for the safety review and the PSAR.



Figure 3. The regulatory compliance processes

In some instances, it is possible to refer to literature for a model, methodology, and/or results for satisfying the regulatory concern. This is applicable only if the proposed reactor design has been analyzed prior; nevertheless, its applicability will be subject to scrutiny from the regulator. In many instances when dealing with novel reactor concepts, it is unlikely that literature can completely cover the regulatory concerns, which would lead to the development of a model specifically to cover the concern presented by the regulator. Note how satisfying a regulator's concern never starts with developing custom models and complex methodologies; but instead, it starts with referring to literature. This is key to optimizing the efforts and workflow of the designers.

3.2. Safety Engineering

Upon reaching a regulatory compliant design, it is suggested to go through a safety engineering process wherein the designers specifically consider the staff and stakeholder needs, standards, and desires to improve the regulatory-compliant design. There are two key aspects of safety engineering (1) the reactor modeling and (2) instrumentation and controls (I&C) choices. The I&C selection should be informed by current state-of-the-art standards in the nuclear industry or similar industries as well as regulatory recommendations. For example, during the regulatory compliance stage, anticipated operational occurrences and design-basis accidents would have been discussed with the regulator, which will in-turn dictate the type and reliability of the I&C equipment that is required. The I&C choice should also consider a balance between operational costs and required maintenance periods, which dictates whether predictive or preventative maintenance is desired.



Figure 4. The safety engineering process.

The modeling part of safety engineering, which is the main subject of this paper, will depend on the successful development of computational models and appropriate optimization implementation as presented in Figure 4. Note that the optimizations are purpose-driven, meaning that optimizing for cost is not necessarily identical to optimizing for performance. Of course, an optimization entails the development of a design that still retains the regulatorycompliant characteristics and improves on them.

4. Proposed Modeling Approach

4.1. Developing the Models

The modeling approach proposed for the NNS, shown in Figure 5, is physics-agnostic and would apply to all models (i.e., neutronics, thermal-hydraulics, solid-mechanics, etc.). This is key because although most accept certain codes to be compliant to regulatory standards, the models developed by such codes are not necessarily up-to-standards; therefore, it is vital for the designers to ensure their models' validity via both verification and validation (V&V).



Figure 5. The proposed model development and V&V approach for the NNS.

The approach presented in Figure 5 focuses on the V&V aspect of the model development, which is arguably the most important aspect. Regardless of the model's complexity, it is important to ensure that it is verified: performs as developed and validated such that the model provides results comparable with reality (to within the desired standards). The V&V strategy should be informed by discussions with the regulator, however, the options presented in Figure 5 provide appropriate options to pursue based on known V&V standards and practices [4-7]. Considering that verification can be performed using numerical stability-and-convergence checks and grid-and-input sensitivity analyses, it is usually a straightforward affair. The validation is usually the costly and time-consuming process, which is what this process attempts to decompose.

Per Figure 5, the modeler should begin by identifying which models require validation (if-any). Upon identifying those models, a literature search must be conducted to find experiments or analytical data that can be used to benchmark such models. A modeler should take advantage of such available knowledge to reduce costs and efforts for validating their models.

In the case that selected model cannot be benchmarked against data from literature, the modeler must still attempt to pursue cost-and-effort savings via further decomposition of the modeled physics. As an example, consider the inlet to the NNS as discussed in other works [8-10], which can be modeled as rectangular channel flow of water experiencing separation into 3 parallel rectangular channels and mixing further downstream. Although it has a unique geometry, fundamentally, the flow evolution through the inlet is resembling typical channel flow mixing experiments found in literature [11-12]. As such, with the approval of the regulator, it may be possible to decompose the physics modeled and validate the mixing component only with the mixing experiments from literature. A modeler must contemplate the answer to this question, and they must also strongly consider any regulator recommendations prior to making a decision on the decomposition of the physics. If it can be decomposed, then the modeler can validate with literature; otherwise, a custom experimental effort will be required, which may be included in the initial startup testing of the reactor. As an example, one may reference NRC's regulatory guide 1.68 for initial test programs for water-cooled nuclear power plants [13] as a guide for setting up their model validations.

4.2. Purpose-driven Design Optimization

Upon successfully completing the V&V process, it becomes possible to pursue a purposedriven optimization study, which is visualized in Figure 6. Any optimization will begin by identifying design inputs and boundary conditions. Such inputs could include the fuel composition, coolant density, operating pressure, etc. Upon identifying the design variables, an optimization type should be selected, wherein Figure 6 identifies cost and performance optimizations. Note that cost and performance optimizations can be a singular optimization under certain conditions.

Depending on the desired optimization, the next step is to identify critical variables that drive the optimization. For example, a performance optimization variable for the NNS may be the cycle length, where maximizing it is desirable to improve fuel utilization and reduce waste. The cycle length can also be a cost optimization variable, wherein maximizing it may be desirable to reduce refueling costs. Note how the purposes are different (cost and performance), but the optimization variable and goal are the same (maximizing the cycle length). An example where cost and performance optimizations may have different variables is when considering safety. Contemplate the choice between highly-enriched (HEU) and high assay low-enriched (HALEU) fuels. Whereas HEU might provide the longer cycle lengths mutually desired by cost and performance needs, HALEU is the preferred option to meet the desired non-proliferation goals. Meeting non-proliferation goals is a performance need, but it can lead to increased costs due to novel fuel fabrication techniques. As such, it becomes a balance of the savings from increased cycle length and increased costs for the HALEU fuel. In this instance, it becomes important to understand the sensitivity of cost and performance to cycle length, which can be accomplished via the computation of sensitivity coefficients.



Figure 6. The purpose-driven design optimization process.

The sensitivity coefficients can be represented as numerical values, fitted correlations, or even simply plots. Essentially, they are the culmination of running multiple scenarios using a model of sorts and understanding the purpose variable's sensitivity to variations in any given design input. Upon obtaining this metric, the designer can identify alternatives for the reactor design and make decisions based on their respective safety engineering standards. It should be noted that such optimization process may be performed even after the building and licensing of the reactor.

4.2.1. Sensitivity Coefficients

The computation of sensitivity coefficients might sound straightforward, but attention should be paid to the fine details. Figure 7 shows the sub-process in detail, where the first step is to determine whether or not a model is available to compute the sensitivity coefficients. If available, then it may be used; otherwise, a model needs to be developed per the process in Figure 5. With the model available, it becomes possible to perform sensitivity or parametric analyses to understand the sensitivity of an optimization-purpose-variable to changes in any design input or boundary conditions. The variation in design inputs is typically a function of some input uncertainty that must be found based on either uncertainty in the design input, or based on available choices for that input. The subject of determining an appropriate input uncertainty is discussed later in the paper.

Once the input uncertainties, and by extension the design input ranges are found, the sensitivity study can be performed via either a deterministic or stochastic approach. Another work gives a simple outline on the differences between the stochastic and deterministic approaches [14], and other works demonstrate it for thermal safety margins in the NNS [15]. Regardless of the adopted sensitivity study approach, the results enable the computation of the sensitivity coefficients in either a linearized or fitted behavior, which comes with its own uncertainty range based on modeling uncertainties.

A final step in this process is to assess the quality of the model used to compute the sensitivity coefficients. If the model's fidelity meets the engineering safety standards, then it becomes possible to adopt the results as-is with no additional computations. However, if the model's fidelity falls short of engineering safety standards, then it becomes necessary to apply a

suitable factor of safety on the computed sensitivity behavior. This factor of safety can be based on probabilistic risk assessments as well as previous experience and knowledge from literature, but it must always be in accordance with the regulator's recommendations.



Figure 7. The sensitivity coefficient computation sub-process.

4.2.2. Input Uncertainties

The input uncertainties used for the sensitivity coefficients in Figure 7 should also consider the approach visualized in Figure 8, which can guide the selection and justification for those uncertainties. Identifying them requires accounting for any historical data from a similar or reference reactor, measurement instrumentation error from the selected I&C equipment, as well as knowledge from other sources like literature, code uncertainties, and manufacturing tolerances to name a few. It is not necessary to include all of the aforementioned sources, but it is appropriate to account for all that is available. Henceforth, a propagated uncertainty can be computed for the design input in question.

Similar to the last step of the sensitivity coefficient computation sub-process, a responsible engineer will ask the pragmatic question of whether or not the computed uncertainty meets given engineering safety standards. The answer to this question is not trivial, because, although the uncertainty sources provide the values sufficiently, it is nearly impossible to account for all sources of error. For example, if the input in question is the thickness of the cladding, then not only does the tolerance and measurement error factor into this input's uncertainty, but also the thermal effects on the cladding. Variation in temperature within the core may yield variations in the cladding thickness for various scenarios, which will introduce additional uncertainties that can be attributed to some sort of physical tight coupling. While it is possible to quantify such uncertainties, it might not be feasible; and at that instant, it becomes appropriate to assign a factor of safety to the computed input uncertainty. Of course, the factor of safety must also be informed by any available regulatory guidance on the topic, and its value should be agreed upon with the regulator to avoid delays in later stages of the design process.



Figure 8. The input uncertainty identification sub-process.

With the clarification on the computation of input uncertainties, the proposed design approach shown in Figure 2 is completed. It should be noted that throughout this process, effective documentation of all efforts and decisions is key to success and continued evolution of the reactor design. This is particularly the case when considering the appropriate input ranges that were used in optimizing the design of the reactor.

5. Conclusions

The proposed design approach for the NNS is presented in this paper, with an emphasis on modeling verification and validation activities. Physics decomposition approach is suggested to reduce costs and efforts for validating models without custom experiments of the complex phenomena. A clear emphasis is placed on regulatory compliance and pre-engagement throughout the process, where optimization is only suggested after reaching a fundamentally compliant design with regulator-influenced safety analysis topics. The optimization process encourages the computation of sensitivity coefficients or behavior that can enable an understanding of the reactor's operation as a function of multiple design parameters. The range of inputs selected for said sensitivity analyses is recommended to be dictated by input uncertainties computed by a process that considers any sources of error that can be quantified in a feasible manner. Factor of safety recommendations are given for both the input uncertainties and the sensitivity coefficients. The approaches shown in this paper will serve as guides for future design activities for the NNS, and will likely evolve with experience.

6. Disclaimer

Certain commercial equipment, instruments, or materials are identified in this study in order to specify the experimental procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

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