PEGASUS: A GENERALIZED FUEL CYCLE PERFORMANCE CODE

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ABSTRACT

This paper introduces a new fuel behaviour code, PEGASUS, as a total-fuel-cycle performance code for the modelling and simulation of nuclear fuel behaviour throughout the entire fuel cycle, from fuel performance in-core to safety evaluation of used-fuel storage and transportation, in a single self-consistent and seamless analysis protocol. Code-unique 3D structural and thermo-mechanical capabilities, built upon a robust finite element computational framework, enables the code to transition from in-core fuel performance analysis mode to ex-core structural analysis mode, maintaining continuity of material conditions between them. In this use, PEGASUS would be the only software needed for complete used fuel integrity evaluation, thereby obviating from current practice of using external structural analysis codes which ignore the effect of damage mechanisms that evolve during in-reactor service and subsequent dry storage.

This paper will describe key and unique features of PEGASUS code, material and behaviour models implemented in the code, applications to Light Water Reactor (LWR) fuels, potential applications to advanced reactors, and status report on the current verification and validation.

1. Introduction

Fuel performance analysis and structural analysis of fuel rods have traditionally been performed separately using different tools: a fuel performance code for the former and a general-purpose finite element code for the latter. Though the structural analysis capability in the traditional fuel performance code is very limited, advances in modelling and simulation technology make it possible to enhance the finite-element modelling capabilities and build them into the fuel performance code. This is the paradigm upon which PEGASUS is built: provide a single tool capable of treating all fuel behavioural regimes of the front-end and back-end fuel cycle as a continuous problem. This removes the uncertainty associated with the simplifying assumptions applied to the fuel and cladding mechanical properties when using a structural analysis code for analyses of spent fuel.

PEGASUS features include a) a robust finite element computational framework, b) a Graphical User Interface (GUI) for input generation, finite-element grids creation, and results visualization, c) modern software development practice of object-oriented programming, continual integration, and testing, and d) a restart capability that adds the flexibility for performing fuel performance and structural analyses.

Focused initially on light water reactor (LWR) fuels and materials, PEGASUS is verified and validated for the modelling of LWR fuels in both test reactor and commercial reactor conditions.
At present, a total of 37 validation cases have been prepared and included in the validation database. Those cases covered several aspects of fuel performance parameters, as well as variations of operating

histories. In addition, a large number of test cases were developed for verifying various aspects of the code/model features.

Following traditional practice, the PEGASUS verification and validation database consists of a number of cases that are available from the International Fuel Performance Experiments (IFPE) database [1] as well as other non-proprietary sources. As examples, temperature predictions for a Halden IFA test rodlet and modelling results for a full-length commercial rod irradiated to high burnup are presented in the paper. An illustrative example of three-dimensional effects is presented for an idealized five-pellet problem with eccentric pellets subjected to a power ramp.

Built upon a proprietary finite element framework written in modern Fortran language, PEGASUS is designed to perform parallel computations on both Personal Computers (PCs) and high-end workstations for different levels of computational tasks. PEGASUS is fully adaptable to address a broad range of applications. The analysis can vary from computing performance parameters for fundamental engineering calculations to advanced high fidelity special-effects simulation. The potential code applications can be extended to the modelling of fuel operations to mitigate fuel failures, the quantification of safety margins for accident conditions, performing structural analysis for used fuels, and modelling of advanced fuel forms with innovative designs. The code’s versatility is designed for broad applications to meet the demands of conventional fuel modelling as well as emerging needs in the development of advanced fuels. Potential applications will be discussed with a few illustrated examples.

2. PEGASUS Overview

The theoretical basis of PEGASUS code consists in 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. To make the solution more effective and efficient, a line-search Newton method is employed, and a pre-calculated Jacobian is also used to provide a Quasi-Newton implementation. In the high-fidelity analysis to capture local response, or in the modelling of accident conditions, such as the ballooning of the cladding, a finite-deformation formulation is used for the modelling of significant stretching in the material deformation as well as the 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 analysis.

Convergence of the solution is determined by comparing the residual norm, that is, the norm of the global residual vector, to prescribed tolerances provided by the user. Those tolerances are provided as a physical parameter in the unit of heat flux for the thermal solution and nodal forces for the mechanical problem.

2.1 Code Features

a) A robust finite element computational framework

PEGASUS utilizes a proprietary finite-element computational framework including a numerical solver without using any third-party libraries. All the numerical algorithms are implemented within one computer code, and this has minimized the dependency on external libraries. Those have been thoroughly tested and can provide a robust platform for the nuclear fuel modelling.

b) A Graphical User Interface (GUI)

A user-friendly graphical user interface is used for the generation of input, finite element grids, as well as for the visualization of analysis results. The output variables for any nodes and elements can be easily accessed through this user interface. The user input can be created using the script languages in a text file and can also be created step-by-step using the GUI.

c) Modern software development practice

PEGASUS is written in modern Fortran using object-oriented programming (OOP), which creates abstract data types for material models that can be inherited for new material model development. This has made the addition of new material models straightforward should the constitutive law for the new material be provided in one of those base material types. This allows the modelling of nuclear fuels for LWR with different new material properties and new fuel types for advanced reactor applications. PEGASUS is managed using a GitLab server. Updates and testing were continually integrated into the code.

d) d) Restart capability

A restart capability is provided in the code that allows the user to save results at specified time steps into a database, and re-run or extend the problem. By loading a previously saved database, the user can resume a new run at any times in the simulation history. In addition, the code allows the user to re-define execution parameters, boundary conditions, and heat source and external forces; therefore, one has great flexibility to use simulation results of an existing case to perform further analysis. This feature can link, for example, the in-reactor fuel performance modelling to the structural analysis of fuel rod integrity in the back-end fuel cycle for dry storage and transportation.

2.2 LWR Fuel Modelling

Using a general-purpose finite-element code for fuel behaviour modelling faces many challenges in the modelling and implementation methods that are unique to the materials and geometries of fuels [2]. This section will emphasize some of those challenges in the Light Water Reactor (LWR) fuel modelling area; those implementations are expected to be transferrable to modelling other fuel types as well.

One well-known issue is the integration with models that involve complex inter-dependency, i.e., the interfacing among multiple models in the code. An abstract data type is implemented in the code for the global communication between multiple components such as, for example, the modelling of the neutronic radial power profile, fission gas release, gap gas pressure, as well as interfacing with a thermal boundary condition governed by the coolant channel flow and heat transfer.

In modelling the fuel thermal and mechanical responses using the finite element solution, the global equation could degenerate such that it is difficult to achieve a converged solution. Numerical techniques are employed in the code to provide a “stabilization” in solving the equation without changing the accuracy.

The modelling of LWR fuel often features a high aspect ratio, which could cause numerical oscillations in the finite element solution under certain conditions. To address this issue, the formation of the finite element integration is optimized for different state and field variables along with an implementation of an adaptive grid meshing technique.

2.3 Material and Behaviour Models

Material and behaviour models in the PEGASUS code consist of a) generic material models for metals (cladding) and ceramics (fuel), and b) specific models used for nuclear materials. Generic material models serve as surrogates for testing and/or creating new material models. The material models [3-8], commonly in most fuel performance codes are available in PEGASUS. A few distinctive models implemented in PEGASUS are described below.

a) Fission gas release modelling

For fission gas release modelling in PEGASUS, we have implemented the Forsberg and Massih fission gas release (FGR) model [6]. The model is based on spherical diffusion from a fuel grain. However, it incorporates a two-stage fission gas release approach, and in contrast to previous models, utilizes time dependent boundary conditions to determine grain boundary gas accumulation, resolution, saturation, and release parameters. Release from the grain boundaries is controlled using a grain boundary saturation criterion.

The implementation of the Forsberg and Massih model included several modifications derived from prior experience and review of previous implementations of the model. These included adjustments and modifications to the applied diffusion coefficients (updated to the recommended values from later publications by the authors [9,10], scaling grain boundary resolution using fission rate (based on evaluation of approaches in work by Turnbull [11], and White and Tucker [12], and calibration of the intragranular resolution rate and fuel matrix hydrostatic stress value used in the saturation and release criterion to available validation test rod FGR data. It is planned that this work will be revisited in the near term to improve the predictive performance of the model as we expand the V&V database and testing regime for PEGASUS. For the modelling of fast transients, mechanistic modelling approach [13][14] can be adapted for PEGASUS code.

b) Nonlinear constitutive material models for fuel and cladding

UO_2 and Zirconium alloys are inherited from two base materials - ceramic and metal. Those constitutive models are nonlinear and have included all the creep-plasticity deformations as well as the empirical deformations in the irradiation environment. Specifically, the relocation, densification, and swelling for UO_2, and irradiation growth of Zirconium alloys are formulated in the constitutive laws. The ceramic UO_2 has a smeared cracking damage model, which was initially used for the modelling of gas-cooled reactors concrete pressure vessels [15], later applied extensively to high velocity impact of reactor containments. Fig. 1 below shows the stress-strain curve implemented in the smeared cracking model for ceramic materials in general.

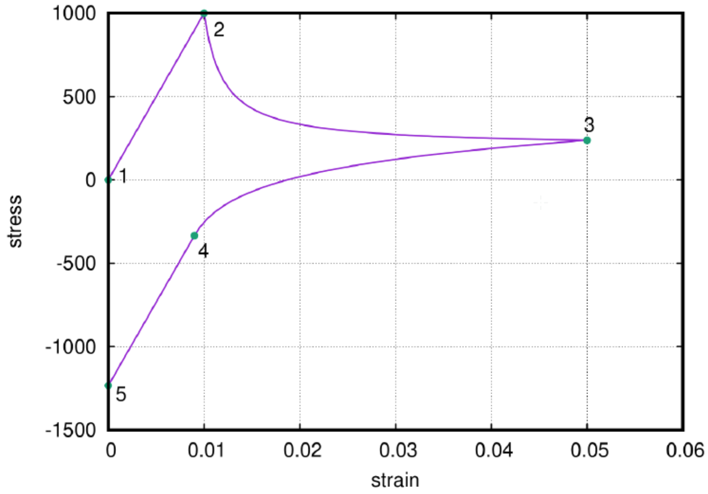

Fig. 1 Stress-strain curve of smeared cracking model for a reversing load cycle.
(1) zero-strain stress-free starting state, (2) material starts to crack,
(3) strain reversal point, (4) material regains original elastic modulus in compression, and
(5) back to the zero-strain state, but with residual stresses due to damage

The dilatational creep model is based on a mechanistic model in Ref. [16], and is implemented to compute evolutionary changes in porosity, i.e., the hot-pressing phenomena at high temperature under hydrostatic pressure, and this is built as part of the default material models in ceramic UO_2.

c) Fuel-cladding gap model

One main challenge in the modelling of LWR fuel is dealing with the contact between fuel and cladding which involves both thermal and mechanical aspects of gap opening and closing. PEGASUS has implemented two distinct thermo-mechanical contact methodologies to address this.

The first methodology is a more general approach that uses a collection of facet-pairs to establish a contact-pressure field. Different than traditional contact methods, this method can describe a smooth contact behaviour in the presence of sliding and can perform a high-fidelity modelling of any contacting surfaces.

The second methodology, which is an alternative approach to modelling pellet-clad contact, is a thermomechanical constitutive model for a “pseudo-material" is developed in PEGASUS. The model does not describe the behaviour of any real material but mimics frictional contact and heat transfer across a thin, gas-filled gap; it can reproduce the thermomechanical behaviour of the gap in both open and closed regimes, with a discontinuity in the transition from open to closed being approximated by sharp, but continuous, changes of material parameters on mechanical and thermal response. To simulate the frictional sliding, a pseudo shear modulus is used to create shear-stress proportional to the contact pressure. Thermal response is characterized by a heat-flux vector computed using a gap conductance model (based on a MATPRO model [3]) in open and closed gap condition. This method can achieve an accuracy at a dimension of the physical presentation of the surface roughness of pellet and cladding while performing a more efficient computation for generating fuel performance modelling results.

Both of these methods have been tested and have shown similar prediction of fuel-cladding gap closure, the second method using gap element is a recommended approach for modeling the fuel problems for its high computational efficiency; it has been used extensively in the LWR fuel verification and validations and have predicted fuel rod dimensional changes successfully. The first method using a contact algorithm has generic applications, and it can be used for high-fidelity computation for checking the accuracy of the gap element method.

d) Coolant channel model

A one-dimensional coolant channel model is implemented in the code to compute coolant enthalpy changes as well as using heat transfer correlations to provide a boundary condition for the modelling of convective heat transfer from fuel rod to the coolant. The coolant channel solves the energy conservation and mass conservation equations in a single channel using the finite element method.

This one-dimensional model is pursued so that it is thermally coupled to a 3D or 2D-axisymmetic finite element model. The governing conservation equations for mass and energy are formulated in the weak-form equations, and then solved approximately on a 1-D mesh consisting of 2-node elements.

The steam table for water properties is implemented using International Association for the Properties of Water and Steam (IAPWS) IF97 standard. The formulation for thermodynamic properties is based on the ASME International Steam Tables for Industrial Use book [17]. The transport property formulations to generate the dynamic viscosity and thermal conductivity are based on the IAPWS 2008 formulation [18][19].

3. Verification and Validation (V&V)

A total of 575 cases are currently available for testing the key functions and subroutines in the code, with an additional 94 cases are available for testing the material models and finite element framework. An automation testing system in the code compares code calculation results to accepted solutions within a specified tolerance to protect against accidental modifications that might break the existing functionalities.

The measurement data is also built-into the code system and is used to compare to model calculations for V&V.

For the validation of integral fuel rod response, 37 cases have been prepared for the validation of LWR fuel modelling capabilities at present. Test rods include instrumented test fuel rods irradiated in commercial and test reactors, and commercial rods with pool-side or hot-cell examination results available. Each case covers several aspects of fuel performance parameters. Overall, those cases can cover all performance parameters of interest to LWR fuel modelling.

The V&V is still on-going as we continue to expand the database to further improve the LWR fuel modelling performance. At present, good results have been achieved in the validation of PEGASUS in the prediction of fuel thermal and mechanical behaviours. Fig. 2 through Fig. 5 show a few examples on the work in progress. Fig. 2 shows the comparison between PEGAUS calculation and measured centreline temperature. Fig. 3 shows the comparison between PEGASUS calculation and measured cladding diametral changes for burnup up to 60 GWd/tU.

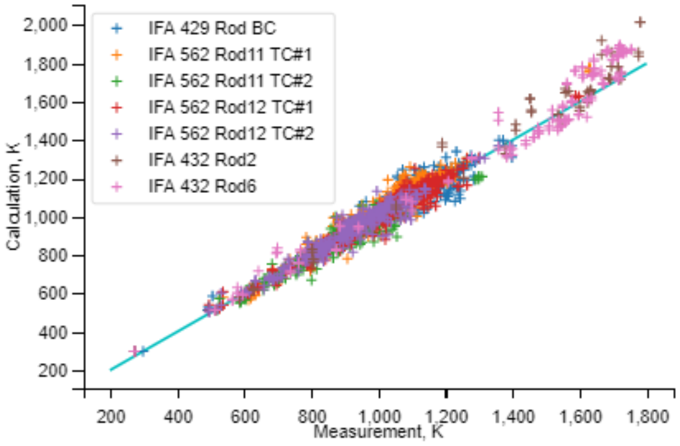

Fig. 2 PEGASUS Validation on fuel temperature prediction

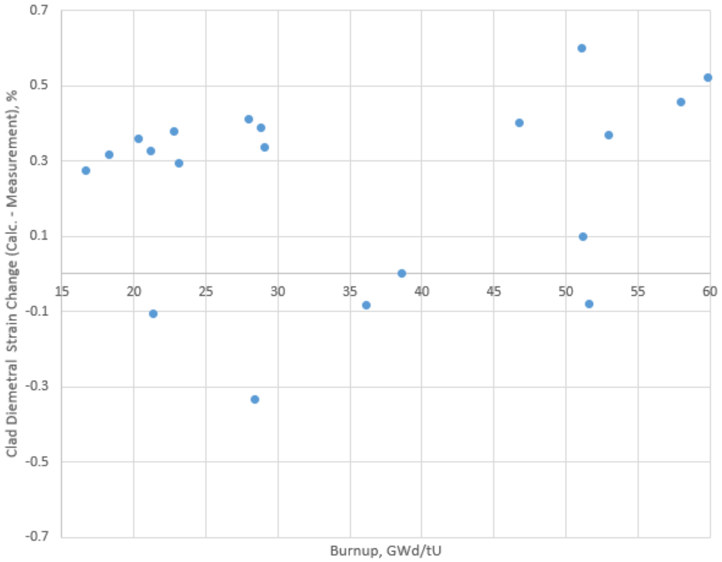

Fig. 3 PEGASUS validation on cladding diametral strain changes (calc. – measurement)

Fig. 4 shows IFA-562.1 rod 12 rod average linear power and PEGASUS calculation results in comparison to the measured temperatures at one thermo-couple location.

Fig. 5 shows an example (TRIBULATION BN1/4) on the prediction of the clad diametral changes in comparison to the profilometry measurement.

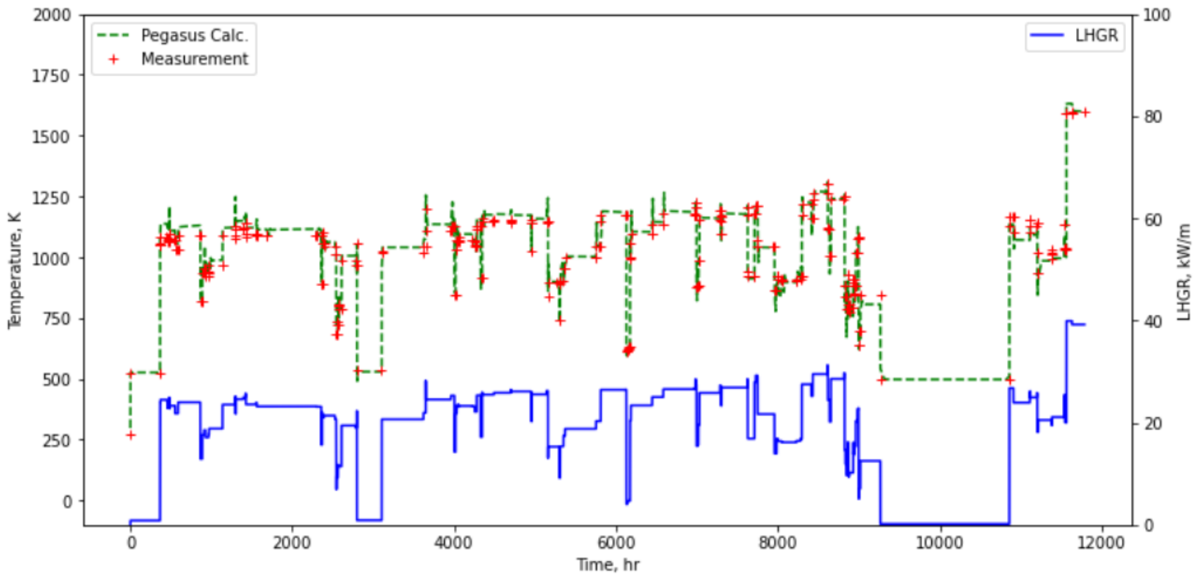

Fig. 4 Input power history and temperature calculations for IFA 562.1 Rod 12

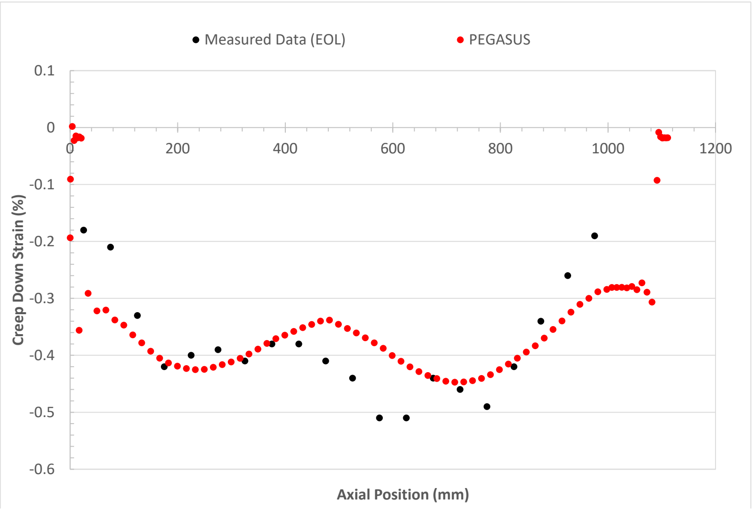

Fig. 5 Creep down strain comparisons for TRIBULATION Rod BN1/4

For the assessment of FGR, the Forsberg and Massih model as implemented in PEGASUS works well for steady-state FGR, however it does not respond adequately to power ramps or transient conditions. Additional work will be needed to address those aspects of FGR as development of PEGASUS continues. Additional areas under consideration for future work include evaluation of the burnup dependency of fuel grain size, intragranular fission gas bubble radius, fuel pellet porosity (especially at high burnups), and addition and integration of gaseous swelling.

4. PEGASUS Applications

PEGASUS application can be extended to mitigating fuel failures in operational conditions, quantification of safety margins in accident conditions, structural analysis for used fuels, and potential applications for new fuel types with various geometries and materials.

4.1 Full Length Rod Modelling

PEGASUS is capable of fuel performance modelling for commercial rods and computing the parameters for evaluating the fuel performance. One example is shown below, the commercial rod BEN013 in the PROTOTYPE high burnup demonstration program at the Calvert Cliffs commercial nuclear power plant [20][21]. Tab 1 shows the key characteristics for the input.

Characteristic	BEN013
Cladding OD, mm	11.176
Cladding ID, mm	9.754
Pellet OD, mm	9.563
Pellet Length, mm	11.430
Enrichment, wt. % U235	3.65
Initial Pellet Density, g/cc	10.395
Active Fuel Height, m	3.472
As-Fabricated Rod Internal Pressure, MPa	2.723
As-Fabricated Internal Void Volume, cm^3	31.58

Tab 1: Design Characteristics, Calvert Cliffs BEN013

PEGASUS-predicted and the measured characteristics, the latter from the end-of-life (EOL) Post Irradiation Examinations (PIEs), are provided in Tab 2.

Characteristic	BEN013	
	PIE	Predicted
Rod Average Burnup, GWd/tU	59.84	58.40
Void Volume, cm^3 (@ STP)	24.71	23.22
Rod Internal Pressure, MPa (@ 25°C)	3.81	3.83
Fission Gas Release, % (Calculated)	2.3	0.61
Average Diametral Strain, %	-0.6755	-0.1551
Elongation Strain, %ΔL/L	0.7937	0.6984

Tab 2: Measured and Predicted Characteristics, Calvert Cliffs

4.2 3-D Modelling

PEGASUS can be used to perform 3-D modelling for high-fidelity analysis. As an example, a rodlet with five discrete pellets is modelled using PEGASUS. The linear power ramps up to 20 kW/m, holds, and then ramps down. Two eccentric pellets were modelled in this case with the second pellet being shifted towards the x direction, and the third pellet (middle) shifted towards the negative x direction. Fig. 6 shows the temperature contour at the full power condition. Due to the eccentricity, the fuel temperature in the second and third pellets are shifted away from the centreline.

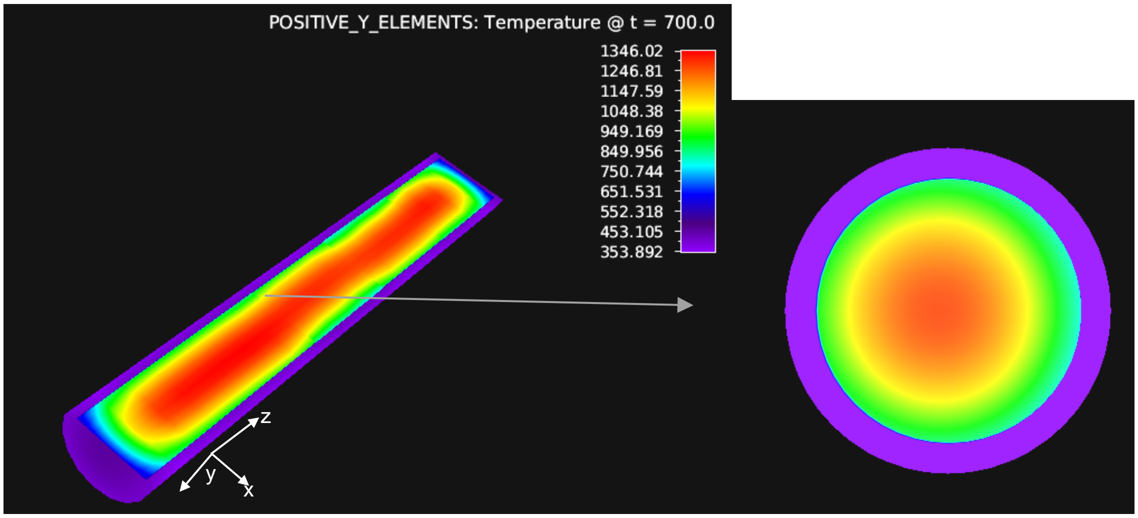

Fig. 6 Fuel temperature response for the 3-D rodlet (with eccentric pellets)

4.3 Structural Analysis for Used Fuel

Current practice of used fuel safety evaluations consists in using structural analysis codes and substituting surrogate fuel with no prior irradiation history for the actual used fuel. To compensate for the absence of in-reactor service effects, assumptions are made for material properties, which ignore the effects of damage mechanisms that evolve during in-reactor service and subsequently during dry storage. The veracity of structural analysis methods of used fuel drop accidents, where fractured fuel pellets, fuel-cladding bonding, radiation damage, corrosion and hydride reorientation play a critical role, is often questioned by the regulators in their reviews of industry submittals. This has contributed in part to a state of high uncertainty in the management of used fuel.

PEGASUS treats used nuclear fuel behaviour as a non-separable part of the fuel cycle, which is at variance with current practice which ignores the very important coupling of the back-end of the fuel cycle to its frontend operational stage. Irradiation and service induced material conditions during normal operations, which undergo further changes during dry storage, constitute the initial conditions for PEGASUS analysis of used fuel subjected to handling and transportation events. Accounting for the evolution of damage mechanisms during in-reactor service and subsequently during dry storage is critical for high fidelity assessment of used fuel failure resistance to impact forces during drop events. This paper describes a new approach to used fuel integrity evaluation as a continuous process with in-reactor fuel performance analysis, using PEGASUS code developed to deal with the entire fuel cycle from initial fuel insertion in reactor to permanent storage.

As an example, Fig**.** 7 shows the axial stress contour by applying a bending moment to a rodlet using PEGASUS code.

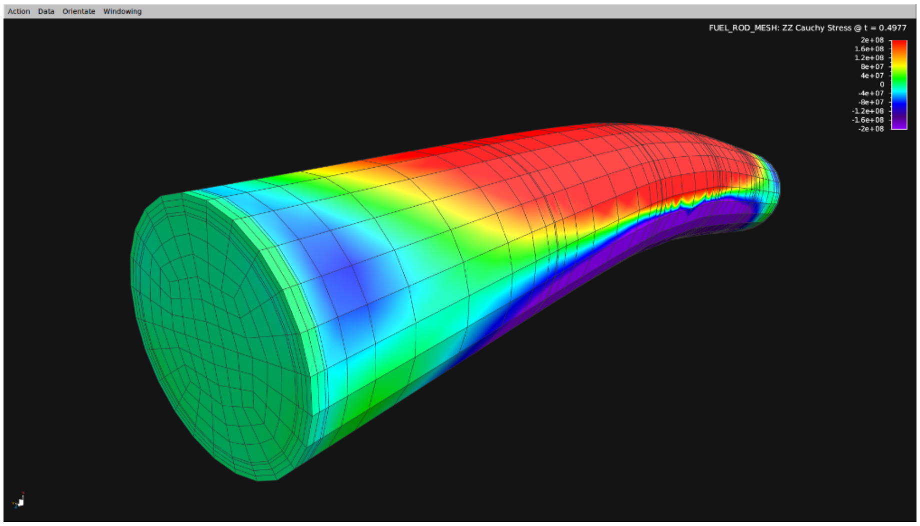

Fig. 7 Illustration of structural analysis of a 3-D rodlet problem

4.4 Advanced Fuels

For advanced fuel designs, PEGASUS has the versatility required to model the unique fuel rod geometries and materials that characterize the leading candidates for implementation in advanced reactor systems. These include modelling of TRISO (TRi-structural ISOtropic particle fuel) and encapsulated TRISO particle fuel matrices. PEGASUS has specific tools to facilitate the modelling of unusual fuel geometries such as those employed for TRISO-based fuel designs. The *spherical mesh object* tool in PEGASUS combined with the code's scripting capability can automatically generate single or multiple fuel particles embedded in a fuel material matrix for fuel performance analysis.

5. Conclusions

PEGASUS is a generalized fuel cycle code to calculate fuel response throughout the entire fuel cycle including in-core fuel behaviour during normal operations and transient events as well as back-end events associated with dry storage and transportation.

Built-upon a robust general-purpose finite element framework, innovative methods were developed in PEGASUS for fuel behaviour modelling to address the complex inter-dependency of behaviour models, contact between fuel/fuel and fuel/cladding, high-aspect ratio of element, and numerical stabilization. A few examples, along with V&V results have demonstrated the code's capability of performing the conventional fuel performance analysis as well as performing structural analysis.

The code's versatility is designed for broad applications to meet the demands of conventional fuel modelling as well as emerging needs in the development of advanced fuels.

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