investigate very detailed mechanical and structural effects in highly complex fuel forms. For example, the mechanical interaction between TRISO fuel layers including the effects of cracking, debonding, and asphericity can be modeled explicitly. Future work is planned to integrate damage-mechanics modeling capability into PEGASUS that is specifically applicable to TRISO-based fuels.

More detailed descriptions and various applications of PEGASUS for fuel performance modeling and analysis both during operation and post-operational storage of standard LWR fuel have been published in several papers recently. These include a review of PEGASUS presented at TopFuel 2021 [1], an article entitled "Nuclear Fuel Performance Modeling of the Fuel Life Cycle with the End in Mind" published online via the Nuclear Newswire [2], a paper on used fuel modeling at the 2022 ANS Summer Meeting in Anaheim, CA [3], and a review of PEGASUS applications for pellet-cladding interaction (PCI) to be presented at TopFuel 2022 [4].

MATERIAL PROPERTIES AND GEOMETRIC MODEL DEVELOPMENT

The current emphasis for the development of PEGASUS is the introduction of material constitutive and behavioral models for ATF (accident tolerant / advanced technology fuel), uranium metal alloy, and TRISO fuel designs for proposed LWR, liquid metal, and gas-cooled advanced reactor applications. This development work is being conducted under several initiatives including an externally funded Department of Energy (DOE) research project and dedicated internal development projects. The progress of those implementations is discussed below. Demonstrations and evaluations of fuel designs using prototypic advanced reactor materials, designs, and operating conditions based on design and/or experimental data are presented where available.

Silicon-Carbide Cladding Material

A project is underway to further the development and irradiation testing of a composite silicon carbide (SiC) material known as SiGA® Technology: **Si**licon Carbide – **G**eneral **A**tomics for application as an ATF and advanced reactor cladding material. This project is supported through a DOE Funding Opportunity Award (DE-FOA-0002308) for the first of a kind irradiation of SiGA® material samples in the guide tube locations of a commercial pressurized water reactor (PWR) in the United States[a]. SI is conducting work under this award with GA – Electromagnetic Systems (GA-EMS) to aid in the design of the SiGA® cladding tube sample irradiation capsule [5].

The potential for SiC as a material in nuclear applications has been recognized for many years with research beginning in the 1950s for applications in nuclear fuel as a component of bi-structural isotropic and later TRISO fuels. This evolved into interest for its application for other components within nuclear systems, such as structural components and cladding due to the material's high temperature and irradiation tolerance, mechanical strength, and inert chemical response. A comprehensive review of research and application of SiC and SiC composites is presented in Katoh and Snead [6]. Examples of SiC composite cladding and BWR channel components fabricated to demonstrate and evaluate this material's capabilities for application in LWRs is shown in Figure 1.

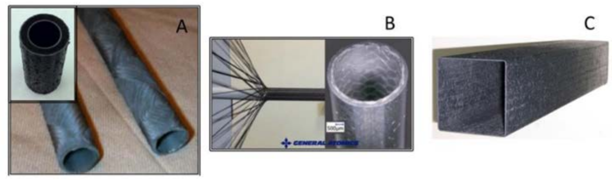

Fig. 1. Examples of SiC and SiC Composite Components: (A) Ceramic Tubular Products triplex LWR cladding, (B) A version of the General Atomics LWR cladding, and (C) A BWR SiC/SiC channel box fabricated and tested by EPRI. (Adapted from Reference [6]).

Key characteristics of SiC include extreme failure resistance, low hydrogen production, and maintenance of coolable geometry under high temperatures (> 1200 – 1700 °C) and pressures/stresses (hoop stresses > 80 MPa) in steam environments as shown during LOCA (Loss of Coolant Accident) burst tests, high stress compression tests, and high temperature (1400 °C) quench tests [5]. These characteristics point to superior accident performance of SiC-based materials like SiGA®.

Prior irradiation testing has been conducted on SiC composites similar to those that are the subject of the current irradiation project. One example of this is an experiment conducted in the HFIR facility at Oak Ridge National Laboratory [7]. This experiment placed several samples of SiC monolith and SiC composite cladding tube into a test canister that contained a surrogate molybdenum "heater" cylinder in place of uranium-based fuel. The heater rod was designed to generate sufficient gamma heating to achieve representative PWR cladding temperatures and heat fluxes. The current project builds upon this work and will expand experimental capability from simulating an LWR environment to placing an experiment directly into an operating LWR.

To conduct this work, SI is implementing a set of generic SiC and SiGA® constitutive models (for both monocrystalline and composite mono/fiber SiGA®) in PEGASUS based on material property data available in the literature and from specific SiGA® design, fabrication, and material testing data provided by GA-EMS. Once completed, the SiGA® models will be used to evaluate the irradiation capsule design and predict the performance of its components throughout the planned irradiation. The results of these studies will be the subject of future publications. It is also anticipated that PEGASUS will be applied for evaluation of post irradiation examination data after completion of the irradiation and hot cell examinations of the SiGA® material samples tested in this experiment.

Uranium Metal Alloy Fuels

Although the subject of research and development for many decades, metallic alloy fuels such as U-Zr and U-Pu-Zr are seeing a resurgence in interest due to the proliferation of advanced sodium-cooled and heat pipe-cooled fast reactor designs proposed through DOE programs such as the Advanced Reactor Demonstration Program [8]. A broad description and review of these fuel types is provided in Crawford et al. [9]. Interest in these fuels is due in part to the extensive operational histories from long term irradiation in DOE research reactors. These would include fuels irradiated in Experimental Breeder Reactor-I (EBR-I), Experimental Breeder Reactor-II (EBR-II), and the Fast Flux Test Facility (FFTF) as part of the Liquid Metal Fast Breeder Reactor and Integral Fast Reactor research programs. The characteristics and potential use of these fuel designs specifically for application in Generation IV (Gen IV) advanced reactors is further examined by Carmack et al. [10]. The conclusion from this review was that given the extensive experience base and generally excellent performance of metallic alloy fuels in historical fast reactor applications, the prospect of use in forthcoming advanced reactors "is excellent."

SI has begun the implementation of metallic alloy fuel and stainless-steel cladding material constitutive models for prototypic fast reactor fuel designs in PEGASUS. Specifically, material properties and behavioral models for U-Pu-Zr fuel and HT-9 (high Chromium, Martensitic stainless steel) cladding have been added.

Regarding U-Pu-Zr fuel, the thermal material models of thermal conductivity and specific heat [10,11] including different compositions and phases for fast reactor application have been completed. The mechanical model implementation includes the elastic modulus and shear modulus as a function of temperature, fuel creep, including both thermal and irradiation components, an isotropic thermal expansion model, and an empirical fuel swelling model that correlates with the fission density [11-14]. For HT-9 a complete set of thermal models and a constitutive mechanical model has been implemented. These models include sub-models for thermal expansion, irradiation and thermal creep, and an elasticity tensor implementation based on data from Hofman et al. [14] and Yamanouchi et al. [15].

Ongoing work includes the implementation of a gaseous swelling and fission gas release behavior model for U-Pu-Zr fuel, a Zr-redistribution model, and a fuel-cladding chemical interaction (FCCI) model that includes the effect on cladding wall thinning.

To evaluate the implementation of these models, benchmark tests were prepared to provide comparative data for assessment of the models' performance. Initially, two test cases were chosen from two experiment series irradiated in EBR-II: X430, a 37-pin hexagonal sub-assembly, and X441, a 61-pin bundle. These experiments were designed to assess numerous fuel rod design variables and fuel response as a function of fuel alloy composition, smear density, plenum-to-fuel volume ratio, power, and coolant conditions [16]. The general experimental fuel rod design corresponds to the typical driver fuel configuration shown in Figure 2.

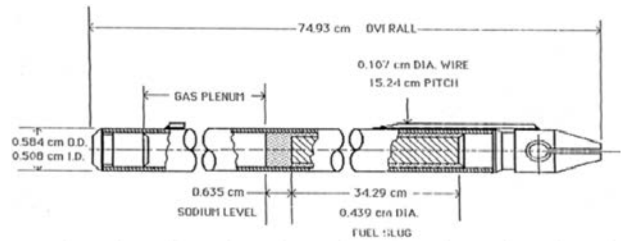

Fig. 2. Typical EBR-II Mark-III/IIIA Fuel Element [14].

Input decks were developed using data from Novascone et al. [17] and Greenquist and Powers [18] for two fuel rods: T654 from X430 and DP21 from X441 using U-Pu-Zr fuel and HT-9 cladding constitutive models and applicable thermal hydraulic and boundary conditions for the coolant channel and the Na-bonded fuel/cladding gap. Table 1 contains data characterizing the two fuel rods and their irradiation history.

TABLE I. Test Rod Description

Rod and Assembly	Fuel Type / Cladding	Pk LHR kW/m	Burnup at. %
T654 X430	U19Pu10Zr HT-9	44	11.68
DP21 X441	U19Pu10Zr HT-9	44	12.5

The X441 experiment consisted of a 61-pin bundle irradiated in EBR-II under steady-state conditions to a target burnup of ~10%. The main objective of the experiment was to determine a design envelope for ternary (U-Pu-Zr) fuel design in EBR-II. The fuel design parameters that were varied include the plenum/fuel volume ratio (1.1, 1.5 and 2.1), fuel smear density (70, 75 and 85% TD), Zr content (6, 10 and 14 wt. %), cladding thickness (0.015 and 0.018 in.) and cladding material (HT9 and D9). Additional goals of this experiment were to provide more input for optimization of U-Pu-Zr fuel and experimental data for validating fuel performance codes.

Illustration of the model and selected results from initial analysis of Rod DP21 are shown in the figures 3 and 4. Figure 3 provides a diagram of the computational model showing the primary components of the model and a plot of the temperature distribution throughout the fueled region of the rod at peak power. Figure 4 provides the radial temperature profile across the fuel rod from the center to the cladding outer surface at peak power near the end of the irradiation period. Temperatures vary from just above 900 K at the pellet

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center to 650 K at the cladding surface. The temperature differential is fairly low at ~250 K as would be expected from a high conductivity metal fuel rod with a Na-bonded fuel cladding gap. Comparison of predicted and measured cladding strains indicates a small under prediction in the analysis (0.4% predicted versus 0.5% measured) likely due to adjustments needed in the fission gas release, swelling, and/or creep models. Overall, however, the results appear consistent with the available experimental measurements and observations. Additional review of the metallic fuel rod analyses and more detailed assessment of the results generated will be completed as the analysis work proceeds with further benchmarking and validation activities.

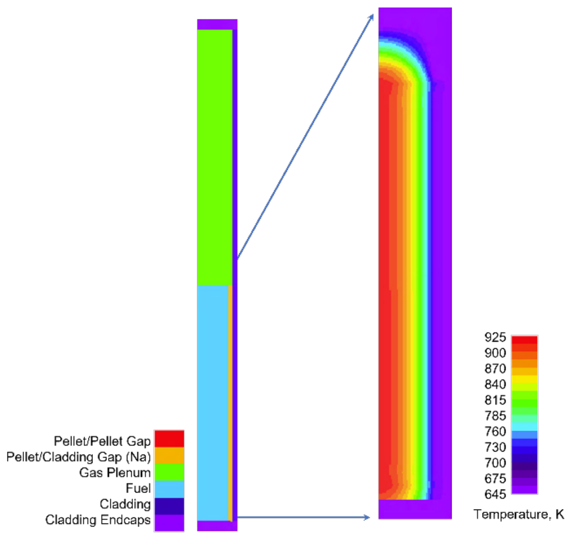

Fig. 3. Left: 2D computational model of rod DP21, Right: temperature contour plot in the fuel stack region at peak power.

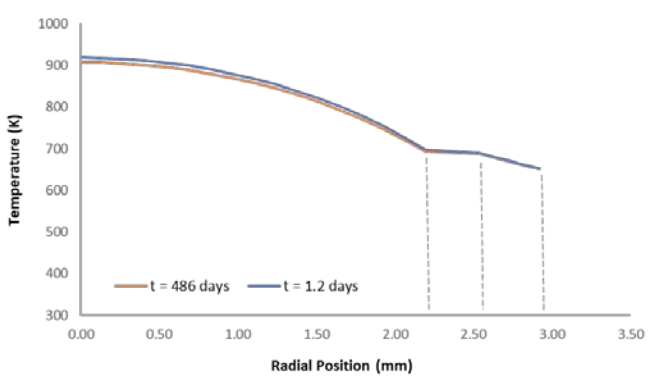

Fig. 4. Computed radial temperature distribution across Rod DP21 at initial and near end of irradiation at full power conditions.

TRISO-Based Fuels

Similar to the recent resurgence of interest in metallic alloy fuels stemming from proposed, next generation liquid-metal and heat pipe-cooled reactors, TRISO fuels have received strong interest from the proliferation of proposed Gen IV high temperature gas and molten salt-cooled reactor designs. Renewed work on TRISO fuels, however, predates the recent “advanced reactor” movement as DOE began the Advanced Gas Reactor (AGR) Fuel Development and Qualification Program in 2002 to support the Next Generation Nuclear Plant (NGNP) Project [19]. Although NGNP never came to fruition, the DOE Office of Advanced Reactor Technologies continued to support the AGR program and now supports the experimental bases for the licensing of proposed High Temperature Reactor (HTR) and other reactor designs that utilize TRISO fuel being pursued by several U.S. commercial reactor designers such as Ultra Safe Nuclear Corporation, X-Energy, and Kairos Power [20].

TRISO fuel modeling development for PEGASUS is in its early stages. Initial research on the needed fundamental material property and behavior model data is ongoing sourcing data from the AGR experimental program [21] and DOE-supported modeling efforts such as those from Hales et al. [22,23]. Until complete models are implemented, simplified material property inputs are being used in testing and benchmark cases. In parallel to those efforts, geometric modeling and meshing techniques specifically to address TRISO fuel configurations are being explored and developed. These efforts exploit the CAD-like modeling environment and other automated meshing tools and capabilities in PEGASUS.

One area of work is developing a consistent methodology for generation of configurations to mimic the distribution of TRISO particles in a fuel matrix. A technique has been developed based on the passive randomization method originated by Sukharev [24] that yields distribution patterns that approximate those observed from TRISO fuel examinations. An example of an early application of this technique is shown in Figure 5.

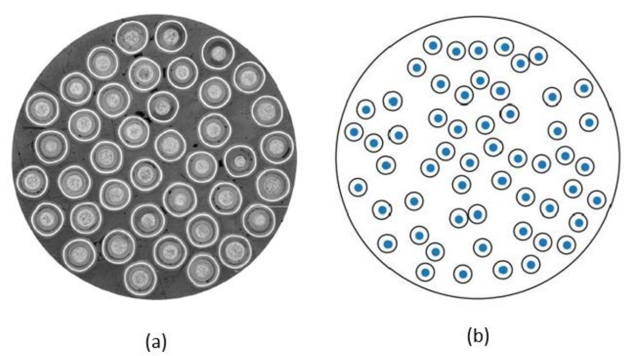

Fig. 5. Example TRISO particle distribution: (a) micrograph of a TRISO fuel compact (adapted from Nelson [25]), (b) random particle distribution pattern algorithm output.

Geometric configurations such as shown in Figure 5b can be converted using automated tools to generate both 2D and 3D FEM meshes with TRISO kernels imbedded in meshed substrates. Models such as these provide the bases for computational studies of TRISO fuel performance from detailed kernel multilayer response to interactions between multiple kernels and their surrounding matrix. Several examples of TRISO meshes generated with PEGASUS are shown in the following illustrations. Figure 6 shows a single TRISO particle 3D mesh model. Figure 7 illustrates the cross section of a 3D TRISO fuel compact with embedded TRISO particles. The appearance of multiple particle sizes is an indication of varying particle depths within the matrix. This figure was generated with the using the spherical object meshing tool in PEGASUS.

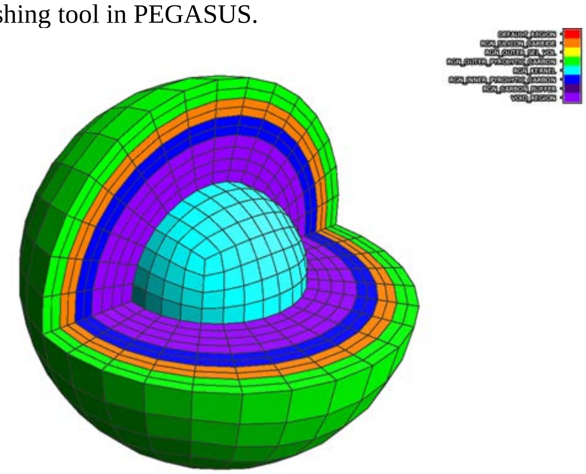

Fig. 6. Single TRISO particle 3D mesh.

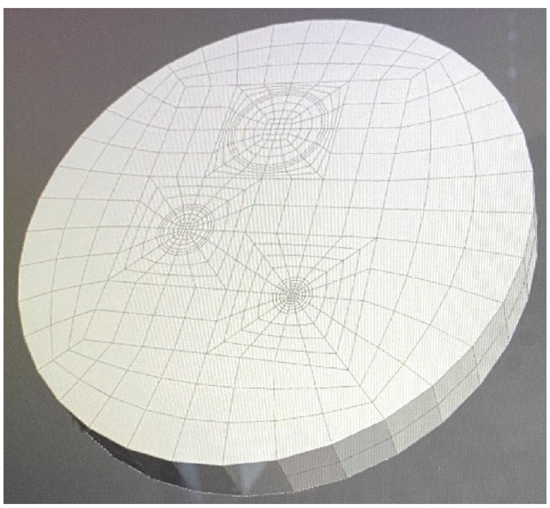

Fig. 7. Cross sectional view of embedded TRISO particles in a 3D fuel compact matrix.

A more complex 3D model of encapsulated TRISO particles is shown in Figure 8. This model features a sparse particle distribution generated by using the randomization technique applied in Figure 5b coupled with 3D automated meshing capabilities. This model was meshed in PEGASUS using an automated scripting tool and tested using simplified approximations of the thermal and mechanical properties of the kernel and matrix materials: UO_2, pyrolytic carbon, SiC, and graphite. Boundary conditions simulating prototypic gas reactor conditions were used in the simulation. A temperature contour plot of a portion of the model in Figure 8 and the resulting temperature distribution is show in Figure 9.

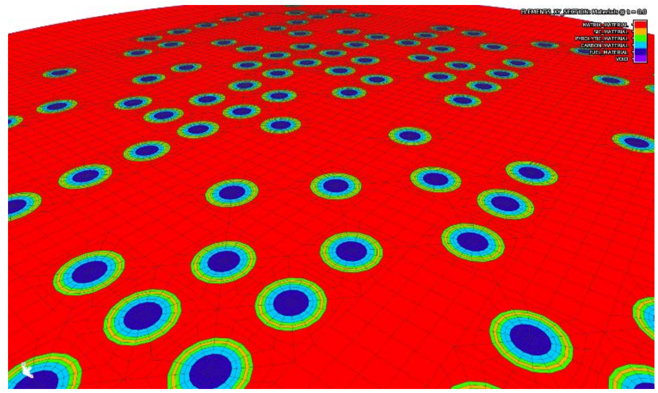

Fig. 8. Cross section of an array of discrete 3D TRISO particles embedded into a graphite compact pellet.

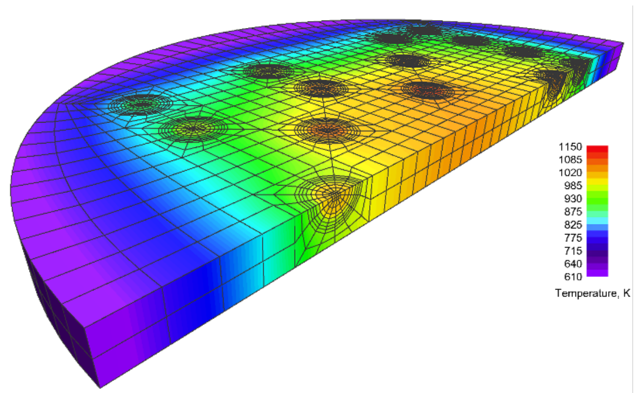

Fig. 9. Temperature distribution in a cross-sectional slab of a TRISO compact matrix model under prototypic gas-cooled reactor conditions.

Further development of the TRISO fuel modeling capabilities in PEGASUS are ongoing. The primary emphasis is on the completion of the requisite material property and behavioral constitutive models. Detailed 3D modeling of TRISO kernels with irregular geometries such as non-uniform thicknesses and shapes of the pyrolytic carbon and SiC layers has been identified as a high priority going forward. Additional options for future development include the implementation of mechanistically based, deterministic TRISO kernel and fuel compact failure models integrated into the material constitutive relations and the calculation and tracking of fission product species diffusion and concentrations which incorporate the effects of chemical interactions and kernel layer and substrate cracking.

SUMMARY

The PEGASUS nuclear fuel behavior code is an advanced and independently developed 3D FEM computational software program capable of performing complex, coupled thermo-mechanical and structural non-linear analyses. The role of Pegasus is envisioned as complimentary to existing regulatory-based assessment and licensing tools, where there is a need to address conservatism, perform an independent assessment, or provide additional fidelity, to laboratory-sponsored research where wider materials, phenomena or fidelity is needed. In summary, Pegasus provides a high fidelity and independent advanced analysis capability that can be used to address existing fuel performance with less conservatism, accelerate development, design, and regulatory processes for new fuel concepts and advanced fuels.

Current development activity is focused on application to proposed advanced reactor designs requiring analysis of unique cladding and fuel materials and design configurations. These materials and designs include ATF fuels and associated materials in LWRs, uranium metal alloy fuels and cladding for application in liquid metal-cooled fast reactors as well in heat pipe-cooled microreactors, and TRISO-based ceramic fuels to be deployed in HTRs and molten salt-cooled reactors. Future development work on PEGASUS will continue along several avenues. Emphasis will continue in the areas outlined in this paper: 1) SiC cladding material property and behavioral model implementation and irradiation test modeling, 2) fast reactor metal alloy fuel modeling and benchmarking, and 3) TRISO-based fuel system constitutive and deterministic failure model development, implementation, and modeling.

ENDNOTES

[a]This report was prepared as an account of work partially sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof nor any of their employees make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of the authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

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