ACCELERATED FUEL QUALIFICATION WHITE PAPER

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1 OCTOBER 2021

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EXECUTIVE SUMMARY

This white paper details a formalized methodology for the development and qualification of new nuclear fuels in an accelerated time frame as compared to the current, conventional methodology of fuel qualification[2]. This methodology is known as Accelerated Fuel Qualification (AFQ). Its goal is to significantly reduce the time to qualify new fuels, from what historically has taken more than 20 years, to an ultimate duration of as few as five years. This white paper lays out the AFQ methodology and illustrates it with examples.

> The goal of AFQ is to reduce the time to qualify new fuels from 20 years to as few as 5 years

The key elements of AFQ include:

- High-fidelity, physics-based modeling and simulation (M&S) tools that adequately describe the fuel performance.
- Out-of-pile and in-pile targeted experiments that efficiently span the range of relevant parameters to provide data that may either be used to construct semi-empirical models or to efficiently validate physics and mechanistic models.
- Execution of coordinated experimental testing and M&S activities, in parallel.
- Incorporation of specialized and accelerated testing methods to obtain relevant data more quickly, such as the Fission Accelerated Steady State Test (FAST) or High Flux Isotope Reactor (HFIR) MiniFuel irradiation methods.

Adoption of the AFQ methodology by industry, and recognition of the methodology by the Nuclear Regulatory Commission (NRC), would facilitate more efficient and timely qualification of new fuel systems. The methodology provides developers a framework to more efficiently develop and perform targeted experiments with the use of M&S, analysis tools and diagnostics to demonstrate fuel performance, with the incorporation of bounding uncertainties and risks for a risk- and performance-based qualification of new fuel systems.

1. INTRODUCTION

The urgent need to deploy new and advanced reactor technologies in the United States and around the world is driven by the retirement of the aging light water reactor (LWR) fleet and

[2] **The objective of fuel qualification** is "*to demonstrat[e] that a fuel product fabricated in accordance with a specification behaves as assumed or described in the applicable licensing safety case, and with the reliability necessary for economic operation of the reactor plant*" (Crawford, D. C., Porter, D. L., Hayes, S. L., Meyer, M. K., Petti, D. A., and Pasamehmetoglu, K.) 2007. An approach to fuel development and qualification. Journal of Nuclear Materials, 371(1-3), 232-242.

need for efficient, low-carbon power sources. In nearly all cases, these technologies utilize new nuclear fuel systems that have not yet been qualified by the NRC.

Nuclear fuel development and qualification requires a process of material development and characterization, out of pile fuel performance testing and analysis, integral irradiation testing and post-irradiation examination, as well as analysis of accident scenarios and other relevant safety evaluations necessary for fuel qualification and reactor licensing. The current approach, without the benefit of modern modeling and simulation tools, depends highly on empirical data and has typically relied on a series of integral fuel tests. Historically, this empirical approach has taken 20 years or longer to acquire data through extensive sequential testing. Thus qualification, and eventual deployment of new fuel systems is a long drawn out process, particularly for non-LWR systems that achieve higher fuel utilization and multi-year lifetimes, such as those used in efficient high temperature gas-cooled or molten salt reactors.

In 2007, Crawford, et al.[3] documented the current approach and rationale, describing a program structure in four phases based on their observations and experience. While sound, this approach is serial, heavily empirically-based, and thus very time-consuming. By more fully incorporating today's multi-scale and mechanistic M&S tools and enhanced experimental capabilities, fuel qualification can be performed much more efficiently, while still maintaining the same high safety standards.

The AFQ methodology brings together a combination of advanced, physics-informed nuclear fuel performance M&S with targeted experiments[4]. See Figure 1. The AFQ methodology aims to consolidate and reduce the number of required integral irradiation tests by developing and using mechanistic models that properly represent the physics of fuel performance, and making use of separate separate-effects tests to inform and validate those models and simulations. These robustly-validated models and simulations can then be used to rapidly optimize fuel designs before undertaking the complex integral irradiation experiments that are needed to demonstrate acceptable fuel performance under prototypical conditions. This approach takes advantage of advances made in microstructurally-informed fuel performance M&S tools and new advanced irradiation capabilities to rapidly converge on an optimized fuel design to be demonstrated.

An ultimate demonstration of the final fuel design, fabricated according to specification, tested at scale, and tested under prototypical conditions, will continue to be a necessary step in fuel qualification. Shortening the time required to advance to this final demonstration phase is where the major time reduction for developing a new fuel would be gained. An overview of the differences between the traditional fuel qualification methodology and the AFQ methodology is given in Figure 2.

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[3] D. Crawford et al., "An approach to fuel development and qualification," *Journal of Nuclear Materials* 371, 232-242, 2007.

[4] J. Opperman, "Original proposal for DOE award No. ARD-18-15066: Combining Multi-Scale Modeling with Microcapsule Irradiation to Expedite Advanced Fuels Deployment" (2018), General Atomics, GA-A29413.

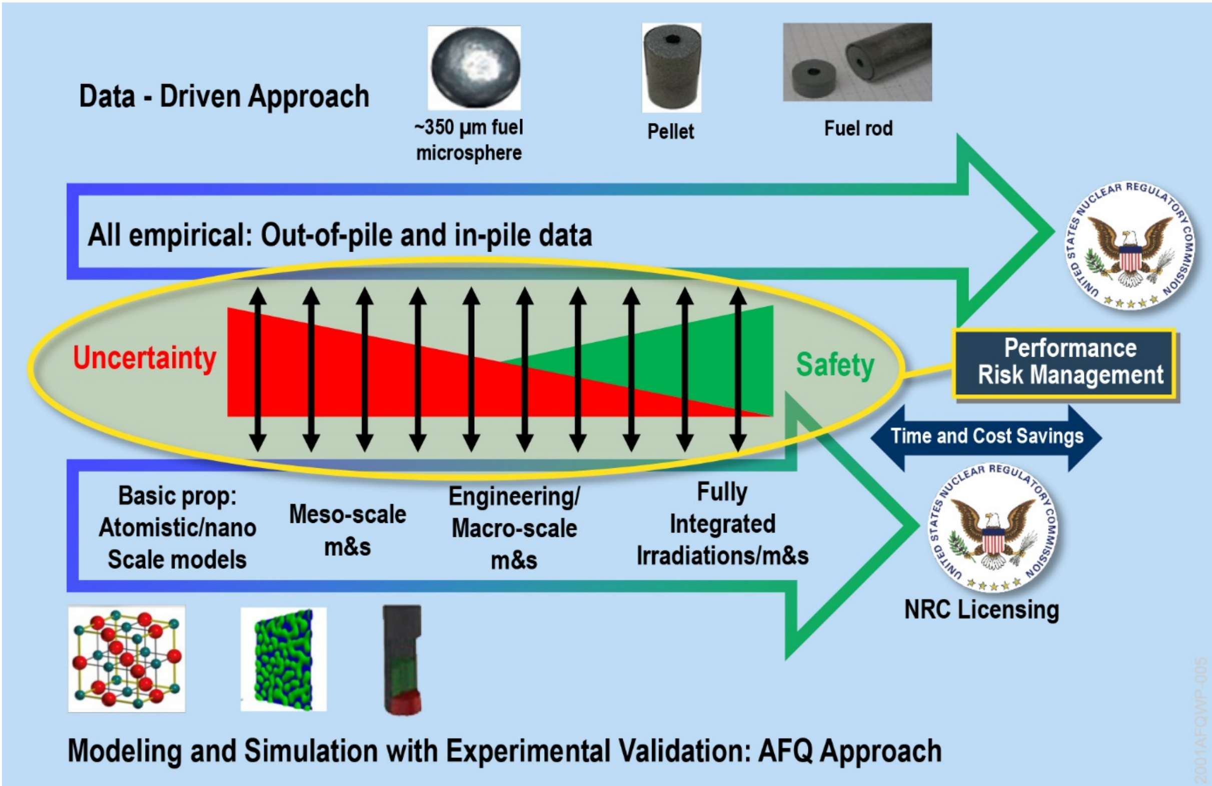

Figure 1. The conventional versus AFQ approaches to nuclear fuel qualification. (Fuel dimensions are for illustration purposes only)

Advances in both computational and experimental capabilities enable the AFQ methodology to be employed today. M&S has advanced by orders of magnitude in computational speed and employs sophisticated algorithms. As a result, in some cases like for UO_2, predictions of fuel behavior are effectively based on first principles calculations. In characterization and experimental test capabilities, new diagnostics can make measurements at higher resolution than ever before, and new techniques enable precision in separate-effects testing. These new diagnostics enable a better understanding of the underlying materials and structures behavior so that the performance of fuel forms does not depend solely on empirical data.

The AFQ methodology consists of a three-phased approach to fuel qualification[5]. Savings in time and cost arise from early identification and focus on the key drivers of the safety case for efficient use of resources. In addition, M&S is performed in parallel with experiments, in an iterative fashion. Importantly, fuel performance codes can make use of empirical materials property data when available, as before, and also use mechanistic, physics-informed models. Note that the development of codes and simulations requires experiments to validate them. The desired result is that use of targeted separate-effects and accelerated experiments enables higher

[5] K. A. Terrani, et al., "Accelerating nuclear fuel development and qualification: Modeling and simulation integrated with separate-effects testing," *Journal of Nuclear Materials* 539, 152267, 2020.

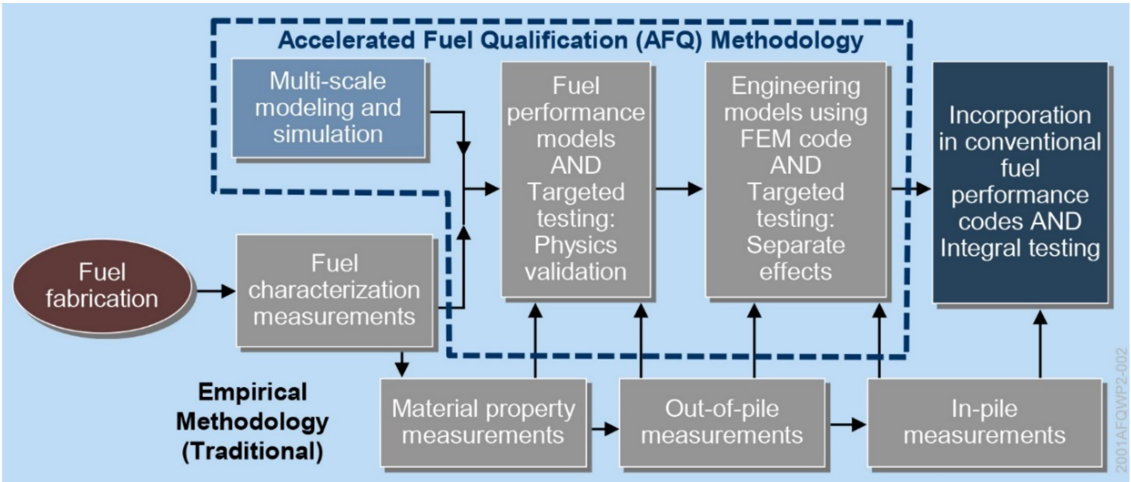

Figure 2. Overview of the traditional vs. the accelerated fuel qualification methodologies

quality, fewer, more effective integral irradiation experiments to validate and acquire the data needed to support the safety case.

AFQ ultimately supports providing data and validation for a specific reactor licensing strategy. It could also accelerate the insertion of new accident-tolerant fuels into existing reactors. The strategy may be based on risk-informed performance or on consequence-based approaches. AFQ is agnostic to this choice and provides the data and validation information for the fuel in an accelerated fashion. It also serves as a deliberate action to bring together advanced M&S tools with a range of advanced experimental tools that include not only separate-effects experiments but other ones that span the gamut from bench-scale all the way to the select number of complete integral tests.

The near-term objectives of the AFQ methodology do not necessitate any wholesale changes to the current NRC regulatory process or timeline. However, familiarity with and involvement in the development of AFQ methodologies could lead the NRC to consider some changes for the sake of efficiency or expediency. The AFQ approach still necessitates a final demonstration of any new fuel technology at near full-scale and under essentially prototypic conditions, as well as delivering a fuel performance code or tool that has been validated using experimental data. Data, analyses, and validated M&S will serve as the basis for any licensing request. The elements of the overall fuel qualification enterprise that are the primary focus of innovation and acceleration are the discovery and development phases that occur at commercial or government laboratories and test reactors, activities which necessarily precede the final demonstration phase. Subsequent to this, the regulatory and licensing phase would proceed essentially as it does now. The objective of the AFQ methodology is to significantly shorten these phases by means of theory-driven discovery and accelerated testing methods, perhaps to as little as a few years.

The following sections include a detailed overview of the AFQ methodology. The discussion focuses on both M&S and experimental elements of the methodology as well as the coupling of the two resulting in this unique new methodology to significantly accelerate new nuclear fuel qualification.

2. OVERVIEW OF AFQ-ENABLING MODELING AND SIMULATION AND EXPERIMENTAL TOOLS

2.1 MODELING AND SIMULATION TOOLS

M&S plays a pivotal role in the overall AFQ methodology. In simple terms, mechanistic models of fuel performance (based on a multiscale methodology, and culminating in a familiar engineering-scale simulation) can be utilized to:

- Accurately interpolate between sparse experimental data on irradiated fuels.
- Provide a detailed analysis of experimental results to reveal and understand governing phenomena.
- Design future experiments to strategically target key unknowns or regimes.
- Potentially identify optimized fuel compositions.
- Be a key aid to informing fabrication studies or manufacturing activities (although this is not the subject of this white paper).

Note that the physics-based methods employed as part of the multiscale fuel performance approach have been under development for the past few decades (and in some cases for almost 50 years). Given the advances in the methods and also in high performance computing, the use of such tools has become effectively commonplace in the field of materials science. Currently, these methods are being used in a linear fashion to improve current fuel materials and design. However, there are also mature multiscale simulation tools in the overall fuel development toolbox that can be used to accelerate fuel qualification. The following is a brief summary of the M&S simulation components.

2.1.1 Multi-Scale Modeling and Simulation

Multiscale fuel performance remains a high priority research area in the DOE-NE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. The phenomena that ultimately govern nuclear fuel performance occur at a wide range of time and length scales. Furthermore, there is a complex interdependence of many of these phenomena. For fuel compositions and operating conditions for which considerable irradiation data exists, it is possible to implement a semi-empirical fit in the engineering-scale fuel performance codes. However, for advanced fuel types where experimental data is relatively sparse, or for cases in which operating conditions that are less well-studied or difficult to fully access experimentally, it is worthwhile to complement experimental efforts with physics-based modeling efforts. Fortunately, there are many computational materials science tools that have been developed and are applicable to the wide range of problems that exist. For example, density functional theory

(DFT), molecular dynamics (MD), dislocation dynamics (DD), cluster dynamics, phase-field simulations, crystal plasticity methods, and more, are readily available to be applied to nuclear fuel problems. Though some features of nuclear fuel complicate the use of these tools, including the presence of actinides in the fuel, the evolving chemical species and states, and irradiation effects. Overall, it is critically important that the appropriate tools are applied to address problems within their range of validity.

These multi-scale tools have been successfully demonstrated for the study of nuclear fuel. As a recent example[6], atomic scale methods were used along with cluster dynamics to generate a fission gas release model for doped-UO_2. The key inputs to this model are the properties of defect clusters that contribute to transport of fission gas and how those properties relate to the state of the fuel, e.g., chemistry and irradiation conditions. The cluster properties are obtained from atomic scale simulations. The model outputs familiar physical quantities or parameters, such as the effective diffusion rate or diffusion coefficient of Xe, that can be used in fuel performance simulations similar to those performed today based on empirical correlations for the same parameters, but with the additional benefit that the multi-scale model allows us to account for changes in operating conditions and fuel chemistry in a more rigorous way.

The mechanistic multi-scale model also offers the opportunity for additional validation, beyond the integral tests traditionally heavily relied upon. The properties entering the mechanistic models may be investigated by separate effects tests relying on probes such as positron annihilation spectroscopy, X-ray and neutron diffraction and imaging, as well as X-ray spectroscopy. The outputs of the multi-scale mechanistic models can be validated against traditional separate effects measurements of thermochemistry and diffusion, which are the same measurements that are currently relied upon as empirical inputs to fuel performance simulations. In addition, validation of fission gas release would be performed based on integral irradiation tests to ensure complete system reliability.

By using mechanistic models that are separately validated, the confidence in the outcome of integral validation tests increases, which offers a pathway for accelerated qualification. As an example, since the mechanistic model accounts for changes in the fuel chemistry, the impact of such modifications on fission gas behavior could be accounted for without embarking on a completely new irradiation campaign. The mechanistic models are also ideal for applying uncertainty quantification and sensitivity analysis, the results of which can be propagated to fuel performance simulations and thus allow identification and execution of validation experiments that reduce the model uncertainty in the most effective way. See footnote 6 and references within for further details on the doped UO_2 study. Although the details are rather involved, the culmination of the lower length scale simulations is a predictive engineering simulation (using

[6] M.W.D Cooper, et al., Fission gas diffusion and release for Cr_2O_3-doped UO_2: From the atomic to the engineering scale, Journal of Nuclear Materials 545, 152590 (2021).

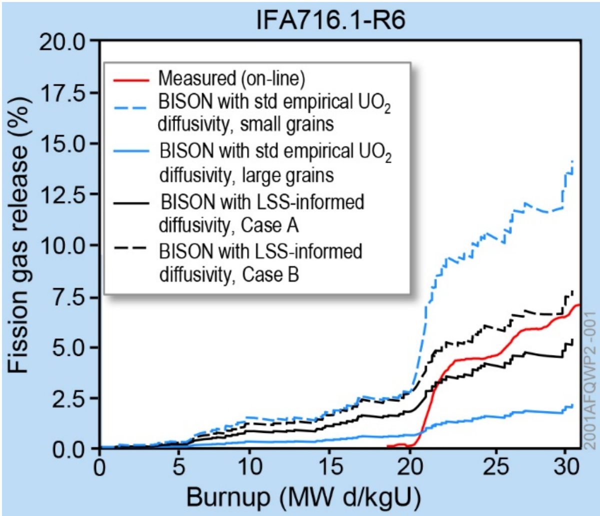

Figure 3. The red lines show the comparison of measured fission gas release (inferred from rod pressure) during the Halden IFA-716.1 test on Cr_2O_3-doped fuel rod 1 and rod 6[7]*. The black lines show the Bison results from using the least linear squares (LLS)-informed enhanced diffusivity model developed in this work, for Case A and Case B. The blue lines show the comparison to results using the standard empirical undoped UO_2 model with small and large grains*

the Bison code, described in the next section) that compares well to experimental data, as shown in Figure 3.

This example illustrates the usefulness of lower-length scale simulations in an AFQ context, by allowing for improved interpretation of limited experimental data and providing insight that enables users to identify new advanced fuels.[8]

2.1.2 Engineering-scale codes

Engineering-scale fuel performance codes with inherent ability to utilize modern high-performance computing (HPC) platforms can assess multiple fuel types and complex geometries. As an example, Bison is a finite, element-based nuclear fuel performance code that is applicable to a variety of fuel forms including LWR fuel rods, TRISO particle fuel, and metallic rod and plate fuel. Bison is based on the Moose framework and therefore can efficiently solve problems using standard workstations or very large, high-performance computers. Bison solves the fully-coupled equations of thermo-mechanics and species diffusion, for one-dimensional spherical, one-dimensional layered, two-dimensional axisymmetric, two-dimensional plane strain, or three-dimensional geometries. Different fuel models can be included to describe temperature and burnup-dependent thermal properties, fission product swelling, densification, thermal and irradiation creep, fractures, and fission gas production and release. Additionally, plasticity, irradiation growth, and thermal and irradiation creep models can be implemented for cladding materials. Models are also available to simulate gap heat transfer, mechanical contact, and the evolution of the gap or plenum pressure with plenum volume, gas temperature, and fission gas addition. Bison has been coupled to the mesoscale fuel performance code Marmot, demonstrating fully-coupled, multiscale fuel performance capability.

[7] T. Tverberg , Update on the in-pile results from the fission gas release mechanisms study in IFA-716, Technical Report HWR-1090, Organisation for Economic Co-operation and Development Halden Reactor Project, Halden, Norway, 2014.

[8] M.W.D. Cooper, C.R. Stanek, and D.A. Andersson, U.S. Patent 10,847,271 B1 "Mn-doped oxide nuclear fuel" (issued Nov. 24, 2020).

2.1.3 Data Science

Advances in data science can be readily incorporated into a multiscale approach. While many data science efforts in the field of materials are directed at identifying optimized compositions, current use of data science is in the area of scale bridging by development of reduced order models (ROMs) from advanced mechanistic performance models and the use of ROMs for uncertainty quantification and sensitivity analysis.

The following are the primary benefits of coupling advanced mechanistic models to engineering-scale simulations through data science methods in both the cladding and fuel examples:

- The ability to extend models beyond the regime with available experimental data (interpolation or in some cases careful extrapolation) with quantified uncertainties, thus reducing the number of tests area needed.
- The ability to identify critical parameters that can be targeted for further testing using separate-effects techniques, rather than lengthy and costly integral tests or simulations to reduce said uncertainties.

These advances in M&S enable more focused and accurate testing. By taking advantage of the increased accuracy and speed of advanced M&S along with advances in testing described below, activities can be performed in parallel to accelerate knowledge of the phenomena associated with fuel performance. These steps are critical for AFQ.

2.1.3.1 Examples of Data Science Applications for AFQ

Prediction of the thermo-mechanical response of cladding is integral to fuel performance and qualification. Accurate and predictive simulations require spatial and temporal resolution of deformation mechanisms that can be active during the operation of a fuel pin, from start-up to high-burnup conditions and from steady-state-operation to transient accident scenarios, such as a loss of coolant accident (LOCA), and how they depend on chemistry, micro-structure, and irradiation conditions. Multi-scale simulations relying on the viscoplastic self-consistent (VPSC) methodology to capture the polycrystal response under various conditions have been used to accomplish this goal for several cladding and structural materials used in reactors[9,10]. The computational cost of using these advanced models for engineering scale finite element analysis (FEA) is prohibitive for most applications. However, data science and ROMs fitted to the advanced models have been developed and interfaced with finite element codes such as Bison to

[9] W. Wen, A. Kohnert, M.A. Kumar, L. Capolungo, C.N. Tomé, Mechanism-based modeling of thermal and irradiation creep behavior: An application to ferritic/martensitic HT9 steel, International Journal of Plasticity 126, 102633 (2020).

[10] W. Wen, L. Capolungo, C.N. Tomé, Mechanism-based modeling of solute strengthening: Application to thermal creep in Zr alloy, International Journal of Plasticity 106, 88-106 (2018).

overcome this limitation. If the ROMs are carefully designed and fitted[11], they allow resolution of the full physical response described by the mechanistic VPSC method at the computational cost of a simple empirical relation traditionally used in fuel performance analysis. This approach enables high fidelity modeling of cladding performance with quantified uncertainties connected to the physical processes in the material that govern performance at the fuel pin scale, thus providing not only improved simulation capabilities, but also a path for model improvement using, for example, separate-effects tests or lower length scale simulations in the spirit of AFQ.

The same data science-based modeling approach may also be applied to other materials in the reactor. One example involves modeling fission gas diffusion in UO_2 under irradiation[6,12,13]. The Centipede code utilizes cluster dynamics simulations to track the point defect evolution under irradiation in nuclear fuels[14]. Successful comparison to available experimental data requires careful consideration of chemistry, tracking a large number of defect clusters and coupling the evolution to the fuel micro-structure. Similar to the cladding example, the Centipede code cannot be effectively coupled to a Bison pin-scale fuel performance simulation directly; instead, simplified analytical models were originally derived for use in Bison[6,10]. These cannot capture all of the dependencies in the cluster dynamics simulations. For this reason, surrogate ROMs have been developed that overcome this limitation. Further, the ROMs enable uncertainty quantification, identification of which parameters are most important from a fuel performance point of view and Bayesian calibration to any experimental data that is or will become available[13].

2.2 ADVANCED EXPERIMENTAL TOOLS

Qualifying a material for a specific function depends on the structure-processing-properties-performance (SPPP) relationship, tied together by material characterization. The materials science tetrahedron visually represents this relationship. The same relationship can be used to visualize accelerated fuel qualification in its efforts to tie together steady state irradiation testing, transient irradiation testing, advanced M&S, and advanced, high-throughput characterization. Material characterization is the capturing of data that pulls together the four corners to understand a given material system, while fuel qualification is the resulting analyses from the efforts in the four corner to ensure reasonable assurance for safe operation. See Figure 4.

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[11] A.E. Tallman, M.A. Kumar, C. Matthews, L. Capolungo, Surrogate Modeling of Viscoplasticity in Steels: Application to Thermal, Irradiation Creep and Transient Loading in HT9 Cladding, JOM 73 (1), 126-137 (2020).

[12] C. Matthews, R. Perriot, M.W.D. Cooper, C.R. Stanek, D.A. Andersson, Cluster dynamics simulation of xenon diffusion during irradiation in UO_2, Journal of Nuclear Materials 540, 152326 (2020).

[13] T. Casey, et al., in progress.

[14] C. Matthews, R. Perriot, M.W.D. Cooper, C.R. Stanek, D.A. Andersson, Cluster dynamics simulation of uranium self-diffusion during irradiation in UO_2, Journal of Nuclear Materials 527, 151787 (2019).

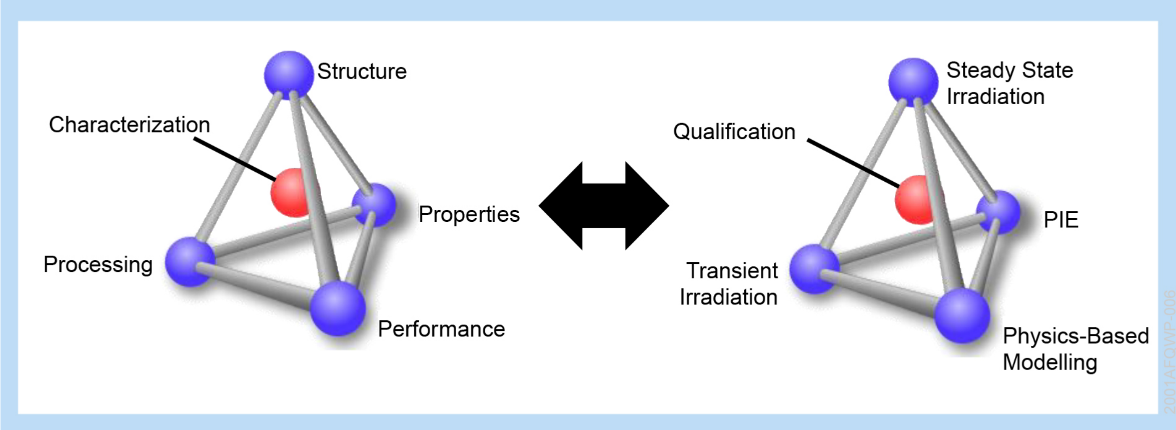

Figure 4. Relationship between materials characterization and qualification

Nuclear fuel qualification ultimately rests on the demonstration that a fuel design will perform predictably during steady state operations, will have constrained effects during transient conditions, and can adequately be represented by performance models that predict fuel burnup (that is, computer codes). Fuel performance codes generally represent an integration of all behaviors within the fuel. Historically, they have been built upon mathematical fits to empirical data sets and as such, are limited to the envelope in which they were fitted, having limited value in projecting fuel behavior beyond the bounding operational envelope (for example, similar fuel form in a new reactor design). Furthermore, empirically-based fuel performance codes are only able to represent bulk fuel behavior. Empirical fits do not have the fidelity to capture the integration of various phenomena that materialize on lower length scales and ultimately impact the engineering scale.

For an accelerated approach to fuel qualification to succeed, these mechanisms need to be physically understood and used to construct physics-based material models to complement and ground integral data sets. Data validation, therefore, relies upon advanced characterization, or post-irradiation examination (PIE), that can provide data to bridge the gap between length scales (atomistic to engineering). This effort must take into account that many of the properties of interest tend to change in nature as length scales are transcended or impacted by other phenomenon not specifically related to the material. One such example is observed when evaluating the macro-scale phenomenon of cladding rupture. This process is driven by the stress being applied to Zircaloy tubes at elevated temperatures. In this example, integral fuel analyses need to evaluate microstructural phenomenon associated with the fuel to accurately predict burst, as shown in Figure 5. This complex relationship between material properties and phenomena is what makes both integral irradiations in a reactor and PIE so critical to fuel qualification campaigns.

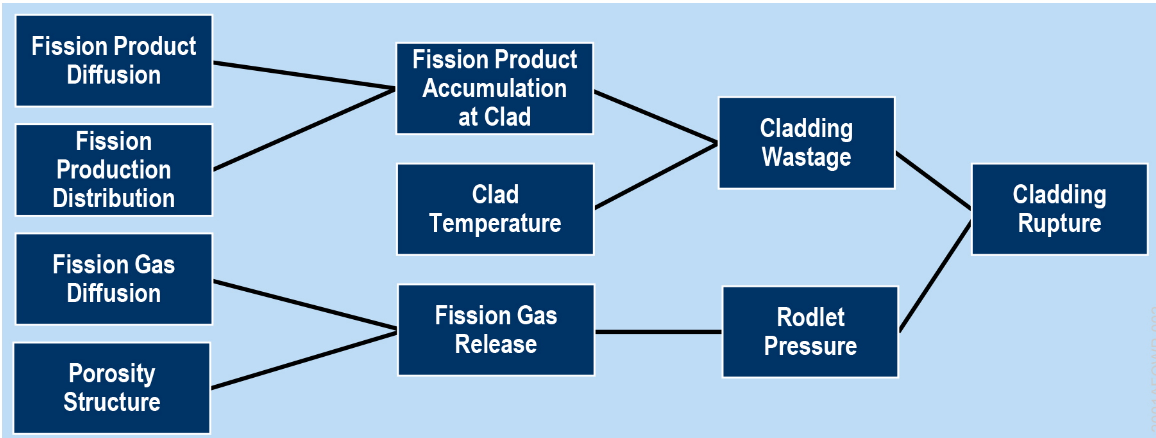

Figure 5. Fuel microstructure phenomenon impact cladding rupture behavior

While the concept to accelerate fuel qualification is clear, thoughtful implementation is necessary for methodologies to succeed in accelerating fuel qualification. Luckily this is not an entirely untrodden path and over the past decade, the US Government (multiple agencies including DOE, Department of Defense, and US Geological Survey) has been championing an effort called the Materials Genome Initiative (MGI), which is a program designed to use advanced materials characterization and testing, in concert with M&S and data science techniques, to physically understand and qualify materials for challenging applications. While examples exist where MGI-type approaches have been utilized to develop new materials tailored for specific applications, there are additional complexities that must be addressed for nuclear energy materials, including their behavior in irradiation environments. Materials science is a relatively data-poor topic – at least as far as "big data" is concerned – and nuclear energy materials are even more data poor. Despite these challenges, there is an opportunity to accelerate the qualification of nuclear energy materials by integrating advanced M&S (including data science methods) described in the previous section with experiments described in this section.

The DOE national laboratory complex is home to world-class instrumentation and technical experts that can support the AFQ methodology. Since fuel is the primary focus of the AFQ methodology, the Advanced Test Reactor (ATR) and Transient Test Reactor (TREAT) at Idaho National Laboratory (INL), the HFIR at Oak Ridge National Laboratory (ORNL), and the Massachusetts Institute of Technology test reactor (MITR) at the Massachusetts Institute of Technology (MIT) are the facilities that can be used to acquire important fuel behavior data at a range of predefined prototypical reactor conditions. In addition, the Argonne Tandem Linac Accelerator System (ATLAS) ion accelerator at Argonne National Laboratory (ANL) can be used for rapid fuel and cladding materials screening experiments as well as verification and validation of mechanistic material behavior models.

ORNL, for example, has developed an experimental capability to perform separate-effects irradiation testing of miniature fuel specimens in the HFIR[15]. These MiniFuel irradiation vehicles have a small sample size (smaller than 4 mm^3) which simplifies the design, analysis, and PIE. By reducing the fuel mass, the total heat generated inside the test capsule can be dominated by gamma heating in the structural materials instead of fission heating in the fuel.

For testing the fuel form, INL has developed a revised capsule design for the accelerated testing of advanced reactor fuels that exploits the use of smaller diameter test rodlets that are operated at increased power densities to reduce the irradiation time required to reach high burnup[16]. The revised capsule design and approach is referred to as fission accelerated steady-state testing (FAST).

An irradiation that would take up to 12 years to complete under prototypic power conditions could be reduced to 2-3 years if the fuel diameter is reduced to one-half, and 1-2 years if the diameter is reduced to one-third.

FAST takes advantage of using a reduced diameter fuel specimen with a linear heat generation rate equivalent to that of the fuel under prototypical conditions, which is achieved by testing in a higher than prototypic neutron flux or increased fuel enrichment. The result is a significant increase in power density that produces an accelerated burnup rate. However, since the test fuel operates at a prototypic linear heat generation rate, the peak fuel temperature experienced by the test fuel will be the same as in the actual application—thus, many aspects of the fuel's irradiation behavior should remain the same despite the acceleration of burnup accumulation. An irradiation that would take up to 12 years to complete under prototypic power conditions could be reduced to 2-3 years if the fuel diameter is reduced to one-half, and to 1-2 years if the fuel diameter is reduced to one-third.

The irradiation capsule is versatile and can also be tailored to experience a large range of temperatures on both the cladding and the fuel, making it very adaptable to a variety of reactor design parameters. In addition, when testing fast reactor fuel in thermal reactors, reducing the fuel diameter can mitigate the radial power depression in the fuel, reducing or eliminating the need to make use of neutron shrouding materials such as cadmium. This benefit also opens up the possibility of testing advanced reactor fuels in small irradiation locations in the ATR at INL.

FAST fuel testing can dramatically accelerate burnup accumulation under testing conditions while keeping the peak fuel temperature at a prototypic value. Since many important fuel behaviors are strongly correlated to operating temperature, there is a strong rationale that

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[15] C.M. Petrie, J.R. Burns, A.M. Raftery, A.T. Nelson, and K.A. Terrani, "Separate effects irradiation testing of miniature fuel specimens," Journal of Nuclear Materials, vol. 526, p. 151783, 2019, doi:10.1016/j.jnucmat.2019.151783.

[16] G.L. Beausoleil II, G.L. Povirk, and B.J. Curnutt, "A Revised Capsule Design for the Accelerated Testing of Advanced Reactor Fuels", *Nuclear Technology* (2019) 444-457.

fuel performance under FAST test conditions will be very similar to fuel performance in the prototypical application. However, while peak fuel temperature is maintained at the prototypic value under test conditions, the temperature gradient in the test fuel will be increased above its prototypic value. Although there are not many fuel behaviors that are strongly correlated to temperature gradient, this aspect of non-prototypicality must be considered when interpreting the results from a FAST test. Furthermore, while fuel burnup accumulation is accelerated under the FAST approach, dose to the cladding is not. Thus, an intimate connection with an advanced, mechanistic modeling activity is necessary to account for such non-prototypicalities in the FAST approach to appropriately utilize the data in an AFQ approach.

Swift ion irradiation at the ATLAS accelerator is capable of irradiating materials using a wide spectrum of swift ions with precise control over irradiation conditions that simulate prototypic in-pile conditions. The diverse beam specifications enable accelerated investigations on a series of irradiation effects including, but not limited to, defects accumulation, interdiffusion (fuel, cladding, matrix), and cavity evolution. The high ion beam flux allows rapid irradiation of fuel and cladding materials to high doses or equivalent burnup. The subsequent investigations of the irradiated specimens in rapid turnaround experiments can be facilitated by the radioactive material characterization capabilities available at ANL.

Ion irradiations at ANL can be utilized in two major aspects of AFQ:

- Screening tests for fuel and cladding materials leveraging the high dose rate feature of ion irradiation.
- Verification and validation of advanced mechanistic models using well-designed ion irradiation experiments with precise condition control.

A combination of those aspects, with advanced M&S methods, eventually powered by physics-aware artificial intelligence, can be used to quantitatively correlate material behavior under ion irradiation and in-pile irradiation, maximizing the merits of ion irradiations in AFQ activities.

Uniquely important to the overall success of AFQ are the high-level capabilities of PIE centers (such as at INL, ORNL, and PNNL), and the type of data necessary to support fuel qualification and benchmark the necessary physics-based fuel performance codes. These suites of instrumentation are grouped based upon the data delivered: microstructure and form, chemistry and composition, thermo-mechanical properties, and lastly three-dimensional reconstructions.

2.2.1 Microstructure and Form

Microstructure and form refer to material characteristics that can be viewed by the naked eye and increasingly with microscopic instruments for more detailed understanding. In essence, this works in reverse of the pyramid shown in Figure 4 in that the user can easily see macroscopic phenomena such as like cladding deformation or rupture can be easily observed by visual inspections to infer performance at the meter to millimeter level (engineering scale). More nuanced phenomena and effects can then be investigated using optical microscopes (mm to greater than 100 µm), scanning electron microscopy (SEM, greater than 1 µm level) or transmission electron microscopy (TEM, greater than1 nm level). While these instruments have become increasingly powerful over the past decade with advanced sensors and computational support, they have truly reached their potential in nuclear fuel research with the introduction of shielded plasma-focused ion beams (P-FIBs) at INL and more recently at ORNL. P-FIBs allow scientists to quickly and accurately modify fuel samples for TEM investigation and micro-mechanical testing while also reducing changes to the material from amorphization during the milling process. This has enabled tremendous growth in nuclear microscopy over the last three years.

2.2.2 Chemistry and Composition

The natural companion to the microstructural observations is that of composition. Many of the tools used for microstructural analysis offer in-situ composition analysis such as energy dispersive spectroscopy (EDS) or wavelength dispersive x-ray (WDX) spectroscopy. Both EDS and WDX are widely available on instruments at both INL, ORNL, and select industries and universities. The combination of SEM with EDS and WDX is excellent for making correlations between microstructure and composition of the fuel, such as distribution of fission product precipitation or redistribution of fuel constituents. EDS is also available on TEM instruments at INL and ORNL via scanning transmission electron microscopy (STEM). The combined method (CHEMI-STEM) is excellent at providing grain-level composition assessments at a scale of at least 100 nm. One additional method of assessing the fuel chemistry is electron probe micro analysis (EPMA also called EMP), which operates in a similar method to an SEM-EDS but has a deeper penetration that can enable the investigation of sub-surface fission gas. Using EPMA and WDX also offers an advantage over EDS as they can resolve low mass elements, such as oxygen or carbon, due to the emission of characteristic x-rays. In addition to the electron-based methods mentioned above, there is also the more traditional analytical chemistry methods of dissolving fuel samples in acid and analyzing the solution through mass spectrometry. The combination of microscopy methods with in-situ chemistry analysis and bulk isotopic analysis is critical in understanding the complete structure and form of an irradiated fuel specimen.

2.2.3 Thermo-Mechanical Properties

After microstructure and chemistry, the next series of PIE assessments pertain to the properties most relevant to fuel performance models: thermal properties such as emissivity, heat capacity, and conductivity, and mechanical properties such as elastic modulus, hardness, and yield.

There are a variety of methods for capturing thermal properties, including those using more traditional equipment such as a laser flash system or more advanced equipment such as the thermal conductivity microscope (TCM) at INL. The TCM uses thermos-reflectance with a laser to derive thermal properties at a resolution of up to 5 µm. At ANL, the suspended bridge method of measuring thermal conductivity can provide measurements of small heterogeneous features in irradiated materials at even lower scale.

Mechanical properties become more complicated because the majority of traditional methods of mechanical testing require machining specific geometries, which is generally not feasible for irradiated fuel. However, the use of laser mills and P-FIBs has enabled the use of smaller scale mechanical testing within SEMs and improved understanding of the impacts of irradiation on mechanical properties of fuel.

2.2.4 Three-Dimensional Reconstructions

The true nature of AFQ depends on coupling the advanced PIE capabilities to multiscale, mechanistic material model development and leveraging data mining, machine learning, and artificial intelligence to take sparse material data sets generated by PIE to identify both intrinsic and extrinsic relationships that occur in the fuel system of interest. PIE capabilities are advancing at such a rate that they enable innovative high-throughput capabilities to generate comprehensive thermomechanical and chemical data sets spanning across a wide range of length scales (atomistic to engineering). This involves developing advanced, high throughput characterization methods for irradiated materials to integrate the data from three tomographic techniques to spatially map the chemistry of an intact fuel rod.

In parallel, numerical M&S capabilities advancements are occurring, and coupled with the rise of supercomputers, new opportunities exist to extend atomistic and microstructural material understandings from the atomistic to the engineering scale. This process of multiscale modeling supports physics-based material model development built on first principles of relevant phenomena and seamlessly couples the relevant mechanisms predictions across broad-length scales to determine the overall system performance. In essence, multiscale models assume that the overall engineering response of the fuel system, or material in general, is directly related to the collective response of lower-length scale phenomenon rather than making phenomenological assumptions regarding fuel system behavior at the engineering scale.

Advanced PIE capabilities and physics-based, multiscale modeling are powerful new tools; however, they can be expensive, and they can introduce additional parameters that must be quantified. Lower-length-scale theoretical methods can provide some of these, and new experiments will be needed to measure others. While seemingly more expensive up front, the robustly validated mechanistic models that result are expected to provide unprecedented insights that will support the accelerated discovery and qualification of new fuels and materials.

As mentioned above, historically, fuel qualification has relied on the generation of extensive data sets that cover a wide range of conditions (such as temperatures, pressure, ramp rates, burnups, and so on). From these data sets, empirical material models are developed and used for engineering scale analyses. This process is both costly and time-consuming. Simply put, this process is ineffective and insufficient to advance nuclear energy in a competitive manner.

AFQ intends to shift the paradigm to theory-guided, data-driven materials research in order to develop a comprehensive understanding of multiscale thermo-mechanics for a given fuel system as well as the potential to develop engineering solutions to target or mitigate detrimental mechanical and functional properties for the fuel system of interest.

3. THE AFQ METHODOLOGY: TYING KEY ELEMENTS TOGETHER

AFQ is part of an overall licensing strategy for a nuclear energy system. Because the licensing strategy is primarily focused on limiting radionuclide release to the public, and fuel is the primary source of radionuclide, AFQ will play a critical role in enabling accelerated licensing for the overall reactor system. The regulator provides general guidelines for risk-informed performance-based or consequence-based licensing approaches. Examples include 10 CFR Part 50/52 for probabilistic risk assessment (PRA)-based approaches and NUREG-1537 for a consequence-based approach as prescribed by the NRC. AFQ methodology may be supporting a PRA-based or consequence-based licensing strategy, and is agnostic to this choice. However, the specific implementation of AFQ needs to be tailored to this specific licensing choice, which is driven by the reactor developer's overall licensing strategy.

3.1 THE OVERALL REACTOR SYSTEM AND AFQ

The ultimate goal of a reactor safety assessment, including its fuel, is to ensure that the safety of power plant employees and the general public is guaranteed. To that end, a series of core safety criteria have been generally developed and used to date, such as the possibility to safely shut down the reactor at any time, the ability to maintain coolability (to control heat generation and prevent fuel melt or phase change, and associated dimensional changes that can impact the shutdown capability or increase radioactive release), and the limitation of radioactive release.

The overall safety of the reactor demands that different criteria are fulfilled based on the reactor type. For example, if the reactor relies on control rods, ensuring that their insertion is possible at all times is required.

To be reactor-agnostic, an overall licensing methodology must have a number of considerations summarized in documentation from the NRC, such as the following:

- The definition of scenarios encompassing normal conditions as well as abnormal occurrences that could expected to happen in the lifetime of the reactor, severe accidents, and natural disasters.
- The definition of failures that will, in these scenarios, lead to endangering the employees or the general population.
- The requirements to have a high certainty that said failures will not happen.

The overall safety is ensured by several pillars, including the safety culture in the nuclear industry, the engineering of safety solutions, the inclusion of generous margins, and the use of advantageous materials. The addition of engineering solutions, such as emergency water supply systems or a chemical mixing tank, is usually expensive and can be limited by choosing adequate fuel materials. The fuel component of the reactor has a large impact, since it is where the heat and radioactive materials are produced. If one were to choose a fuel that is well-known and characterized, with years of operating experience, uncertainties will be smaller, and so will the required margins to avoid failures. Similarly, margin can be created if the fuel material has advantageous properties, such as a high melting temperature, passively safe neutronic feedback, or low hydrogen pickup. These properties can also increase margins to failure or push the operating conditions to improve economics.

AFQ relies upon a three-phase methodology of fuel development and qualification.

- Phase 1 involves identifying the operational and environmental envelope and considering basic irradiation effects, along with equilibrium thermodynamics, to identify suitable constituents of the fuel system.
- Phase 2 involves identifying governing phenomena and quantifying associated parameters through separate-effects testing and integral fuel performance analysis.

During Phase 3, the fuel system design is fully developed and integral fuel fabrication is finalized to allow integral fuel irradiation and transient safety testing to develop the licensing basis.

The principles of AFQ during Phase 1 enable expedited material testing and screening of fuel systems. Fuel material optimization is generally performed after finishing the preliminary reactor design. First, the reactor designer must answer questions such as the power output, the reload frequency, the size of the core, the type of neutron spectrum, the coolant properties, and so on. From there, what the NRC calls a “fuel performance envelope” can be determined. Fuel materials must be able to perform acceptably under all of these operating conditions, with an additional margin that depends on how well the fuel performance can be predicted. In this phase, it is common for the designer to consider various materials, to get a preliminary idea of feasibility. However, to do so, many properties must be known at a fundamental level. This can be a problem when moving away from the most conventional options, or when small but unknown design tweaks are needed, such as changing an alloying concentration. Thus, in a material selection phase, it is very useful to have a process that can quickly and reliably provide preliminary results to screen out options and allow for focus on select promising materials.

After choosing the reactor fuel and structural materials, the developer must ensure that the data is reliable, which begins in Phase 2 and is finalized during Phase 3 of the AFQ process. To develop sound material behavior models, the developer must also provide uncertainties on the final results. This begins in the design for manufacturability environment, where specifications of the materials are defined, with a balance between precision and reproducibility on the one side, and economics on the other one. Dimensions, microstructure, and microchemistry must be defined because the models will have to be valid for the full range of specifications. The impact of designing for manufacturability, and the influence of the manufacturing process on the material properties and design parameters is recognized.

Phase 2 iteratively develops the safety case through separate-effects testing coupled with integral fuel analyses such that Phase 3 integral testing is designed to validate the safety case developed in Phase 2. In traditional model development, quality assurance is provided by using proven empirical processes to generate data. This method requires a significant amount of time and is very expensive. AFQ is modernizing this approach to make data acquisition faster and economical by using novel experimental methods, real-time data acquisition sensors, and advanced modeling. Combining these principles with a prioritization of model development based on a given parameter's particular uncertainty and its impact of the final uncertainty as suggested in footnote 4 may reduce the amount of time required to ensure adequate design margins for safety. An important step is to adequately characterize these new methods so that they are acceptable to safety and regulatory agencies and that their uncertainty is well-known and accepted. The iterative analysis and testing activities in Phase 2 support effective integral fuel design testing within Phase 3. The intention is to focus on tests designed to successfully demonstrate the safe and acceptable operation of the fuel under prototypic and transient and accident conditions.

Especially relevant for new materials is novel failure modes, an aspect that must be considered. To utilize new materials, or even current materials, outside of the range on which experience exists, it is essential to verify that no unexpected failures will occur. Once again, AFQ testing methods coupled with M&S facilitate results in a shorter timeframe compared to traditional material development approaches.

As previously noted, industry will follow all updated guidance issued by the NRC. The NRC is actively working on a new part to Title 10 of the Code of Federal Regulation (10 CFR Part 53) to establish regulations that account for advanced reactors. Due to the 10 CFR Part 53 development schedule, a reactor vendor may use the current regulatory framework (10 CFR Part 50/52) where applicable while considering any impacts due to anticipated potential future rulemaking.

NRC guidance provides recommendations for Industry to follow in licensing new reactors and fuel materials. Additionally, developers can use the Licensing Modernization Project (LMP), as discussed in NEI 18-04, "Risk-Informed Performance-Based Guidance for Non-Light Water Reactor Licensing Basis Development" and Regulatory Guide 1.233 "Guidance for a Technology-Inclusive, Risk-Informed, and Performance-Based Methodology to Inform the Licensing Basis and Content of Applications for Licenses, Certifications, and Approvals for Non-Light Water Reactors" to develop the foundation for a reactor's safety case. The licensing application may be developed using a combination of NUREG-1537, "Guidelines for Preparing and Reviewing Applications for the Licensing of Non-Power Reactors" and the process and format of the Technology Inclusive Content of Application Program (TICAP), and the Advanced Reactor Content of Application Project (ARCAP). The LMP, TICAP, and ARCAP are currently in development and in combination with AFQ tools, the qualification process stands to accommodate new non-LWR reactor fuel systems much more efficiently.

3.2 THE IMPORTANCE OF PHENOMENA IDENTIFICATION AND RANKING TABLES (PIRTS)

Once the system constraints (reactor system and operating parameters) during normal operation and postulated accident scenarios and the fuel design concepts are identified, potential failure mechanisms are considered with respect to achieving basic design functions. Design criteria are based on meeting three fundamental safety functions: control of the reactivity, removal of heat, and confinement of the radioactive material, as well as limitation of accidental radioactive releases. Failure mechanisms are identified and associated either with failure of the first fission product barrier, or fuel system performance degradation, such that reactivity control or heat removal capabilities become compromised and reactor safety systems are adversely impacted. The evaluation of the risks of the fuel systems to meet safety criteria during normal operation, transients, and postulated accidents is assessed through identifying the failure modes, the mechanisms associated with those modes, and the phenomena associated with those mechanisms.

A failure mode is a specific loss of functionality of the fuel system that results in failure or degradation. It is the way in which a fuel component or system fails and is defined by function and behavior. The failure mechanism is the factor that causes a failure mode and is defined by states or conditions of the system that contribute to the causes of the failure. A system may have many different failure mechanisms that lead to a failure mode. The states or conditions involved in a failure mechanism are considered phenomena that contribute to the failure mechanism. These phenomena are usually determined by testing and modeling. Once phenomena associated with failure mechanisms are identified, they are ranked according to their impact on the failure mechanisms and the knowledge about the phenomena.

The phenomena involved with the potential failure or damage mechanisms of the fuel design operating within the reactor system constraints are identified and ranked according to the impact on the mechanisms and the knowledge of the phenomena. The phenomena should be given a high, medium, or low ranking of importance, and the current level of knowledge should be assessed as unknown, partially known, or known. A simple matrix of knowledge versus impact is used to identify phenomena with low knowledge and high impact in which to focus, as depicted in Table 1.

TABLE 1. MATRIX OF KNOWLEDGE VERSUS IMPACT				
		Importance		
		High	**Medium**	**Low**
Knowledge Level	**Known**			
	Partially Known	*		
	Unknown	*	*	
* Fuel systems falling into areas indicated by an asterisk benefit from AFQ the most				

The PIRT is a systematic way of organizing information to help guide research or development of regulatory requirements. This ranking occurs through an iterative process involving expansion of material databases, developing and using mechanistic models of fuel behavior, and conducting integral fuel performance analyses. A substantial amount of experimental data and an understanding of irradiation effects in materials are available.

A collaborative effort between fuel developers and national labs along with academia should be utilized in the iterative process of ranking the phenomena to prioritize the use of engineering-scale M&S tools in combination with separate-effects testing to improve understanding of the phenomena involved with the performance of the fuel design with respect to failure and damage mechanisms. The goal is to support the definition of the design bases and associated acceptance criteria for the safety analyses involved in the licensing strategy identified by the developer. Additionally, technical gaps are identified where knowledge or experimental data is lacking, and additional test programs are needed, including integral effects testing.

The PIRT becomes more detailed and complex as a reactor system matures. For example, during Phase 1 development focusing on fuel-cladding matrix selection as described in the next section (see Table 2), the determination of gaps within fuel and cladding material properties and associated physics-based models is very simple as illustrated. Once the design develops further into Phase 2 and more knowledge is gained by separate effect testing and the models used to perform simulations to define bounding variables and operating envelope become more involved, PIRTs become more interdependent. Phenomena start to become interrelated as the failure and damage mechanisms become understood. In phase 3 of AFQ, PIRTs identify gaps in the understanding of these mechanisms to focus integral irradiation testing and continued development of M&S.

3.3 THE ESSENCE OF AFQ: TARGETED EXPERIMENTS AND M&S VALIDATION[17]

The heart of the AFQ methodology is the ability to reduce the overall experimental data required to qualify a new nuclear fuel system by developing targeted experiment plans informed by mechanistic models to fill data gaps.

The paper by Wen et al.[18] provides an example of how a reduced number of data points can accurately represent behavior (strain) as a function of an important parameter (time) when a good physics-based model exists. This example shows a mechanism-based model of the thermal and irradiation creep of HT9 and experimental data. A rate-theory-based dislocation climb law was developed including the contribution of irradiation-induced point defects. The climb approach is coupled with a constitutive model describing the effects of solute strengthening and Coble creep mechanisms. The model was benchmarked using the experimental results of Toloczko et al.[19] for both thermal and irradiation creep tests, as shown in Figure 6. The comparison shows that the model can quantitatively assess the relative roles of the physical mechanisms. This also indicates that the model can be effectively used to predict the thermal and irradiation behaviors of the silicon carbide (SiC) composite being developed for the application to the high temperature and high-dpa applications.

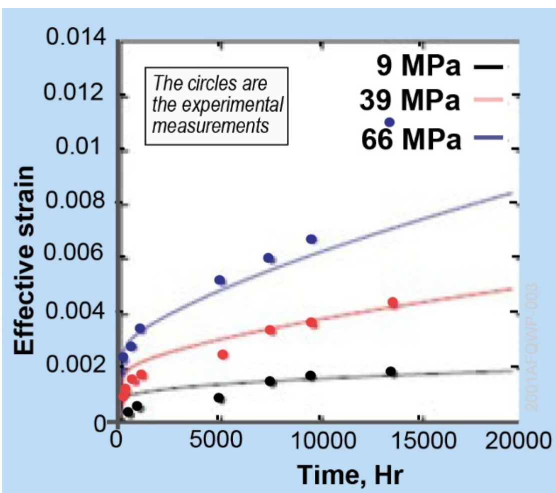

Figure 6. Predicted thermal creep behavior of HT9 steel as a function of von Mises stresses at 600 °C[17]

In comparison to the approach outlined in the Crawford paper[2], the AFQ methodology essentially consolidates Phases 2 and 3 into a single phase. The initial Phase 1, selection of a fuel form and matrix, is still the starting point for both approaches as shown in Table 2. However, many irradiation experiments have now produced useful materials property data that can already be used to refine the initial selection, potentially obviating some of the Crawford Phase 2 activities. Furthermore, M&S can be pursued in parallel with separate effects measurements of material properties and component level tests. Both of these enable a time-savings.

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[17] Information in this section is based on a General Atomics Electromagnetic Systems (GA-EMS) report: "Energy Multiplier Module (EM^2) Accelerated Fuel Qualification Strategy," GA-EMS document 30533R00003/A, May 6, 2021".

[18] W. Wen et al., "Mechanism-based modeling of thermal and irradiation creep behavior: An application to ferritic/martensitic HT9 steel," LA-UR-19-28064, Los Alamos National Laboratory, 2019.

[19] M. Toloczko et al., "Comparison of thermal creep and irradiation creep of HT9 pressurized tubes at test temperatures from ~490ºC to 605ºC," S. T. Rosinski, Ed., *Effects of Radiation on Materials: 20th International Symposium*, ASTM International, 2001.

TABLE 2. PHASES OF THE AFQ METHODOLOGY		
PHASE	**FUEL SYSTEM COMPONENT**	**AFQ ACTIVITY**
Phase 1	Fuel-cladding/matrix selection	Choice of fuel system components for the expected operating environment based on irradiation, thermochemical, and thermodynamic behavior from literature searches, separate effects data, and so on.
Phase 2	Fuel	Fissile material properties and component level performance testing and M&S.
	Material encapsulating the fuel (tube, plate or matrix)	Non-fissile material properties and component-level performance testing and M&S.
	Prototypic combinations of fuel and encapsulating material	Thermochemical and thermomechanical prototypic interaction testing and M&S.
	Analysis by M&S and testing, where possible	Determination of uncertainties and safety margins in transients, DBA.
Phase 3	Integral fuel and cladding/matrix	Fuel system performance in prototypic conditions - fuel burnup.
		Fuel system performance in prototypic conditions - cladding/matrix corrosion, heat transfer.
		Transient testing.
		Anticipated operational occurrence (AOO), design basis accident (DBA).

Executing each phase involves a well-defined coupled experimental and M&S plan, which includes the following actions per each phase[20]:

3.3.1 Phase 1: Data Compilation and Physics-Based Modeling

1. Compile and evaluate existing data.
2. Identify gaps in data (PIRTs). See Table 3 and Table 4 for examples.
3. Develop physics-based models that describe the phenomena to be implemented in codes such as Bison.
4. Identify the driving physics phenomena and experimental observables that are important to the safety case.

Table 3 and Table 4 contain generic lists of fuel and cladding properties, respectively, applicable to existing LWR fuel. These tables have the following columns:

- Uncertainty: Based on the quality and consistency of existing data due to availability of measurements and their variations.
- Importance: Based on the impact of the property or model on fuel damage, fuel failure, and coolability.

[20] General Atomics project 30533 under DOE grant agreement DE-NE0008831.

- Priority: Reflect the combined impacts of uncertainty and importance to indicate the relative need and urgency to collect new data and improve modeling to reduce uncertainties in the fuel safety analysis.

The objective of modeling and measurement data gathering is to reduce the uncertainties in the safety decision making such that reasonable and acceptable design margins exist to preclude fuel damage, fuel failure, and loss of coolability.

TABLE 3. GAP ASSESSMENT IN FUEL FORM PROPERTIES AND MODELS

PROPERTY OR MODEL	UNCERTAINTY	IMPORTANCE	PRIORITY
Melting temperature	Low/moderate/high	Low/moderate/high	Low/moderate/high
Specific heat	Low/moderate/high	Low/moderate/high	Low/moderate/high
Thermal conductivity	Low/moderate/high	Low/moderate/high	Low/moderate/high
Emissivity	Low/moderate/high	Low/moderate/high	Low/moderate/high
Density	Low/moderate/high	Low/moderate/high	Low/moderate/high
Elastic modulus	Low/moderate/high	Low/moderate/high	Low/moderate/high
Poisson's ratio	Low/moderate/high	Low/moderate/high	Low/moderate/high
Yield stress	Low/moderate/high	Low/moderate/high	Low/moderate/high
Fracture stress	Low/moderate/high	Low/moderate/high	Low/moderate/high
Thermal expansion	Low/moderate/high	Low/moderate/high	Low/moderate/high
Swelling	Low/moderate/high	Low/moderate/high	Low/moderate/high
Creep	Low/moderate/high	Low/moderate/high	Low/moderate/high
Diffusion coefficients	Low/moderate/high	Low/moderate/high	Low/moderate/high
Fission gas release	Low/moderate/high	Low/moderate/high	Low/moderate/high
Densification	Low/moderate/high	Low/moderate/high	Low/moderate/high
Relocation	Low/moderate/high	Low/moderate/high	Low/moderate/high

EXAMPLE

TABLE 4. GAP ASSESSMENT IN FUEL CLADDING PROPERTIES AND MODELS

PROPERTY OR MODEL	UNCERTAINTY	IMPORTANCE	PRIORITY
Specific heat	Low/moderate/high	Low/moderate/high	Low/moderate/high
Thermal conductivity	Low/moderate/high	Low/moderate/high	Low/moderate/high
Emissivity	Low/moderate/high	Low/moderate/high	Low/moderate/high
Thermal expansion	Low/moderate/high	Low/moderate/high	Low/moderate/high
Density	Low/moderate/high	Low/moderate/high	Low/moderate/high
Elastic modulus	Low/moderate/high	Low/moderate/high	Low/moderate/high
Poisson's ratio	Low/moderate/high	Low/moderate/high	Low/moderate/high
Yield stress	Low/moderate/high	Low/moderate/high	Low/moderate/high
Fracture stress	Low/moderate/high	Low/moderate/high	Low/moderate/high

EXAMPLE

TABLE 4. GAP ASSESSMENT IN FUEL CLADDING PROPERTIES AND MODELS			
PROPERTY OR MODEL	**UNCERTAINTY**	**IMPORTANCE**	**PRIORITY**
Swelling	Low/moderate/high	Low/moderate/high	Low/moderate/high
Creep	Low/moderate/high	Low/moderate/high	Low/moderate/high
Stress-strain	Low/moderate/high	Low/moderate/high	Low/moderate/high

3.3.2 Phase 2: Model Validation

1. Use the physics-based models that describe the phenomena of interest. Do not rely solely on empirical models.
2. Validate the models with targeted experiments (separate effects testing). That is, measure key experimental observables and results compare to simulations.
3. Use the models to perform more simulations to optimize and help define the bounding variables (pressure and temperature) and determine and define an operating envelope of parameters in which the simulations are validated.
4. Use M&S to determine sensitivities and uncertainties with more fidelity than can be obtained with purely empirical models. Continue doing separate effects testing and sub-scale integral testing, as necessary.

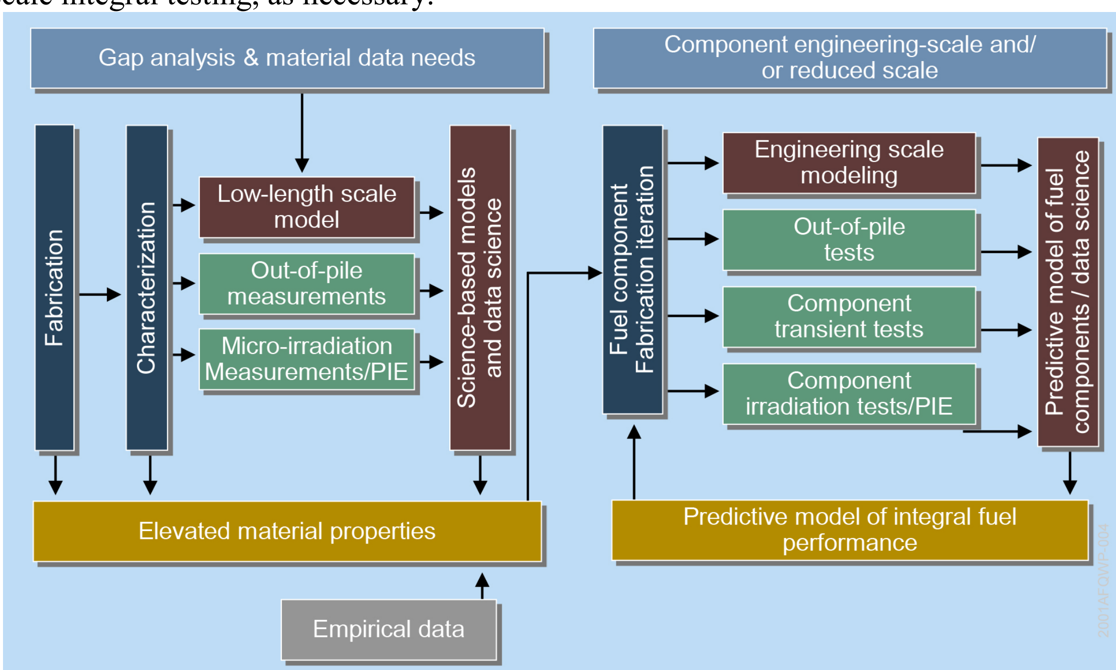

Figure 7. Detail of Phase 2 of the AFQ methodology[20]

In this phase, M&S is performed for the low-length scale modeling and separate effect tests are also carried out to validate the M&S results. Figure 7 portrays a flowchart with the details of Phase 2 that is more explicit in showing the fabrication and characterization steps implicit in Terrani et al[5], and shows the contribution of the low-length and engineering-scale modeling as they contribute to the evaluated material properties and the predictive model of integral fuel performance.

Phase 2 is where most of the benefits of AFQ will be realized. Engineering-scale tools become well developed based on integrating separate effects testing with science-based models. These models are developed and validated by component irradiation testing and data science to become predictive. Once the engineering-scale modeling becomes well-informed and mature and the fuel design specification is established through manufacturing development, the Phase 3 integral testing is planned for specific facilities based on a targeted prototypical or accident-based environment. Phase 3 integral testing is based on the test designs, specifications, and analysis results from Phase 2.

3.3.3 Phase 3: Essential and Limited Integral Testing

1. Carry out essential integral demonstration tests under prototypic or nearly prototypic conditions, which are expected to be limited in number given information already obtained in Phases 1 and 2.
2. Produce a final fuel qualification topical report for licensing purposes.

As discussed in the previous sections, in Phases 1 and 2, the modeling of the nuclear fuel form uses atomistic and mesoscale approaches to derive key model parameters and to inform irradiation testing. These material properties and models are used to build continuum-scale models of the fuel. The cladding also uses continuum-scale modeling and test data due to its engineered composite structure. With science-based models, integral irradiation tests can focus more on validating parameters and confirming expected trends and inflection points in the models, compared to irradiation testing to collect data to build empirical-based models. Science-based models may also allow greater flexibility in interpolation and extrapolation beyond the irradiation database, allowing implementation of new designs with sufficient safety margins.

Phase 3 will be informed by Phase 2 for integral testing. Integral fuel testing may initially be performed using reduced size fuel elements. These scaled-down fuel elements could be irradiated in the ATR in a test capsule adopted from the Advanced Gas Reactor (AGR) fuel program. After the versatile test reactor (VTR) is built and finished commissioning tests, specific fuel elements would be able to be tested in more prototypical conditions of temperature and neutron flux, such as in gas, molten salt, sodium, and perhaps additional test loops. Both the ATR and VTR tests can be accelerated using higher than normal fission density. Use of ^{235}U enrichment greater than 20 weight % could be used to accelerate the burnup. The data from these integral fuel tests will be used to establish the safety case for the fuel sufficient for use in a reduced-scale demonstration reactor with prototypic conditions.

Engineering-scale M&S tools, along with early irradiation testing, provide feedback to the materials data and design parameters, which will be used to refine subsequent integral fuel testing. Targeted separate-effects testing can further refine the safety case and minimize efforts on parameters with little or no effect on fuel performance. Integral tests under prototypical conditions to full burnup will ultimately be required to fully qualify the fuel system for its entire lifecycle. For a long-life fuel, this testing to acquire qualification data may be obtained in a bootstrapping way with a demonstration reactor.

3.3.4 Summary of the Three Essential Elements of AFQ

Use of atomistic and mesoscale modeling to develop mechanistic models that can be validated by experimental data: Science-based modeling will add confidence and reduce uncertainty, particularly when extrapolating to higher burnup and when compensating for effects of accelerated irradiation at much higher-than-normal fission density. The mechanistic models will reduce the dependence on models that are derived from “fits” to purely empirical data because the functional relationships of key dependent variables are science-based.

Intentional use of pre-irradiation characterization and PIE with enhanced microstructural analysis techniques to inform, refine, and validate the advanced M&S tools: The goal of developing advanced M&S is a set of science-based models that can be used to predict long-term irradiation behavior of the fuel system to avoid fuel damage and failure, and ensure fuel coolability during severe accidents. Completely empirical models are inherently limited to the database used to create them. Science-based models use better mathematical descriptions of the physics and mechanisms of the underlying material properties to enable them to have a much more robust fidelity than the limitations of a purely empirical database. Variations and uncertainties in specifications can be accommodated in science-based models to reduce excess margin that is normally required by the use of empirical models. The integral testing, in addition to providing the data that may be used in empirical models, also serves as validation of the science-based models, verifying the safety-related margins.

New experimental techniques, such as the advanced M&S, FAST fuel irradiation, and MiniFuel capsule irradiation used in tandem with M&S: Specialized experiments can provide separate effects data that are expected to inform and thus, reduce the number and total cost of fuel irradiations. The number of irradiations is greatly reduced because the models are more science-based with less emphasis on empirically-based models. Empirically-based models require a much larger database to establish the foundation of the empirical model. In particular, FAST irradiations are accelerated, and when validated and used appropriately, will reduce both the cost and schedule, as compared with prototypic irradiation. Fuel qualification will ultimately rely on integral fuel data from a reduced-scale prototype or demonstration reactor to validate performance.

4. SUMMARY AND PATH FORWARD

The AFQ methodology articulates a path to qualify new nuclear fuels in a timely and cost-effective way by leveraging the most advanced M&S and experimental tools that are available today. The long and protracted fuel qualification process has always been considered the "long pole in the tent" of the licensing process. Achieving widespread adoption of AFQ as common practice will help address this challenge and provide the NRC with a rigor and consistency in approach to aid in evaluation of the fuel form. Using the AFQ framework would enable a more efficient overall licensing of new reactor systems. If implemented appropriately, the AFQ methodology could significantly reduce the time to qualify new fuels, from what historically has taken more than 20 years, to a target of as few as five years, along with a significant cost reduction resulting from the reduced number of costly integral tests and the associated use of special testing facilities, labor, and materials.

> The AFQ methodology offers a path to qualify new nuclear fuels in a timely and cost-effective way by leveraging the most advanced M&S and experimental tools available today.

The AFQ methodology is a suggested guide to the qualification of new nuclear fuels. It is up to each fuel developer to adopt all, part, or none of this approach. It is hoped that developers will realize the benefits inherent in adopting as much of the methodology, as appropriate, to the fullest extent practicable.

The AFQ methodology must be tailored for the specific reactor type, fuel form, and safety case. Users will realize the benefits of AFQ more rapidly if it is demonstrated for a variety of reactor technologies and fuel systems (for example, new fuel design development for existing reactors). Users are recommended to document and analyze any lessons learned from specific applications of the AFQ methodology to further improve and refine the generic methodology and to provide best-practice updates to its tools and their implementation.

To facilitate the wide adoption of the AFQ methodology, continued engagement by the NRC is necessary to implement the key elements of the AFQ methodology with each developer and enable an expeditious path to qualification of their specific fuel system. Additionally, DOE support through funding opportunities that strengthen the elements of AFQ is essential for industry-wide adoption. Establishing merit criteria that value modeling and simulation together with targeted experiments may be a way to encourage this aspect of AFQ which stands to bring the most benefit in reducing implementation time required, especially in Phase 2.

TABLE 5. ACRONYMS	
ACRONYM	**DEFINITION**
AFQ	Accelerated Fuel Qualification
AGR	Advanced Gas Reactor
ANL	Argonne National Laboratory
AOO	Anticipated Operational Occurrence
ARCAP	Advanced Reactor Content of Application Project
ATLAS	Argonne Tandem Linac Accelerator System
ATR	Advanced Test Reactor
CFR	Code of Federal Regulation
DBA	Design-Basis Accident
DD	Dislocation Dynamics
DFT	Density Functional Theory
DOE	Department of Energy
EDS	Energy Dispersive Spectroscopy
EM^2	Energy Multiplier Module
EPMA	Electron Probe Micro Analysis
FAST	Fission Accelerated Steady-State Testing
FEA	Finite Element Analysis
GA-EMS	General Atomics Electromagnetic Systems
HFIR	High Flux Isotope Reactor
HPC	High-Performance Computing
INL	Idaho National Laboratory
LLS	Least Linear Squares
LMP	Licensing Modernization Project
LOCA	Loss of Coolant Accident
LWR	Light Water Reactor
M&S	Modeling and Simulation
MD	Molecular Dynamics
MGI	Materials Genome Initiative

TABLE 5. ACRONYMS	
ACRONYM	**DEFINITION**
MIT	Massachusetts Institute of Technology
MITR	Massachusetts Institute of Technology Reactor
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NRC	Nuclear Regulatory Commission
ORNL	Oak Ridge National Laboratory
P-FIB	Plasma-Focused Ion Beam
PIE	Post-Irradiation Examination
PIRT	Phenomena Identification and Ranking Table
PNNL	Pacific Northwest National Laboratory
PRA	Probabilistic Risk Assessment
ROM	Reduced Order Model
SEM	Scanning Electron Microscopy
SiC	Silicon Carbide
SPPP	Structure-Processing-Properties-Performance
STEM	Scanning Transmission Electron Microscopy
TCM	Thermal Conductivity Microscope
TEM	Transmission Electron Microscopy
TICAP	Technology Inclusive Content of Application Program
TREAT	Transient Test Reactor
VPSC	Visco Plastic Self-Consistent
VTR	Versatile Test Reactor
WDX	Wavelength Dispersive X-ray