LA-UR- 09-02409

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Title: On the Extension of Modern Best-Estimate Plus Uncertainty Methodologies to Future Fast Reactor and Advanced Fuel Licensing – Initial Evaluation of Issues

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Intended for: The 13th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-13)
Kanazawa City, Ishikawa Prefecture, Japan,
September 27-October 2, 2009.

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On the Extension of Modern Best-Estimate Plus Uncertainty Methodologies to Future Fast Reactor and Advanced Fuel Licensing – Initial Evaluation of Issues

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ABSTRACT

Closing the fuel cycle is the major technical challenge to expanding nuclear energy to meet the world's need for benign, environmentally safe electrical power. Closing the fuel cycle means getting the maximum amount of energy possible out of uranium fuel while in turn minimizing the amount of high-level waste that must be stored. DOE's Advance Fuel Cycle Initiative (AFCI) program addresses this challenge by recycling the transuranic (TRU) isotopes contained in spent nuclear fuel; recycling, in turn, minimizes the amount of high-level waste that would require storage in repositories.

Developing new fuels and the plants that burn them is a lengthy and expensive process, typically spanning a period of two decades from concept to final licensing. A unique challenge to meeting the AFCI objectives in this area is that the experimental database is seriously incomplete. As such, using a traditional, heavily empirical approach to develop and qualify fuels and plant operation over the operational conditions of a AFCI plant will be very challenging, if not impossible, within the expected schedule and budgetary constraints.

To address this concern AFCI has launched an advanced modeling and simulation (M&S) approach to revolutionize fuel development and fast reactor design. This new approach is predicated upon transferring the recent advances in computational sciences and computer technologies into the development of these program elements.

The licensing process that has historically been used by the NRC for fuels qualification is based upon using a large body of experimental work to qualify and license a new fuel. If a modeling and simulation approach with more directed experimentation is to be considered as an alternative approach for licensing, then a framework needs to be developed that can be agreed to with the NRC early in the developmental process. The use of modeling and simulation as a means of demonstrating that a design can meet NRC requirements is not new and has precedence in the NRC. The method is generically referred to as a "Best Estimate plus Uncertainty" approach (BE+U), since the goal of the methodology is to compare the model value (best estimate) plus any uncertainty to a figure of merit like cladding temperature.

The challenges for extending the BE+U (1) method for fuel qualification for an Advanced Reactor Fuel are driven by: schedule, the need for data, the data sufficiency, the identification of important phenomenon, the process of validation (with focus on the multi-scale model), and the need to produce and extended best estimate plus uncertainty methodology. This paper examines these issues an offers up a proposed set of methods that extend the current BE+U methodology address most if not all of these challenges.

KEYWORDS

Advanced Reactor Fuels, Verification and Validation, Best Estimate Plus Uncertainty

1. INTRODUCTION

The increased use of nuclear energy in the nations energy portfolio has been suggested recently by various social, economical and political organizations. Several options for the extension of nuclear energy being considered are; 1- Life Extension of Current Nuclear Reactors, 2-Advanced New Generation Reactors (Gen III systems), 3- Generation IV Nuclear Energy Systems (particularly Next Generation Nuclear Plant (NGNP) concentrating on high temperature applications), and Advance Fuel Cycle Initiatives (AFCI) (fast reactor and advanced transmutation fuels). These new technology concepts will require new types of fuels (except the first option that may require more understanding of fuel behavior than development or minor modifications of fuels), and the new fuels have to be developed and qualified. Our discussion focuses on the qualification of fuels, primarily fuels AFCI program is pursuing at this point.

The advanced fuels of interest to AFCI programs are more complex than the traditional fuels previously and currently used in existing reactors. The added challenges are primarily caused by the inherent variability in fuel compositions used in a closed-fuel-cycle system. Furthermore, the fabrication of new fuels must take into account impurities and final product form with actinides, both of which may vary depending upon the separation technologies ultimately deployed for recycling spent fuel. It is clear that using a traditional, heavily empirical approach to develop and qualify fuels over the entire range of variables pertinent to AFCI on a timely basis with available funds would be very challenging and costly, if not impossible.

The primary objective of the Advanced Fuel Cycle Initiative (AFCI) Transmutation Fuel Campaign (TFC) is to qualify the transmutation fuel(s) for use in fast burner reactors over the entire range of compositions to obtain closure of the fuel cycle while maintaining the commercial competitiveness for nuclear energy. Within the context of the TFC, qualification means demonstration that the fuel will perform predictably and acceptably under normal operations and transient conditions. The qualification objective is achieved
by:

- Targeted testing for *a limited number of fuel compositions*, fabrication processes, and clad materials up to the level of lead-test assemblies, and
- An *extensive modeling and simulation* approach to quickly extend the empirical database to the entire range of variables that are needed to meet the AFCI objectives.

As a result, AFCI TFC has launched an advanced modeling and simulation campaign to revolutionize fuel development. The Nuclear Energy Advanced Modeling and Simulation

(NEAMS) program is natural extension of the TFC M&S program with a consideration of a larger scope. The primary objective of the NEAMS fuels Integrated Performance and Safety (IPSC) project is to deliver a coupled, three-dimensional, predictive computational tool for nuclear fuel pins and assemblies, applicable to both existing and future reactor fuel design, fabrication and for both normal and abnormal operating conditions. The validated tools can be used for lifetime extension, development of more informed safety margins, and the design of future fuels for potential new nuclear systems. It is important to re-emphasize that the NEAM fuels IPSCs objective of a successful modeling and simulation program is not a luxury but an indispensable necessity for the future of the nuclear energy. Without NEAMS fuels IPSC capabilities the use of extended nuclear energy in the nation's energy portfolio will take an unacceptably long time with an increased cost. NEAMS is targeting a 10 year accelerated program to achieve its goal.

2. CHALLENGES TO EVALUATION MODEL DEVELOPMENT

From the aforementioned description of program goals and targets, a list of challenges that may arise in the in the regulatory process can be postulated. The challenges for developing an evaluation model for fuel for an advanced reactor are driven by:

- Schedule,
- The need for data,
- The data sufficiency,
- The process of validation for multi-scale models,
- The identification of important phenomenon, and
- Effective review process.

Some of these issues can be addressed by modifying the current methodologies and some of them depend upon the programmatic decisions between the DOE and NRC. These issues are discussed below.

2.1. Schedule

The NEAMS and AFCI program requires a schedule to develop and "qualify" an advanced reactor fuel in a time frame of about 10 years. A qualified fuel is defined as a fuel that can be demonstrated to perform predictably and acceptably under normal operations and transient (accident) conditions. This schedule is far faster than the historic time of 20 to 25 years for fuel qualification that traditionally would overcome any lack of data by a large experimental program that develops the necessary data before the an evaluation model is developed. For applications in programs like AFCI and NEMAS, time will not allow a serial approach to the problem. Instead a parallel effort is needed to perform the V&V and Uncertainty Quantification at different length scales. This needs drives the other issues that are discussed below.

2.2. Need For Data

The licensing process that has historically been used by the NRC for fuels qualification is based upon using a large body of experimental work to qualify new fuel. If a modeling and simulation approach with more directed experimentation is to be considered as an alternative approach for licensing, then a framework needs to be developed that can be agreed to with the NRC early in the developmental process. The use of modeling and simulation as a means of demonstrating that a design can meet NRC requirements is not new and has precedence in the NRC. The method is generically referred to as a "Best Estimate plus Uncertainty" approach (BE+U), since the goal of the methodology is to compare the model value (best estimate) plus any uncertainty to a figure of merit like cladding temperature. The method is typically done in conjunction with the validation and verification effort for the model.

The current methodology used by the NRC for performing V&V and BE +U are outlined in Reg-Guide 1.1.57[1] and Reg-Guide 1.203[2]. The Reg-Guide methodology was designed for validating and determining the uncertainty of a model for a situation where the data necessary to achieve this end is *already* available. The situation for a new advanced reactor fuel is different in that the necessary data *does not exist* for new fuels. The new fuels will be experimentally tested in parallel to the development of evaluation models that will require validation. This means the existing Reg-Guide Methodology must be modified to allow for a parallel development of data while the models and associated V&V and BE+U are being performed. The modified process must allow for feedback from the V&V and BE+U effort to direct experimental testing of new fuel.

2.3. The Data Sufficiency

The review of program plans of AFCI TFC and NEAMS indicates that the programs aims to test a limited number of fuel compositions. This is because the number of design parameters (actinides-plutonium, americium, neptunium etc.) in new fuels is high and testing in every potential combinations of fuel composition is practically impossible (possible but very expensive and timely). The other factors limiting the testing requirements are testing facilities are not readily available in US. This is one of the main reason the programs introduced the concept of the science-based modeling and simulation enhancing ability to interpolate and extrapolate within design space; perform sufficient and relevant experiments in limited but critical portions of the design space, validate models, and interpolate (or extrapolate when possible) within untested regimes.

Testing/experimentation is a critical element of any product delivery when there are significant consequences should the product fail, e.g. loss of life, significant loss of investment, inadequate time to replace the failed product. Testing in such a situation validates that the product works, at least initially but many questions will remain such as how long will it work, how efficiently and will that remain acceptable, what if a part within the product fails, etc. Thus while a single experiment/test may provide useful information about a product, questions often remain and even multiple tests may not address them all.

A similar discussion can be undertaken with respect to modeling and simulation when no experimental information is available to guide theory, models and simulation or to validate that the simulations adequately represent the real world. This is actually the perspective from which we approach the question, i.e. what physics models are needed, and once build do they reproduce the test results adequately? A second question is: Are predictions made with the codes robust or, to the contrary, vulnerable, to the assumptions upon which the models and numerical algorithms are based? These two questions form the basis of a predictive accuracy assessment. The degree to which simulation codes can be used with confidence to support fuel development activities depends on the answers brought to these two questions.

Traditionally, the predictive accuracy assessment is done by simple statistics using an excess of experiments. Same or similar experiments are performed at different facilities to eliminate the designer biases. How many experiments are enough is answered by simple statistical criteria. In the data sparse environments, not only the predictive accuracy assessment becomes difficult, but also the quantification of predictive maturity is necessary. The predictive maturity scales were somewhat subjected to interpretation by experts when there is plenty of data. It is also difficult to quantify the effect that different levels of maturity may have on risk and decision-making.

Thus, the validation in data scarce environment motivates the need for another, more objective, approach based on a mathematical model that develops a metric of predictive maturity. Such a model is expected to quantify the sufficiency of simulation maturity, while accounting for prediction uncertainty, and increase the credibility of safety predictions.

The other deficiency of the state-of-the-practice is that levels of maturity are always assessed relative to experimental datasets that are available to the analysts. Unfortunately, these may not be representative of regimes or regions of the design space where one may need to extrapolate the predictions of a code. The difficult question of extrapolation requires a rigorous methodology for code scaling ("How to scale the results of table-top experiments to full-scale systems?") and inference of uncertainty in prediction ("How to extrapolate uncertainty bounds to regimes or regions of the design space that cannot be tested experimentally?"). Addressing this challenge can leverage techniques based on the concept of similarity and recently proposed the predictive maturity concept to infer uncertainty for complex physics experiments. Such a model is expected to increase the credibility of safety predictions and quantify the sufficiency of simulation predictions.

2.4. The Process of Validation with Focus on Multi-Scale Validation

The traditional validations in large scale computer codes such as Transient Reactor Analysis Code (TRAC[3]) was to develop closure relations for local models from tests where the boundary conditions are controlled (separate effects) tests. The closure relations include empirical and semi-empirical and mechanistic models. The appropriate constants in these models are determined from the experimental data. These models are then implemented into the large-scale computer models. The integral assessment of the large-scale computer models was done against data obtained from scaled prototypes (integral tests). In most of the cases some of the constants in local closure relations again is adjusted to predict the integral test data. It is very rare that the closure relations are obtained from purely theoretical models or another large-scale simulations.

AFCI TFC road map and NEAMS Fuels program plan definitely introduces a multi-scale coupled calculations of the fuel performance. This means several different simulations at large scale should occur instantaneously or serial fashion. The validation of these schemes has challenges. The lower length scale simulations may require same level of rigor in validation. In some cases the validation of a lower length scale have to be done at a higher length scale. These issues raises challenges how multi-scale coupled validation requirements and its process requirements should be address in the current regulatory guidelines.

The closest example of multi scale validation comes from defense applications where some models are purely theoretical while others have limited data for validation in different scales (Unal[4]). The defense applications depend primarily upon simulation capabilities. Therefore, the simulation uncertainty estimation becomes a key issue in the assessment of margin. The primary uncertainty quantification method that is being proposed is the forward propagation method used in the current the NRC methodology. Defense simulations are much more complex than the current tools used for reactor accident analysis and involve multi-physics codes and data. The number of potential model parameters involved is considerably high. The methodology to reduce the number of significant parameters is a key part of the overall approach.

It is best to visualize the simulations as simply consisting of two-fundamental parts- the hydrodynamic and nuclear parts. The process for the hydrodynamic portion is shown in
Fig. . The key models in the hydrodynamic simulations are the material equation of state, material strength and damage models.

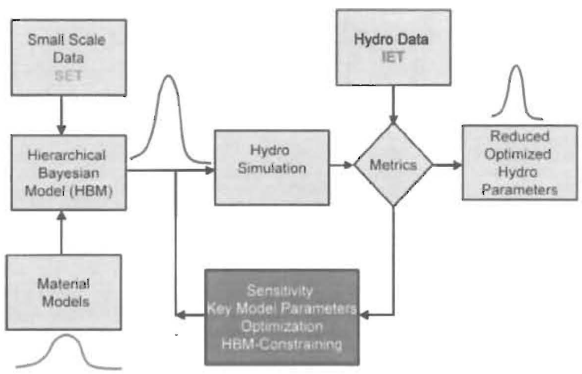

Fig. 1. The Process for the Hydrodynamic Phase.

Physics models are developed using a classical hierarchical decomposition approach (Simon[6]) from small-scale data (the corresponding nuclear industry term is separate-effect tests, SETs). The Hierarchical Bayesian Model (see Unal[5], Higdon[7], Higdon[8], Kennedy[9] and Williams[10]) is used to characterize the uncertainty in SETs initially. The models developed from SETs are applicable to a certain range of parameters. The analyst often extrapolates these models to more extreme conditions at which the data is lacking. The validation of material hydro models is done using small-scale data as was done in the development of closure relations in TRAC code. However, the regime the materials models are applied to are more extreme than the regime than that for which the model was developed. In order to justify these extrapolations the analyst can assess the IET data where the ranges of parameters are typical of the desired conditions.

The initial uncertainty distribution obtained from SETs is shown conceptually in
Fig. colored in red. It represents the uncertainty in each model parameters (multiple model parameter distributions). After applying HBM to SETs, uncertainty distributions are obtained that are prior estimations for the hydro simulations and are shown as blue colored. (Within the HBM the initial distributions are referred to as "prior" distributions while those obtained by applying the HBM are referred to as the "posterior" distribution.) The hydro simulations are

further constrained against the integrated effect test (IET hydro data). At the end of this step, we obtain key model parameters, their contributions to the hydro model uncertainty, and the posterior model parameter distributions. (If extrapolation of the SET conditions to the IET conditions were not required and the various physics models employed in the IET were truly uncoupled then we would expect the prior and posterior distributions results from the application of the HGM were be very similar if not the same.)

A similar process is followed for the nuclear simulations as shown in Fig. .

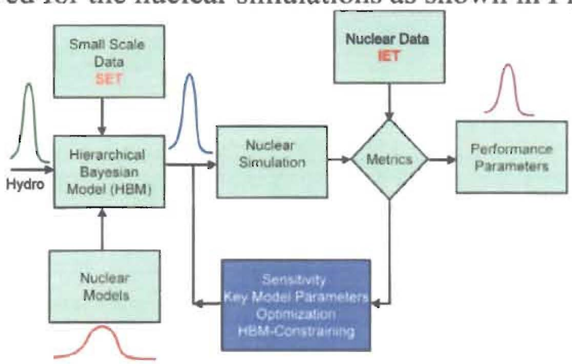

Fig. 2. Nuclear QMU process.

In the nuclear phase, the analyst must consider cross sections, opacities and various other model parameters that may affect our performance parameters. The paper does not contain an example of the nuclear phase.

The complexity in the multi scale modeling of nuclear fuels is similar to those we discussed above for the defense applications. In the short term, the plan is to use a hierarchal mutli-scale approach where the analyst will calibrate each scale results with its own data base (that could be coarse). The ultimate safety calculations will be done with an engineering scale code where uncertainties from lower length scale will be input. The overall validation approach is not mature and an evolving subject. This paper discusses the anticipated issues that may change as the multi-scale approach evolves.

2.5. The Identification of Important Phenomenon

Because the V&V process may be parallel with the model development and experimental programs, the identification of limiting or key phenomenon in Reg-Guide type of BE+U methodology has risks. The Phenomena Identification and Ranking Table (PIRT) process for fuels for example, would produce insight based on old experimental studies and potentially yield limited insight or information on a new fuel form. However, the computational sensitivity studies can be used to enhance the PIRT process. The computational tools could be used to identify where the models would have low level of confidence to simulate a physical phenomenon. In order to this result, sensitivity methods enabling uncertainty quantification may be needed. These methods with the help of a predictive maturity assessment may help to design better experiments in areas where the uncertainty is high. Thus, the experimental design and interaction with modeling becomes important for discovery of potentially important phenomenon and characterization of the phenomenon under different conditions or component variations.

2.6. Effective Review Process

The traditional review process for license applications is defined in the standard review plan (NUREG-0800[11]) produced by the NRC. Generally speaking, the vendor follows these guidelines and submits an application to NRC. The NRC then reviews the application and gives comments back to the vendor if they feel that the application is incomplete or they need more specific information. After this interaction the NRC makes a decision on the application's ability to satisfy the requirements if the vendor's design can be certified.

This process usually takes on the order years depending upon the specifics of the reactor design. The NEMS program is trying to reduce the time for fuel development to a time frame (10 years) that is substantially less than historical precedence. One reason is that the process has traditionally been reactive on the part of the NRC to the industry. The industry submits information and the NRC reacts (reviews and provides feedback) to the information. There are understandable reasons why the review period is long, however, the NEAMS program requires a different strategy due to the challenges mentioned above. These programs require NRC's involvement in the early stage of process and methods development (data, model, design etc). In other words, the NRC has to be pro-active during the program development. How the NRC becomes pro-active and what role they play in the program development needs to be defined.

3. PROPOSED APPROACH

In order to address the challenges just presented, a proposed approach and method have been developed. First an overview of the approach is presented. A brief description of the major attributes of the approach, the extension of the current methodology, the use of a predictive maturity model and the need to validate lower length scales models is presented with a description of how this overcomes many of the current challenges to fuel licensing.

3.1. Overview of Proposed Approach

The approach needs to have the following qualities:

- It must have a feedback mechanism to the experimental program developing data to direct experiments to the needed data that can satisfy the figures of merit specified for the evaluation model of the fuel. The mechanism will be described later, but in essence its goal is to develop an efficient process for directing the model development and experimental program.
- A method for determining when enough experimental data has been developed to satisfy the figures of merit is needed in the method. Essentially it answers the question "When is the answer provided by the model good enough?" This method will be referred to as defining the "maturity" of the model.
- The use of lower length scale models will be necessary to replace some separate effects testing (SET). Traditionally, SET would be developed given the level of data needed for the final evaluation model (called here the engineering level model.)

In order to develop data that may be needed, the approach would include using a lower length scale model, for which data may already exist and use the output from this model as data input into the higher-level length scale model. Note it is understood that the uncertainty and bias that this method may introduce must be carefully evaluated when characterizing the uncertainty of the overall evaluation (engineering) model.

3.1. Extending the Reg-Guide Methodologies for Best Estimate Plus Uncertainty

To address the challenges presented earlier it is proposed to extend the basic approach that the NRC has developed and advocated in both Reg-Guide 1.157 and Reg-Guide 1.203. This is extended process is shown in flow chart form in Figure 3.

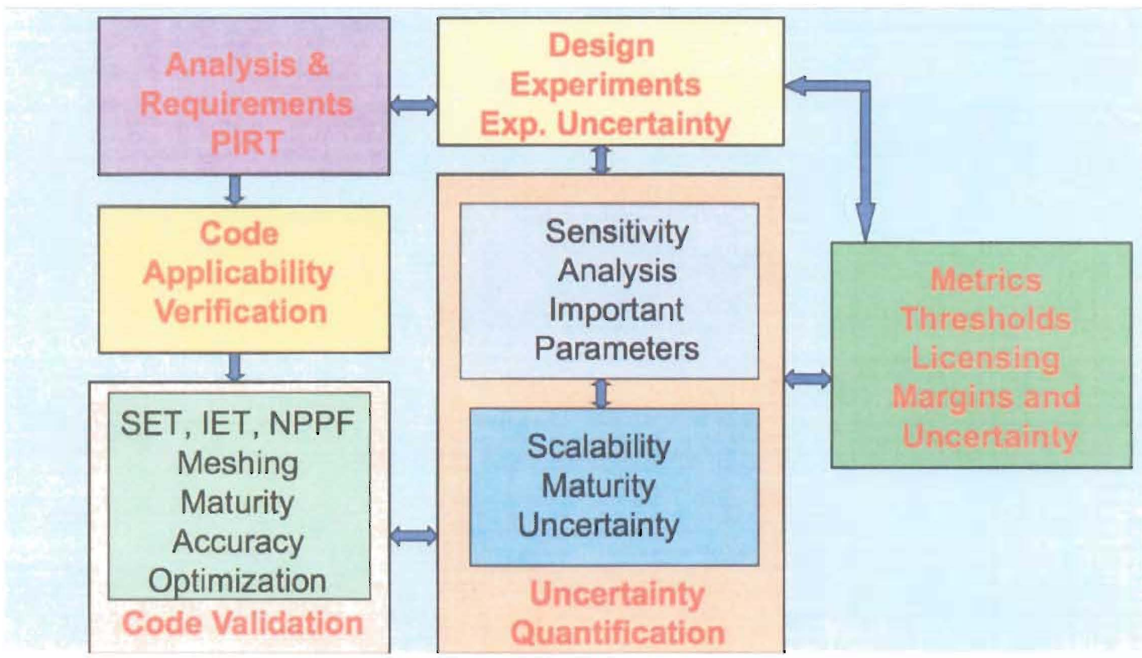

Fig. 3. Extended V&V and Best Estimate Plus Uncertainty Methodology

The approach has several important features. First, the basic elements outlined in the Reg-Guide are retained. The second important feature is the is the inclusion of a feedback loop for both the process of code validation and verification and also for the estimation of uncertainty. This feature is shown by the double arrows in Figure 3. The feedback loop is an important feature to this methodology. Experiments may be terminated or the types of experiments redirected in order for the overall evaluation model to satisfy the figures of merit (example, the figure of merit may be a best estimate calculation plus uncertainty compared to success criteria such as a fuel cladding temperature.) A methodology is being proposed that uses Bayesian statistics to update the input data into the evaluation model. This process of updating occurs with each successive iteration of the system. Given the desire to lower overall uncertainty this method has the ability to direct the experimental program to end state that either produces no improvement in maturity (to be discussed) or to satisfy the figure of merit.

It is worth note that the approach separates the code verification and validation into two steps. As shown in Fig. 4, the code verification is required for all different scales early in the code development process. The code validations consider physics models used in each scale simulations. At this step, the method aims to ensure each physics model is matured, robust and the biases in predictions relative to separate effect or integral effect tests are determined. At the end of this step, a baseline model of the nuclear power plant (or fuels or both) is developed for sensitivity analysis for prototypical calculations. The use of prototypical design and safety test and assessing the maturity against this data is the last step before we perform uncertainty quantifications.

Fig. 4 shows conditional pathways form one box to another one to indicate that there is a possibility that required maturity cannot be demonstrated and additional experiments may be required. In that case we return the design and experimental box to either change design or obtain new experiments to address the validation issues in both physics models or integral simulations and apply the methodology again until we reach a reasonable maturity and bias estimations. As a result of this process there is also possibility that the process may result in a situation that enough experimental data may be accumulated to qualify fuel with the use of empirical closure relations rather than mechanistic models that may give undesirably high uncertainties. Again, the purpose of this paper is to introduce an idea to the community to start the discussion of what we need to do in the licensing and validation in the data sparse environment.

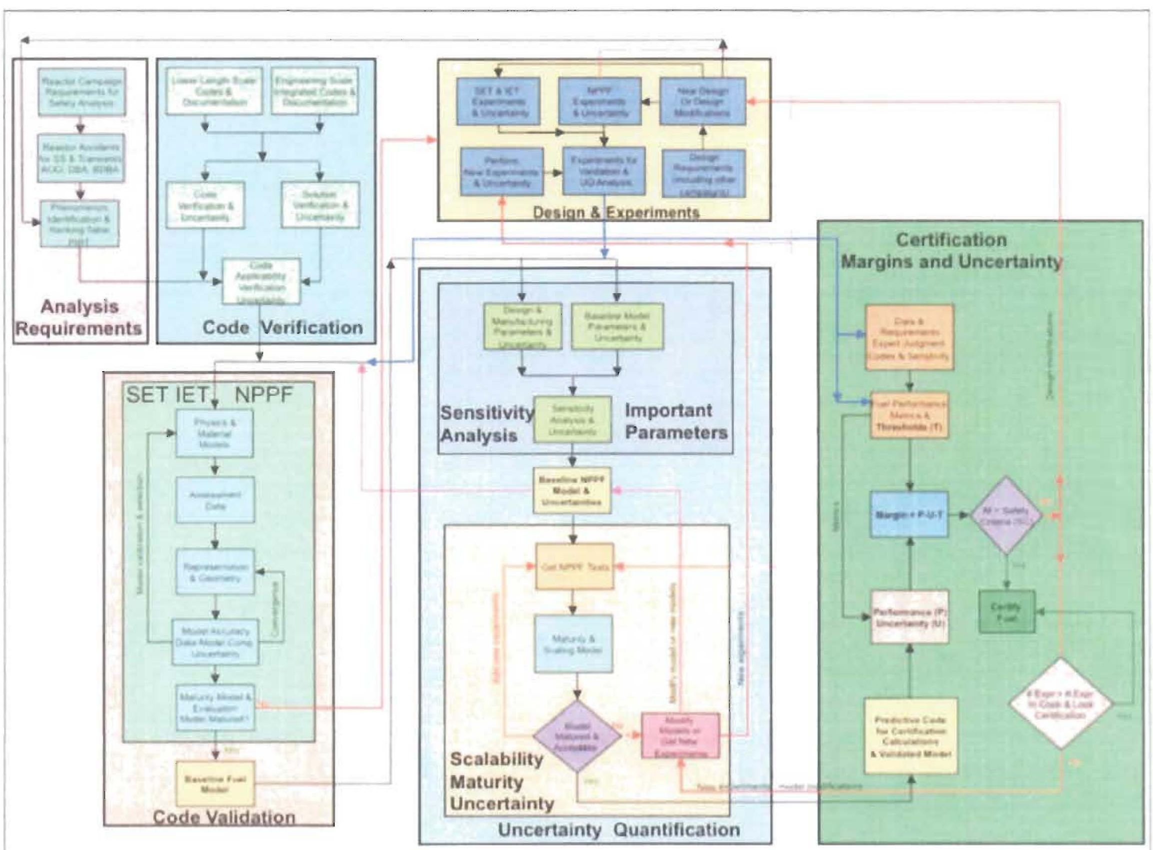

Fig. 4. Details of Extended V&V and Best Estimate Plus Uncertainty Methodology

3.2. Maturity of the Model (i.e. When is the Answer Good Enough?)

A question that has always arises for any methodology is "when is the answer good enough?" In the past when no other method was evident, expert judgment was used to make this determination. For this approach the idea of the "maturity" of the model result will be introduced. Maturity will be defined as numerical value that is a measure of the "change" of a result, very close to determining a value reaching an asymptote. This criterion will be measured and used as a means of determining when further experimentation is needed or the maturity of the model has been reached and no further reduction in uncertainty can be achieved or the figure of merit has been achieved. An example of a recent Los Alamos National Laboratory application of predictive maturity is shown in Figure 5 and based upon the work by Hemez[12].

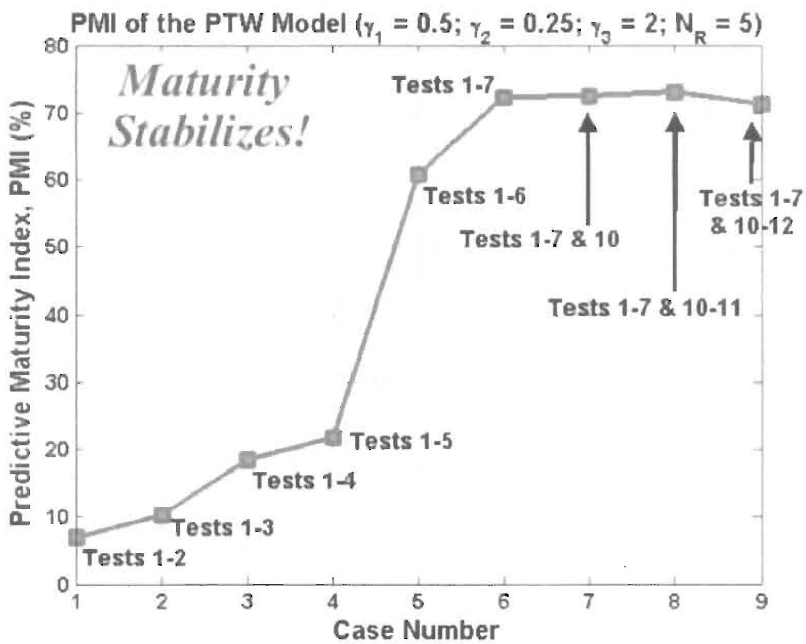

Fig. 5 Example of Predictive Maturity Index (Ref. 5)

3.3. Use of Lower Length Scale Models to Supplant SET Data

In the absence of some SET data an alternative is to supply data from a lower length scale model shown in Figure 6. An example of different length scale models for an advanced reactor fuel could be models at the: 1) atomistic level 2) single crystal level 3) polycrystalline level and 4) at the fuel pin level (referred to here as the engineering level.)

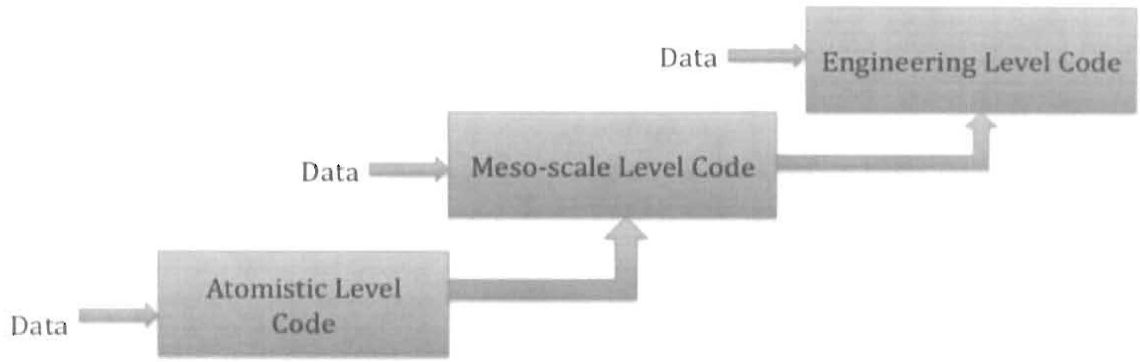

Fig. 6. Schematic Presenting Use of Lower Length Scale Models

The number and depth of lower length scales models may vary, but typically will be limited to two levels deep. One issue that must be addressed by this approach is to ensure that all uncertainty and bias in the lower length scale data and model is accounted for. So, when uncertainty is propagated though the evaluation (or engineering level) model, the uncertainty from the lower level length scale models must be propagated as well.

4. CONCLUSIONS

The advanced fuels of interest to AFCI program are more complex than the traditional fuels currently used in existing reactors. The complexity arises from the inherent variability in fuel compositions used in a closed-fuel-cycle system. Using a traditional, heavily empirical approach to develop and qualify fuels on a timely basis with available funds would be very challenging and costly. Instead, the AFCI program has embarked on a program with targeted testing for a limited number of fuel compositions and to use extensive modeling and simulation approach to extend the empirical database.

The use of modeling and simulation will require that evaluation models conform to the current NRC regulatory requirements and guidelines. There will be challenges adequately developing an evaluation model for fuel for an advanced reactor in the necessary time frame. These challenges include, schedule, the need for data, the data sufficiency, validation of multi-scale models, identification of important phenomena and efficient review.

These issues have been examined and a methodology has been proposed that extends the current NRC best estimate plus uncertainty methodology. The method focuses on using a feedback loop that uses baysian statistics to direct experimentation used to verify and validate the process. The method also advocates the use of a predictive maturity methodology to provide feedback to the experimental program when enough data has been produced. Finally, the validation process must account for the use of multi-scale models that are used in place of separate effects testing for data input for models at a larger scale.

ACKNOWLEDGMENTS

The DOE-NE AFCI NEAMS program directed by Alex Larzelere has funded the work. We want to thank AFCI Fuels Campaign Manager Dr. Kemal Pasamehmetoglu for encouraging and funding us to develop new concepts for licensing applications and his valuable suggestions and guidance.

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