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ABSTRACT

The U.S. Department of Energy Advanced Fuels Campaign (AFC) is currently funding research and development on a number of fuel technologies for light water reactors (LWRs) that could provide enhanced performance under accident scenarios relative to the current zirconium alloy-uranium dioxide (UO_2) fuel system. The overall mission of the accident tolerant fuel (ATF) research is to develop advanced fuels/cladding with improved performance, reliability and safety characteristics during normal operations and accident conditions, while minimizing waste generation. Evaluating the performance of candidate ATF concepts is a topic of significant discussion among researchers, fuel vendors and utilities to ensure that the developed concepts can meet minimum performance and economic requirements, can be developed within a reasonable time, and can be approved for insertion as a lead fuel rod in a commercial reactor by the 2022 goal established in the U.S. Characterizing the performance enhancements of candidate ATF first requires understanding the performance of the current Zr-UO_2 system under equivalent operations and accident scenarios. Proper evaluation of each concept is dependent on development of data through focused out-of-pile and in-core experiments to support modeling of the fuel and cladding behavior in fuel performance and systems analysis codes; complementary irradiation of ATF concepts will be discussed in a separate paper. This paper will provide an overview of the key evaluation tools and evaluation scenarios currently being considered within the LWR community for ATF. The evaluation toolset includes standard neutronic and thermal-hydraulic analysis for normal operating conditions and transient/accident conditions and analysis of severe accident behavior using modified versions of the MELCOR code for preliminary concept screening. Development of advanced fuel performance analysis using the BISON application based on the Multi-physics Object-Oriented Simulation Environment (MOOSE) at Idaho National Laboratory (INL) has also been initiated. Evaluation scenarios (e.g. accident scenarios) currently being discussed for use across the international ATF development teams are also presented.

1. Introduction

The safe, reliable and economic operation of the nation's nuclear power reactor fleet has always been a top priority for the nuclear industry. Continual improvement of technology, including advanced materials and nuclear fuels, remains central to the industry's success.

1.1 Motivation

The current nuclear power industry is based on mature technology and has an excellent safety and operational record. The current UO_2 – zirconium alloy fuel system meets all performance and safety requirements while keeping nuclear energy an economically competitive clean-energy alternative for the United States. With the exception of a few extremely rare events, the current fuel system has performed exceptionally well.

The goal of accident tolerant fuel development is to identify alternative fuel system technologies to further enhance the safety, competitiveness, and economics of commercial nuclear power. The development of an enhanced fuel system supports the sustainability of nuclear power, allowing it to continue to generate clean, low-CO_2-emitting electrical power in the United States. Details on the applicable development phases, key ATF attributes, and proposed evaluation metrics are included in previous publications [e.g., 1, 2].

1.2 Constraints

Any new fuel concept proposed for enhanced accident tolerance must be compliant with and evaluated against current design, operational, economic, and safety requirements [2]. The constraints associated with commercial nuclear fuel development and deployment that are applied to ATF designs include:

- *Backward Compatibility*— Compatible with existing fuel handling equipment, fuel rod or assembly geometry, and co-resident fuel in existing LWRs.
- *Operations*— Maintains or extends plant operating cycles, reactor power output, and reactor control.
- *Safety*— Meets or exceeds current fuel system performance under normal, operational transient, design-basis accident (DBA) and beyond design-basis accident (BDBA) conditions.
- *Front end of the nuclear fuel cycle*— Adheres to regulations and policies, for both the fuel fabrication facility and the operating plant, with respect to technical, regulatory, equipment, and fuel performance considerations.
- *Back end of the nuclear fuel cycle*— Cannot degrade the storage (wet and dry) and repository performance of the fuel (assuming a once-through fuel cycle); should consider potential issues associated with a possible future transition to a closed fuel cycle.
- *Economics*— Maintains economic viability with respect to additional costs (e.g., fabrication) and potential cost reductions realized through improved performance (higher burnup for extended cycles and power upgrades) or increased safety margin.

Analysis of proposed fuel and cladding concepts must be conducted using a number of different tools to evaluate potential performance under normal operating conditions, anticipated operational occurrences (AOOs), and DBAs, and prediction of possible behavior under BDBAs. It is also necessary to assess the possible magnitude of enhanced accident tolerance offered by a proposed concept. Analysis tools rely on availability of experimental data to properly model the performance of the candidate materials under each of the modeled scenarios. In many cases, only limited data is available for proposed fuels and cladding materials, or on the interaction between fuel and cladding or cladding and coolant. Hence, some analyses must apply approximations and assumptions early in the development stage before data becomes available. These approximations result in increased uncertainty in the predicted performance until improved data become available.

This paper provides an overview of the set of analysis tools that are currently being employed in screening and evaluation of ATF concepts in the U.S. Department of Energy Advanced Fuels Campaign.

2. Standard Analysis Suite

Design of an advanced fuel system demonstrating enhanced performance and safety relative to the current fuel system first requires understanding the current state-of-the-art fuel system performance under the various system operating regimes. These “regimes” include:

fabrication / manufacturability; normal operations and AOOs; postulated accidents (DBAs); severe accidents (BDBAs); and used fuel storage / transportation / disposition. This paper focuses on analysis over the three operational regimes; it does not address evaluation of fabrication or handling issues (either before or after irradiation).

An assessment of the potential beneficial impact or unintended negative consequences of candidate ATF concepts must address the obvious “fuel-specific” characteristics of the concept, but, perhaps more importantly, the assessment must address how implementation of the concept will affect reactor performance and safety characteristics. This assessment would include neutronics and thermal-hydraulics analyses to ensure that the reactor would operate as intended with the candidate fuel system. Coupled thermal hydraulic-neutronic analysis of candidate ATF concepts is essential in understanding the synergistic impact of the thermal properties and reactivity feedback.

2.1 Standard Screening Analyses for ATF Concepts

Standard evaluation of ATF concepts includes neutronics, thermal-hydraulic analyses, fuel performance, and detailed systems analyses. Each of these analyses is briefly described below. For additional detail on the code set employed in screening analysis for fuel and cladding concepts, see Todosow, et al. [3]. As noted in Bragg-Sitton et al. [2], the analysis fidelity and level of detail depends on the development stage of the modeled concept. During the initial “screening” stage analyses will have limited detail, based on the current state of knowledge for the concept. The level of detail may range from literature reviews and expert judgment through limited experiments and computational analyses. In evaluating the potential performance of an ATF concept, the goal is to have sufficient confidence in the assessment, given a reasonable investment of time and resources, that identified changes relative to the reference fuel system (UO_2-Zr-alloy) are known well enough to proceed with continued development, or to conclude that the concept should be modified or abandoned.

Researchers at Brookhaven National Laboratory (BNL) working within the U.S. DOE Advanced Fuels Campaign have developed and benchmarked a method for screening the reactor performance and safety characteristics of proposed advanced concepts [3]. Key elements in the methodology include: initial screening, three-dimensional core analysis, and transient analysis. Initial screening analysis entails infinite lattice calculations at the fuel assembly level to estimate ATF impact on cycle length/burnup, reactivity and control coefficients, etc. as a function of a selected fuel enrichment. Subsequent 3D core analyses include thermal-hydraulic and temperature feedback, providing a platform for fuel cycle analysis and time-dependent accident analysis. Analysis of selected transients is then conducted to provide an estimate of “coping time” (i.e. time to failure of key components) under the modeled conditions. Screening analyses must indicate a reasonable increase in the coping time for candidate ATF concepts relative to the reference fuel system (e.g. on the order of hours) to be considered “accident tolerant.”

Many light water reactor fuel concepts have been analyzed using the described screening analyses [3]. Some specific examples of the application of screening analyses to date include assessment of inert matrix fuel [4], fully ceramic microencapsulated fuel [5, 6], high-density ceramic composite fuels [7], candidate advanced cladding materials [8], and “drop-in” ceramic composite fuels [8]. These screening analyses provide information on the potential impact of fuel and cladding materials on reactor performance and safety characteristics. In addition, the screening analyses can help identify limitations in state-of-the-art modeling tools that may impact the ability to accurately model all aspects of some concepts. One specific example is identification of the need to implement best-estimate thermal models to accurately model fast transients with fully ceramic microencapsulated fuel [6].

The constraint of “backward compatibility” noted in section 1.2 means that a candidate fuel should be able to replace the current reference fuel without significantly impacting handling operations, core thermal-hydraulics, emergency systems, etc. This requirement also places reasonable limitations on the possible enrichment of proposed fuels, recognizing that the current limit on fuel enrichment for commercial reactor applications is <5 w/o ^{235}U. Maintaining the backward capability constraint could restrict opportunities for performance optimization, but also reduces issues with licensing the fuel and implementing it in the current LWR fleet. The ability of concepts to adhere to this constraint can be addressed in the initial suite of screening analyses.

Initial Neutronic Screening Analyses: Initial analyses are often performed at the fuel-assembly level (especially for PWRs) using the linear reactivity model (or an appropriate enhancement) [9]. This model is used to estimate the cycle length and discharge burnup as a function of the number of batches in the fuel management scheme, power peaking, etc., and to estimate reactivity and control coefficients relative to the reference UO_2 configuration. Codes selected to conduct these analyses at BNL for candidate ATF include the deterministic TRITON/NEWT code [10] or Monte Carlo codes such as MCNP [11] and Serpent [12]. The Monte Carlo codes provide results that are essentially benchmark quality and are constrained only by the available nuclear data and the geometric detail and statistics employed in the modeling.

Three-Dimensional Core Analyses: Ultimately, core-level analyses are required to assess the potential benefits, as well as any negative aspects, associated with the implementation of a specific concept. The assembly-level lattice analyses described above provide the nuclear data (e.g., neutron cross sections, etc.) for subsequent full-core, three-dimensional analyses that include thermal-hydraulic and temperature feedback. These analyses can be used for fuel cycle analyses and some time-dependent accident analyses. For the ATF concepts both the thermal properties and the reactivity coefficients will change relative to the reference UO_2-Zr alloy system. BNL researchers have selected the PARCS nodal code for this analysis step [13]. Thermal hydraulic analyses can be performed at the assembly or core level for steady-state estimates of the Departure from Nucleate Boiling Ratio (DNBR) or Minimum Critical Power Ratio (MCPR). Codes that can be used for these analyses include VIPRE and COBRA. Coupled thermal-hydraulic – neutronic analysis of candidate ATFs is essential in understanding the synergistic impact of the thermal properties and reactivity feedback.

Transient Analyses: As noted above, ATF concepts must be evaluated over the full spectrum of AOOs, DBAs and BDBAs to estimate potential safety enhancements in addition to evaluating the potential performance enhancements under normal operating conditions. The full spectrum of accidents can be found in Chapter 15 of a standard Safety Analysis Report for the nuclear plant. Thermal hydraulic transients are typically modeled in the TRACE code, but PARCS (standalone) or PARCS-TRACE is used to study reactivity transients where 3-D kinetics effects are important. While this analysis is again limited by the available data on the proposed fuel system, it can provide a preliminary estimate of “coping time.”

One important caveat is that the screening analyses frequently require assumptions for the properties of candidate materials. The best available material properties are used in these analyses, but it is noted that material properties of candidate fuel and cladding materials depend on radiation damage, fraction of cold working, temperature, and other conditions. These dependencies may be unknown or have significant uncertainty for proposed novel candidate fuel or cladding materials, resulting in significant uncertainty in the predicted performance.

2.2 Advanced Fuel Performance Modeling Tools

Detailed measurement of material properties and characteristics is necessary to perform a fuel performance calculation. Behavioral models will include concept-specific material properties, which must be derived from validated models, experimental data or assumptions. In some cases, the proposed fuel and cladding concept may be similar to the current fuel system, such that existing behavioral models can be applied with limited modification. However, cases in which the concepts deviate significantly from the current system will require development of material-specific behavioral models. The ATF concept development team would be expected to develop such models during the course of fuel and cladding development and testing. If the developed models are sufficient to support fuel performance analysis, then work can proceed using the available analysis tools with the correct behavioral models inserted.

The U.S. DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program is developing an advanced modeling and simulation toolset for application in a wide array of problems. Several NEAMS tools function within the Multi-physics Object-Oriented Simulation Environment (MOOSE) [14] framework. MOOSE provides a high-level interface to sophisticated nonlinear solver technology, and it provides the framework upon which other analysis tools are created. The associated fuel performance code, BISON, is a finite element-based code applicable to a wide variety of fuel forms. It solves the fully-coupled equations of thermomechanics and species diffusion, for either 1D spherical, 2D axisymmetric or 3D geometries. MARMOT is a lower-length-scale code that interacts with BISON to predict the effect of radiation damage on microstructure evolution, including void nucleation and growth, bubble growth, grain boundary migration, and gas diffusion and segregation. In addition, MARMOT calculates the effect of the microstructure evolution on various bulk material properties, including thermal conductivity and porosity.

In the absence of specific data on the properties and behaviors of many of the candidate fuel and cladding materials, specific fuel performance modeling within BISON is limited. Hence, a preliminary sensitivity study was conducted at INL to identify trends and to determine the overall impact of the variation of multiple thermophysical parameters on fuel performance [15]. Using a simplified loss of coolant accident scenario, the impact of thermal conductivity, specific heat capacity, Young's Modulus and thermal expansion coefficient on the maximum creep strain, peak cladding temperature, maximum principle stress and maximum von Mises stress was calculated. Note that although creep is the primary nonlinear deformation mechanism for most cladding materials, this parameter does not lend itself to a simple parametric study. A specific creep model must be adopted in future studies of specific ATF candidates. This simplified study was essentially a proof-of-concept in using BISON to investigate ATF performance under a postulated accident condition. Despite the simplified approach to the program, the work points to a few key conclusions. Under LOCA conditions, it was found that creep strain is most sensitive to thermal conductivity and specific heat. Hence, new cladding materials with low thermal conductivity and low specific heat will have the least creep strain.

A recently initiated three-year research task under NEAMS is focused on expanding the existing BISON/MARMOT fuel performance modeling and simulation capability to enable evaluation of leading ATF concepts. Efforts will be made to expand the NEAMS fuel performance code BISON to perform a representative assessment of accident tolerance for selected concepts. Concept-specific material and behavioral models are expected to require experimental data generated by R&D activities under AFC, and it will also rely on lower-length-scale models developed under the NEAMS program (i.e. MARMOT).

3. Analysis of Severe Accident Behavior

Scoping simulations performed using a severe accident analysis code can be applied to investigate the influence of advanced materials on BDBA progression and to identify any existing code limitations. MELCOR is a systems-level severe accident analysis code that is being developed and maintained at Sandia National Laboratories in New Mexico (SNL/NM) for the Nuclear Regulatory Commission to support licensing activities. MELCOR includes the major phenomena of the system thermal hydraulics, fuel heat-up, cladding oxidation, radionuclide release and transport, fuel melting and relocation, etc.

MELCOR is designed for current LWR core material configurations. As such, the code contains material property definitions for UO_2, Zircaloy, ZrO_2, steel, steel oxide and Inconel for the fuel, cladding, spacer grids, support plates and channel boxes. However, an effort to extend the MELCOR capability to include candidate accident tolerant cladding materials was undertaken beginning in fiscal year (FY) 2012. To date, INL researchers have added properties and behaviors for silicon carbide (SiC) and FeCrAl to the MELCOR reactor core oxidation and material properties routines [16]. These code versions also decouple material composition assignments, such that changes can be made to the composition of one component (e.g. the cladding) without affecting other core structures. These alternate materials may be selected as the sole cladding material or as a coating (or sleeve) on a standard metallic cladding (e.g. SiC sleeve over metallic cladding, such as a Zr-alloy; FeCrAl coating on Zr-alloy). Modifications to include additional fuel materials (beyond UO_2) have not yet been addressed.

Scoping evaluations for candidate materials can be performed using the revised MELCOR models if sufficient data is known from characterization activities. The manner in which a candidate cladding material oxidizes will determine which code version should be used (e.g. SiC or FeCrAl versions). The FeCrAl version of the code should be selected for candidate cladding materials that demonstrate parabolic oxidation behavior (similar to FeCrAl and other metals); in this case, the FeCrAl properties could be overwritten by the user to assess performance of an alternate candidate material. For materials that exhibit both parabolic oxidation and linear volatilization, similar to SiC, the SiC version should be employed, with material-specific properties entered as appropriate. Key material properties and behaviors necessary for MELCOR simulation include:

- Properties of the base material (e.g. SiC) and its oxide (e.g. SiO_2), as a function of temperature and irradiation
  - Melting temperature of the base material, oxide and any eutectics that may form
  - Thermal conductivity
  - Specific heat
  - Density
  - Emissivity
- Oxidation reactions, including oxidation rate, heat of reaction, reaction products, etc.
- Arrhenius relationship for parabolic oxidation rate behavior

In the absence of specific property and behavior data or significant uncertainty in the available data for selected materials, MELCOR can be employed to perform parametric studies. Key parameters, such as the oxidation rate or the material thermal conductivity, can be varied over a reasonable range to determine the overall impact on behaviors of interest, such as peak cladding temperature. In this manner the properties that most impact the accident performance of the fuel system can be identified.

The INL-modified version of MELCOR has been applied in the analysis of a pressurized water reactor accident (specifically Three Mile Island Unit 2 [TMI-2] and the associated loss of coolant accident sequence) to determine potential safety enhancements that could be realized with SiC or FeCrAl cladding materials [16]. Analysis of the impact of FeCrAl replacement of all zirconium alloy components in a boiling water reactor (specifically, Peach Bottom) station blackout scenario (as occurred at Fukushima Daiichi) has been conducted by Oak Ridge National Laboratory (ORNL) [17].

3.1 PWR Severe Accident Analysis

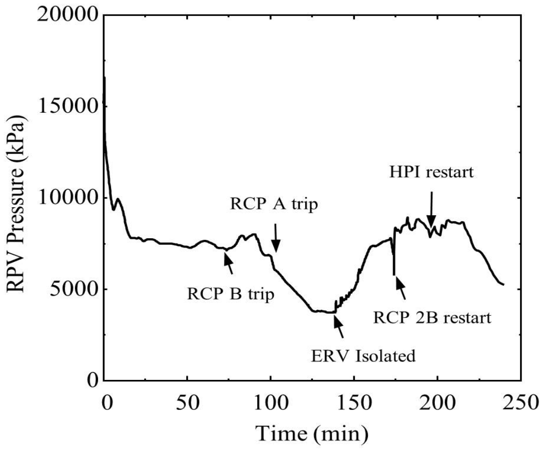
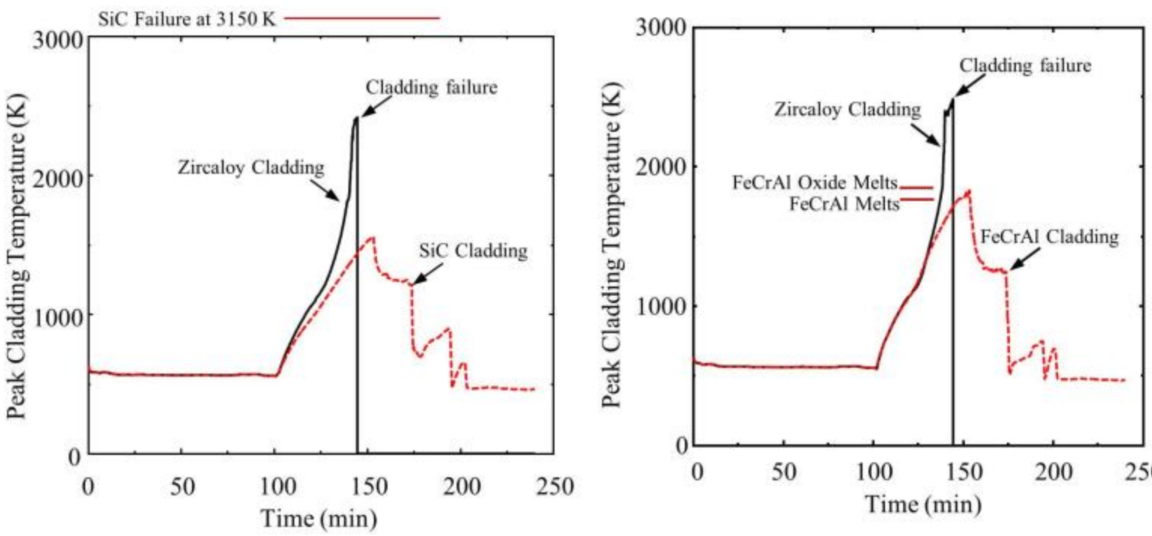


Figure 1. RPV pressure during the TMI-2 loss of coolant accident.

The reactor pressure vessel (RPV) pressure during the TMI-2 accident sequence is shown in Fig. 1; times at which reactor coolant system (RCS) pumps were tripped and restarted are shown. The INL-generated SiC code version substitutes the properties of CVD SiC for Zircaloy in MELCOR's reactor core oxidation (oxidation in air and steam) and material property routines (properties such as thermal conductivity, specific heat, density, emissivity, and heat of formation). See Merrill and Bragg-Sitton [18] for additional detail. The SiC version of MELCOR was benchmarked against available experimental data [e.g., 19] to ensure that present SiC oxidation theory in air and steam were correctly implemented in the code. The FeCrAl code version was also verified against available data to ensure that the code returns oxidation rates that match the adopted oxidation correlations [20]. Benchmarking of the FeCrAl version has not yet been completed.

As an example of the results that can be derived from MELCOR analysis, Fig. 2(a) shows the peak cladding temperature as a function of time during this accident sequence for both Zr-alloy and SiC cladding. The MELCOR-predicted cladding temperature is below the melting temperature of the silica protective scale that forms on the outer surface of SiC (~1873 K) and is well below the decomposition temperature of SiC (~3150 K), such that core geometry would be expected to be maintained. Fig. 2(b) shows results for FeCrAl cladding. In this case the predicted cladding temperature is estimated to be very close to the assumed failure criteria (FeCrAl melt temperature) and also approaches the assumed melting temperature of the FeCrAl oxide (1870 K). Data on the specific melting temperature of FeCrAl oxide is necessary to attain higher confidence in the potential that the FeCrAl cladding would remain intact in this scenario. Additional output information useful in evaluating potential safety enhancements include heat input due to cladding oxidation and total combustible gas production (e.g. H_2, CO, etc., depending on the cladding material selected). Note that the MELCOR analyses are only used for scoping evaluations early in the development of an ATF concept and are not intended to support down-select decisions.



(a) (b)

Figure 2. MELCOR-calculated peak cladding temperature for Zircaloy, SiC and FeCrAl cladding during a TMI-2 event sequence.

3.2 BWR Severe Accident Analysis

MELCOR analyses have also been conducted for a baseline BWR case, namely the Peach Bottom plant (GE BWR4/Mark I) [21]. In this case several station blackout scenarios were modeled in which the loss of all AC power occurs at the time of scram, and DC power is lost at a specified time. This scenario is similar to what occurred at the Fukushima Daiichi plant in Japan. In this example, FeCrAl cladding material was modeled using the most recent material properties available including appropriate oxidation kinetics. Although additional material properties are still required (e.g. production of eutectics), the MELCOR evaluation has been useful in estimating the additional time to the onset of cladding melt and radionuclide release offered by FeCrAl cladding relative to Zircaloy. Other data tracked include the mass of combustible gases (H_2) produced and the cumulative energy release due to material oxidation in the core.

4. Evaluation Scenarios Under Consideration

As noted in section 3, preliminary INL and ORNL analysis of severe accident conditions modeled the TMI-2 and Fukushima accident scenarios. Selection of appropriate “illustrative scenarios” that can be employed across the international community is currently under discussion within the Nuclear Energy Agency (NEA) Expert Group on Accident Tolerant Fuels. This group is conducting work under three task forces: (1) Systems Assessment, (2) Cladding and Core Materials, and (3) Fuel Concepts. Scope for the Systems Assessment task force includes definition of evaluation metrics for ATF, technology readiness level (TRL) definition, definition of illustrative scenarios for ATF evaluation, parametric studies, and selection of system codes. Task forces 2 and 3 focus on compiling data on ATF materials currently under development.

Several countries are actively developing and testing ATF materials. In many cases, similar materials are being investigated in multiple countries. It is of interest to the international nuclear community to have these independent teams adopt common TRL definitions, adopt similar evaluation metrics, and apply similar evaluation scenarios. March 2015 discussions among the Systems Assessment task force members identified two simplified scenarios that can be applied by ATF development teams for LWR plants (PWR, BWR and VVER):

- *Station Blackout:* This scenario is postulated to occur with high system pressure and allowed to continue to the point of RPV failure.
- *Large-break LOCA:* This scenario provides a low-pressure condition in which coolant is lost while there is high decay heat in the reactor.

The proposed scenarios are intended to provide bounding cases for fuel performance. It is expected that each country or development team will utilize fuel performance and system analysis codes that are accepted within the associated organization to conduct these evaluations. All ATF evaluations under the selected accident conditions should be allowed to progress to the point of core failure in the analysis. This allows one to estimate the potential increase in coping time that might be offered by candidate ATF concepts and to assess potential outcomes should failure occur (e.g. if the fuel fails, how does it fail?). Pressure is a very significant parameter in the accident progression, as reflected in the selection of both a high-pressure and low-pressure scenario. Following completion of bounding analyses, researchers should perform parametric studies for these illustrative scenarios to develop a better understanding of the impact of additional variables. Such parametric studies could include variation of the point in the operating cycle that the accident occurs (how much burnup has been accumulated in the fuel?) and the time after reactor scram that core cooling is lost.

These illustrative scenarios will be documented in a future report issued by the NEA Expert Group.

5. Conclusions

Analysis of ATF concepts entails preliminary screening analysis, development of behavioral models to support fuel performance modeling and detailed system analysis. Existing tools can often be applied but may require significant assumptions due to limited data availability for the candidate materials. As more data becomes available material-specific behavioral models can be developed and employed in detailed analyses intended to predict the potential performance enhancements offered by an ATF concept over the reference fuel system (UO_2-Zr-alloy).

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