Used Fuel Modeling: An Integral Approach using PEGASUS Code

Wenfeng Liu, Joe Rashid, Bill Lyon, and Michael Kennard

*Structural Integrity Association, Inc., 9710 Scranton Rd., Suite 300, San Diego, CA 92121, wliu@structint.com

INTRODUCTION

The current safety evaluation methodology applied for used fuel is generally based on applying structural analysis codes to surrogate fuel with no prior irradiation history. This approach often ignores the effects of material degradations that evolve during in-reactor service. Therefore, assumptions must be made on material properties and damage mechanisms, and the important roles of fuel cracking, fuel bonding, irradiation damage, corrosion/hydriding and their synergies are neglected. Because these effects are not explicitly represented in used fuel modeling, the validity of such analyses is often questioned by regulators, and thus, has contributed in part to a state of high uncertainty in used fuel management.

To obviate the flaw in this approach, i.e., removing simplifying assumptions applied to the fuel and cladding mechanical properties, a new modeling paradigm is being developed and implemented in the PEGASUS code. PEGASUS treats used nuclear fuel issues as an integral part of the entire fuel cycle and models all fuel behavior regimes as one continuous problem. Irradiation and service induced material conditions during normal operations, which undergo further changes during dry storage, would provide the initial conditions for PEGASUS analysis of used fuel subjected to handling and transportation events. Therefore, the evolution of material properties during in-reactor service and subsequently during dry storage is seamlessly accounted for in the analysis procedure. This integral approach makes it possible to perform high-fidelity assessments of used fuel failure resistance in accident conditions. In such use, only one code, is needed for the fuel integrity evaluation in the entire fuel cycle.

This paper highlights a few key aspects of LWR fuel modeling using the PEGASUS code, reports ongoing development efforts to facilitate used fuel modeling, and shows an example of the spent fuel analysis as a continuation of in-reactor fuel modeling.

PEGASUS FEATURES FOR USED FUEL MODELING

An overview of PEGASUS code's material, behavior models, and modeling capability was presented in Ref. [1]. The theoretical basis of the PEGASUS code consists of the coupling of the mechanical equilibrium equations and the energy conservation equation to solve for displacement and temperatures described at each node in the multi-dimensional finite element grid. The non-linear global field equations are solved for the incremental displacements and temperatures using the Newton-Raphson method. In high-fidelity analyses to capture local response, or in the modelling of accident conditions, a finite-deformation formulation is used for the modelling of significant material deformation as well as for geometrical rotation. Along with the implementation of nuclear fuel material and constitutive models, PEGASUS has the capability of a general-purpose finite-element code for performing structural analyses.

PEGASUS analysis simulation of the backend fuel cycle represents subjecting the fuel to a temperature history typical of dry storage conditions. This phase of the analysis continues with the behavioral models and thermo-mechanical and physical states of the fuel and cladding inherited from the operational phase. These include cladding irradiation hardening, hydrogen content and corrosion thickness; PCI damage if any; fuel burnup distribution and gas inventory; fuel swelling, cracking and relocation; and fuel-cladding bonding if developed during high-burnup. Material and behavioral models needed for modeling used fuel consist of those used in the in-reactor analysis phase plus additional models specific for ex-reactor analysis, which include burnup-dependent decay heat time history; cladding and fuel thermal creep; He production and fuel swelling due to α decay; hydride precipitation and reorientation model; multiphase (metal, circumferential hydrides and radial hydrides) damage model for accident analysis; and critical strain energy model (CSED) for cladding failure evaluation under impact and bending loading.



Fig. 1. PEGASUS Prediction of Fuel Temperatures using 2-D Grids used for Validation Cases

At present, a total of 37 validation cases have been developed using test reactor fuel and commercial fuel rods



based on information from the literature [2-3]. Fig. 1 shows an example of code validation for fuel temperature calculations. A few features to facilitate used fuel modeling include a) generic finite element modeling capability, b) database to support restart analysis, and c) unlock and lock simulation to re-assign boundary conditions and thermal and mechanical loads.

One area of ongoing development is the adoption of a hybrid 2D/3D modeling capability to further improve integral fuel rod analysis capability.

The hybrid model construct is illustrated in Fig. 2, which depicts a full-length fuel rod as a composition of several finite element mesh zones, each of which is suited for simulating a behavior regime in the fuel cycle, with high-fidelity treatment of their interfaces. Zone A is a 2D axisymmetric, smeared-pellet representation that is suited for global behavior calculation. Zone B is a 3D fine grid of smeared pellets intended for spent fuel bending and pinch loading analysis, And Zone C is a highly detailed, fine grid 3D representation of individual pellets intended to simulate the local fuel response such as required for PCI phenomena including pellet defects. The dimensions of these zones are parametrized so that they can be easily changed to make the finite-element mesh compatible with the axial power profile (i.e., placing Zone C at the peak power location).



Fig. 2. Schematic of Fuel Rod Model for Fuel Cycle Analysis

The fuel rod finite element constructs, which are not visible in the Fig. 2 schematic, constitute the only geometric input utilized for fuel behavior analysis in-reactor as well as for spent fuel storage and transportation. Fig. 3 shows the temperature distribution for all fuel rod zones at a 35 kW/m power level. Note that Zone A, being axisymmetric, appears as a half rod. Zone C has a middle pellet with an MPS and a radial crack.



Fig. 3 Schematic of 2D/3D Hybrid Modeling

This first-of-a-kind, high-fidelity approach could provide enormous savings in engineering cost and work force utilization by focusing computational detail only where needed.

USED FUEL MODELING EXAMPLE

As an example, we start with the modeling of in-reactor irradiation of a commercial rod using PEGASUS. Material models are described in Ref. [1] where most of the fuel and cladding material properties are based on [2][3]. Table I shows the primary fuel design parameters. The fuel rod is subjected to a constant power of 25 kW/m in a two-year irradiation to reach a burnup level of 26.9 GWd/tU. A 3-D model is created at the mid-section of the fuel rod. In-reactor irradiation results for this case are reported in Table II.

TABLE I. Design Characteristic of Fuel Rod	
Parameter	Value
Cladding OD, mm	10.77
Cladding ID, mm	9.25
Pellet OD, mm	9.21
Initial Pellet Density, %TD	94
As-Fabricated Rod Internal Pressure, MPa	3.6

TABLE I. Design Characteristic of Fuel Roo

TABLE II. Base Irradiation Results

Parameters	Value
Void Volume, cm3 (@ STP)	10.47
Rod Internal Pressure, MPa (@ 25°C)	3.8
Fuel radial displacement, micron	8.0
Elongation Strain, %ΔL/L	0.126



(a) Hoop stress contour



(b) Axial stress contour Fig. 4 Spent Fuel Rod Segment under Combined Bending and Pinch-Loading in 9-m Drop Accident



PAGE | 2

Using the code's advanced modeling capability, a restart run is performed after the base irradiation and new mechanical load and boundary conditions are assigned to model the fuel response during spent fuel transportation and storage.

Fig. 4 shows the resultant stress contours of the fuel segment under combined bending and pinch loading that could result from a hypothetical 9-m drop of a spent fuel cask.

Note that using the same base irradiation result, which is automatically stored in a PEGASUS-specific analysis database, different mechanical loads can be imposed in any number of subsequent analyses. This capability offers great flexibility for used fuel safety evaluation.

CONCLUSIONS

This paper presents a new approach to used fuel safety evaluation, treated as a continuation of in-reactor fuel performance modeling. This new modeling paradigm preserves the damage states and material property evolutions during base irradiation as the initial conditions for used fuel storage and transportation analyses. This approach eliminates the uncertainties of current practice in which commercial finite element codes are used with no ability to simulate the used fuel material conditions. The new modeling and simulation methodology is implemented in a generalized fuel performance code, PEGASUS. Built upon a robust finite element computational framework, PEGASUS' highfidelity, 3-D structural, thermo-mechanical capabilities enable the modeling of fuel response in the entire fuel cycle from in-core fuel performance analysis mode to ex-core structural analysis mode.

REFERENCES

1. W. Liu, et. al., "PEGASUS: A Generalized Fuel Cycle Performance Code," TOPFUEL 2021 (2021).

2. International Fuel Performance Experiments (IFPE) Database. OECD-NEA, http://www.oecd-nea.org/science/fuel/ifpelst.html.

3. G.P. Smith et. al., Hot Cell Examination of Extended Burnup Fuel from Calvert Cliffs-1, Volume 1, Final Report, November 1993, EPRI, Palo Alto, CA, TR-103302-V1.

4. G.P. Smith et. al., Hot Cell Examination of Extended Burnup Fuel from Calvert Cliffs-1, Volume 2, Final Report, July 1994, EPRI, Palo Alto, CA, TR-103302-V2.

5. MATPRO version 11: A Handbook of Materials Properties for Use in the Analysis of Light Water Reactor Fuel Rod Behavior. Technical Report NUREG/CR-0497, TREE-1280



R3, Idaho National Engineering Laboratory, Department of Energy, 1979.

6. SCDAP/RELAP5-3D Code Manual. Volume 4: MATPRO a Library of Materials Properties for Light-Water-Reactor Accident Analysis. Technical Report INEEL/EXT-02-00589, Idaho National Engineering and Environmental Laboratory, 2003.

PAGE | 3