Transactions, SMiRT-23
Manchester, United Kingdom - August 10-14, 2015
Division III

REACTOR PRESSURE VESSEL INTEGRITY ASSESSMENTS WITH THE GRIZZLY SIMULATION CODE

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ABSTRACT

Grizzly is a simulation tool being developed at Idaho National Laboratory as part of the US Department of Energy's Light Water Reactor Sustainability program to provide improved safety assessments of systems, components, and structures in nuclear power plants subjected to age-related degradation. Its goal is to provide an improved scientific basis for decisions surrounding license renewal, which would permit operation of commercial nuclear power plants beyond 60 years. Grizzly is based on INL's MOOSE framework, which enables multiphysics simulations in a parallel computing environment. It will address a wide variety of aging issues in nuclear power plant systems, components, and structures, modelling both the aging processes and the ability of age-degraded components to perform safely.

The reactor pressure vessel (RPV) was chosen as the initial application for Grizzly. Grizzly solves tightly coupled equations of heat conduction and solid mechanics to simulate the global response of the RPV to accident conditions, and uses submodels to represent regions with pre-existing flaws. Domain integrals are used to calculate stress intensity factors on those flaws. A physically based empirical model is used to evaluate material embrittlement and evaluate whether crack growth would occur. Grizzly can represent the RPV in 2D or 3D, allowing it to evaluate effects that require higher dimensionality models to capture. Work is underway to use lower length scale models of material evolution to inform engineering models of embrittlement. This paper demonstrates an application of Grizzly to RPV failure assessment, and summarizes on-going work.

INTRODUCTION

The effects of age-related degradation mechanisms on critical systems, structures, and components play a key role in decisions related to renewing nuclear power plant licenses to permit service beyond 60 years. In considering extended operation, aging issues must be considered in a wide variety of nuclear power plant components. The reactor pressure vessel (RPV) is an example of a critical component for which aging must be considered. RPVs must maintain integrity during both normal and off-normal operating conditions. Off-normal conditions of concern include pressurized thermal shock (PTS) loading events, which are characterized by rapid cooling and depressurization of the RPV and can potentially be followed by a rapid repressurization. In the unlikely event that a vessel subjected to such loading contains a large pre-existing crack, the crack could propagate through the wall of the vessel (Odette and Lucas, 2001). Such a failure is more likely to occur if the material is brittle. The steel used to construct RPVs becomes more brittle at lower temperatures. Aging due to long-term exposure to elevated temperatures and irradiation such as that experienced in the vicinity of the core also embrittles the material, as manifested by an increase in the ductile to brittle transition temperature and a drop in the upper shelf energy. Because of this, failure of RPVs due to PTS is an important consideration for life extension beyond 60 years.

The susceptibility of aged RPVs to fracture is a function both of the material embrittlement due to aging and of the loading conditions imposed on the vessel. Because of this, an assessment tool for RPV fracture must model both the aging processes and response to loading. This is an inherently multiscale problem, involving microstructure evolution at the nanometer scale, fracture mechanics at the millimeter scale, and global RPV thermomechanical response at the meter scale. A variety of modeling techniques are needed to simulate response to aging mechanisms and loading at all of these scales.

MULTIPHYSICS SIMULATION ENVIRONMENT

The Grizzly simulation code is being developed to provide an improved scientific basis for life-extension decisions. Grizzly is intended to provide a multiphysics, multiscale computational platform to simulate both the aging processes and the effects of aging on the ability of these components to safely perform their intended tasks. Ultimately, Grizzly will address a wide range of aging issues in key components, including the RPV, core internals, containments, piping, concrete structures, and cables. The RPV has been chosen as the first application for Grizzly because of its critical role in ensuring safe operation of nuclear power plants, and because of the extreme difficulty involved in replacing or repairing the RPV.

Grizzly is based on Idaho National Laboratory's Multiphysics Object Oriented Simulation Environment (MOOSE) framework (Gaston et. al., 2009). MOOSE is a finite element based framework for solving tightly coupled systems of partial differential equations (PDEs) on parallel computing platforms. MOOSE solves user-defined physics equations, and has been applied to a variety of applications. As of 2014, MOOSE is released as open-source software, and is being used by research organizations worldwide.

MOOSE solves the system of equations using the preconditioned Jacobian-free Newton Krylov (JFNK) method. This technique uses Newton iterations to minimize the residual of the full system of coupled equations. The classical Newton method forms the Jacobian matrix and uses it to solve for the iterative update to the solution vector. To avoid forming the Jacobian matrix, JFNK employs a Krylov iterative method (GMRES) to perform linear iterations to solve for each nonlinear Newton update to the full solution vector. Krylov methods do not require the actual Jacobian matrix, only the action of the Jacobian on a vector, for which a finite-difference approximation is employed.

To accelerate convergence, the system of equations is preconditioned using a matrix that is an approximation of the Jacobian matrix. Improved convergence is typically obtained as the preconditioning matrix better approximates the Jacobian matrix. A major benefit of preconditioned JFNK is that for modeling coupled physics problems, the coupling terms between physics equations often do not need to be included in the preconditioning matrix for reasonable performance. This facilitates rapid development of coupled physics applications, and has been successfully applied to a variety of types of multiphysics problems.

MOOSE has a modular architecture, providing pluggable interfaces for users to implement their own physics equations. Users define the system of PDEs to be solved, including the solution variables, the volume and surface integrals, material models, and other auxiliary operations required to solve the weak form of the coupled system of PDEs. These are defined by a combination of input file commands and code modules that can be user-defined for specific applications. A variety of applications have been developed based on MOOSE for a variety of engineering and physics problems, including nuclear fuel performance, neutron transport, thermal-hydraulics and microstructure evolution. MOOSE provides a set of modules for modeling common physics that are shared across these applications. These include general capabilities for solid mechanics, heat transport, and phase field methods, for example.

Grizzly builds on the capabilities in MOOSE to solve the physics equations of interest for nuclear power plant component aging problems. As mentioned previously, the initial focus of Grizzly is to address the RPV fracture problem. Work is also currently underway to model aging mechanisms in nuclear power plant concrete structures, and future work is planned for other components as well.

MODELS FOR RPV SIMULATION

Capabilities are being developed in Grizzly to calculate both the engineering fracture response of the RPV and material aging mechanisms. Evaluating the fracture behavior of an RPV involves modeling both the global thermomechanical response, as well as the local response of the region in the vicinity of a pre-existing flaw in the material that could serve as the fracture initiation point. In addition to calculating the loading on flaws, it is also important to characterize the material capacity. Grizzly incorporates an engineering-scale model for aging-induced embrittlement, and development is underway to develop a bottom-up capability to model aging mechanisms and their effect on the fracture toughness. A given RPV can contain a potentially large population of flaws of a variety of sizes and orientations. A probabilistic approach is ultimately necessary to make engineering decisions on the serviceability of a degraded RPV with such a flaw population. The approaches employed in Grizzly for these aspects of the problem are summarized in the sections below.

Global RPV Thermomechanical Response

The first task in an assessment of RPV integrity during PTS loading conditions is to compute its response to the thermal and mechanical loading imposed on it. The beltline region of the RPV experiences the highest fluence, and is thus the most susceptible to embrittlement and fracture. Because this region is far away from the ends of the vessel, it can be idealized as an axisymmetric, infinite cylinder for the purposes of computing the thermal and mechanical response if the pressure and temperature loading are uniform. This property is typically exploited to simplify modeling of the RPV, as is done in the FAVOR code (Dickson et. al., 2012), which models the beltline response in 1D. Grizzly can represent the RPV using 2D axisymmetry or 3D, the latter of which permits the analysis of features or loading that depart from axisymmetric conditions.

Grizzly uses MOOSE to solve the coupled equations of heat transport and solid mechanics. The PDE governing heat transport can be expressed as shown in Equation 1:

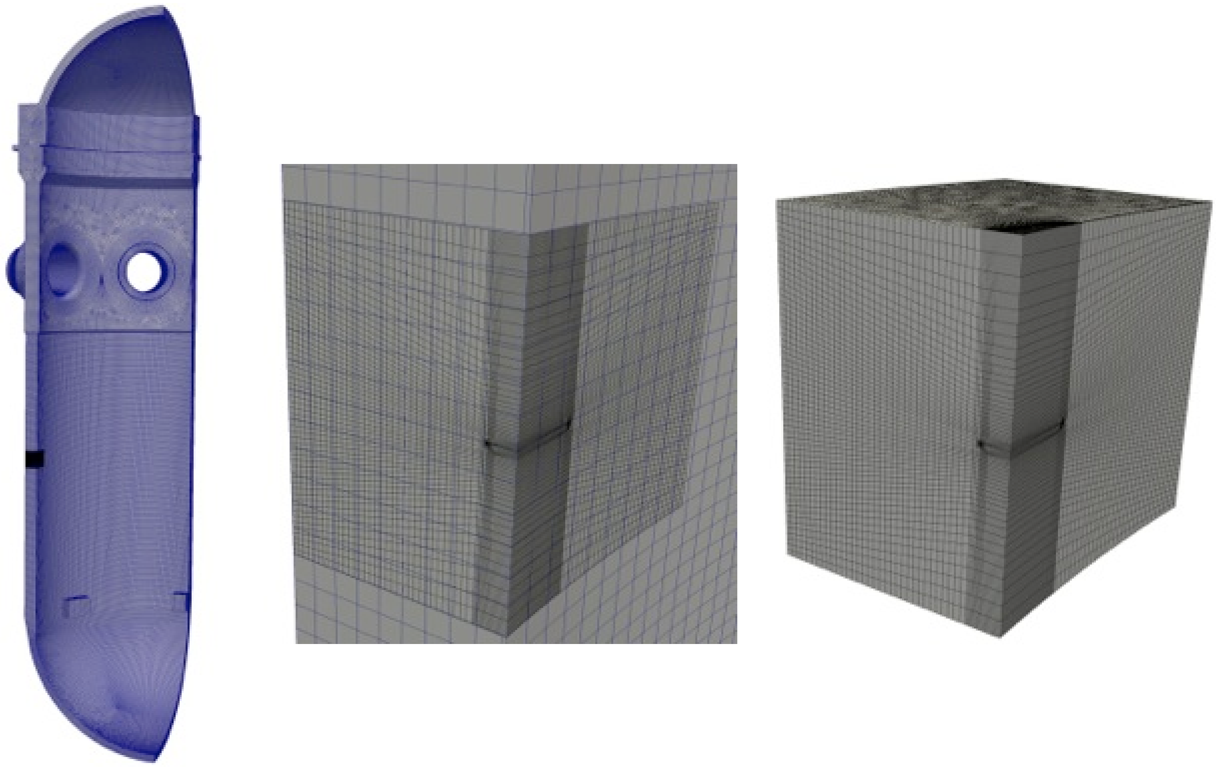
$$\rho C \frac{\partial T}{\partial t} = \nabla \cdot K \nabla T + Q \tag{1}$$

where T is the temperature, t is time, ρ is the density, C is the specific heat, K is the thermal conductivity, and Q is a volumetric heat source, which is zero for the RPV analyses here. The specific heat and thermal conductivity are functions of temperature. The PDE governing mechanical response is the expression of stress equilibrium given in Equation 2:

$$\nabla \cdot \boldsymbol{\sigma} + \boldsymbol{b} = \mathbf{0} \tag{2}$$

where $\boldsymbol{\sigma}$ is the stress tensor and $\boldsymbol{b}$ is a body force vector (assumed to be zero here). It is assumed here that the stainless steel liner and base steel both behave elastically, with temperature-dependent Young's Modulus and Poisson's ratio. Thermal expansion is temperature-dependent, and is defined using a function that provides the mean thermal expansion relative to a reference temperature. The methodology described by Niffenegger and Reichlin (2012) is employed to compute incremental thermal expansion from this function.

Grizzly employs the MOOSE framework to perform a tightly coupled solution of the discretized weak form of Equations 1 and 2 with the finite element method. The 3D mesh shown in Figure 1(a) is used in the present work to demonstrate the application of Grizzly to an RPV fracture analysis. This model has 9 linear 8-noded hexahedral elements through the thickness of the base metal, and 1 element of the same type through the thickness of the stainless steel liner. This model represents an idealized geometry, and is not for a specific reactor. Two symmetry planes are employed, with appropriate boundary conditions, to represent a quarter of the vessel. This model is subjected to transient temperature and pressure, and computes the displacement and temperature at each time in the simulation. The global model represents the RPV without any defects. Separate submodels, described in the following section, are used to capture the local response in the vicinity of a defect.



(a) Global Mesh (b) Detailed view of overlaid meshes (c) Submodel mesh

Figure 1: Computational meshes to model global RPV response and local response in flaw region. Submodel is embedded in global mesh as shown by black region on left side of (a), and in detail in (b).

Fracture Simulation

The assessment of whether fracture propagation would occur at the location of a pre-existing flaw is performed using linear elastic fracture mechanics (LEFM). A 3D model of the material surrounding a flaw, such as the one shown in Figure 1(c) is used to calculate the mechanical response in that region, including the stress intensity along the tip of the flaw. The submodel includes a flaw, represented in this case as a surface-breaking elliptical crack incorporated in the finite element mesh. The submodel is geometrically positioned to coincide with the geometry of the RPV model. Figure 1(a) shows both the global mesh (blue element lines) and the submodel (black region on left side of global model). The submodel is positioned adjacent to the symmetry plane on the left side of the figure. A detailed view of the two superimposed meshes is shown in Figure 1(b), with blue lines for the global mesh and black lines for the submodel mesh.

The domain of the submodel is made sufficiently large that the crack has little effect on the response at the far boundaries of that model. On all boundaries of the submodel that are embedded within the global model, the interpolated displacement on the global model is interpolated at each time in the analysis and imposed as a displacement boundary condition. It is assumed here that the pre-existing crack has no effect on the thermal response, so the global temperature is imposed on the submodel, and only the equilibrium equations (Equation 2) are solved in the submodel. The same material properties are used in both models.

Grizzly employs fracture domain integrals to compute the stress intensity along the 3D crack front. Grizzly can compute the J-integral (Rice 1968, Shih *et al.* 1986), from which the mode-*I* stress intensity factor can be calculated for elastic material and cracks subjected to pure mode-*I* loading. In the beltline region of an RPV subjected to spatially uniform thermal and pressure boundary conditions, flaws aligned with the axes of the RPV would be subjected to pure mode-*I* loading. In general, however, if flaws were not aligned with the RPV axes, if there are local irregularities in the RPV, or if the boundary conditions are non-uniform, cracks would be subjected to mixed-mode loading. Axial flaws in the belt-line region of an RPV experience mode-I loading and hence the corresponding stress intensity factor can be calculated from the J-integral. However stress intensity factor calculations from the standard J-integral become prohibitive for arbitrarily oriented cracks or mixed mode loading conditions.

To handle the general mixed-mode loading case, Grizzly also employs the interaction integral method (Yau *et al.* 1980). This is based on the J-integral, and makes it possible to evaluate mixed-mode stress intensity factors K_I, K_{II} and K_{III}, as well as the T-stress, in the vicinity of 3D cracks. The formulation relies on superimposing Williams' solutions for stresses and displacements around a crack tip (in this context called 'auxiliary fields') and the computed finite element stress and displacement fields (called "actual fields"). The total superimposed J can be separated into three parts: the J of the actual fields, the J of the auxiliary fields, and an interaction part containing the terms with both actual and auxiliary field quantities. The last part is called the interaction integral. To obtain individual stress intensity factors, the interaction integral is evaluated with different auxiliary fields.

Material Embrittlement

The models described in the previous sections are used to compute the time history of the loading on the flaw, characterized by the stress intensity factor. To determine whether crack growth would occur, it is also necessary to characterize the material's resistance to fracture, expressed as the fracture toughness. Grizzly currently can employ the correlation of Eason et. al. (2013) (EONY model) to compute the embrittlement due to neutron irradiation and thermal aging, characterized by the shift in the ductile to brittle transition temperature. In the words of the authors, this is a "physically motivated, empirically calibrated" model. It represents the underlying mechanisms leading to embrittlement, such as precipitation, and is represented by the chemical composition of the alloying elements. Other correlations are then used to ultimately compute the transition temperature shift. All of these correlations are calibrated based on extensive experimental data, which means that this model is quite reliable within the range of experiments. However its application to irradiation times exceeding those of the experimental data, which goes out roughly to the life of the current reactor fleet, may not be reliable. Once the transition temperature shift is calculated, the fracture master curve (ASTM E1921-14a, 2014) is employed to compute the fracture toughness at a given temperature.

In an effort to have more confidence in predictions for longer-term irradiation exposure, which are needed for decision making for license extensions, an effort is underway as part of the Grizzly project to develop bottom-up, lower length scale models of the processes leading to material embrittlement. This includes modeling of irradiation damage to the bcc Fe matrix using molecular dynamics and rate theory, and modeling solute precipitation using molecular dynamics, atomistic kinetic Monte Carlo and phase field methods. Crystal plasticity is being used to compute material hardening, and cohesive fracture models are used to compute the fracture toughness as a function of temperature and irradiation dose. It is expected that these models can ultimately be integrated to provide an engineering-scale model that can be more robust for predicting the life of RPV steels exposed to longer irradiation times.

Probabilistic Fracture Mechanics

The current work demonstrates a deterministic analysis of a single crack. Ultimately, however, a probabilistic approach must be taken to characterize the probability of fracture of the vessel with random distributions of cracks. This is the approach taken in the FAVOR code. To use Grizzly in a probabilistic setting, it will be used in conjunction with RAVEN, a probabilistic risk assessment tool also based on the MOOSE platform.

FRACTURE VERIFICATION TESTS

The interaction integral capability developed in Grizzly provides post-processors for calculating mixed-mode stress intensity factors as well as T-stress. A set of verification problems have been developed to compare values computed by Grizzly for the Mode I stress intensity factor using J-integral and interaction integral methods with known solutions. One of these problems is shown here.

A model of a semi-elliptical flaw in a semi-infinite medium under a remote tensile stress was developed to verify Grizzly's ability to compute the mode-I stress intensity factor on a 3D model with a curved crack front. A close-up of the crack area of the mesh is shown in Figure 2. Results for K_I using the Grizzly interaction integral as well as the J-integral capability are compared in Figure 3 with an equation fit to finite-element simulation results (Newman and Raju 1981). The position $\Phi = 0°$ is at the free surface and $\Phi = 90°$ is at the symmetry plane. Benthem (1977) showed that for a crack that intersects a surface at a right angle, the stress intensity factor is zero at the surface. Since the K_I values at a node represents an average over a segment of the crack front, the value at the surface will be unreliable and has been omitted from Figure 3. In general, the results agree well with the reference solution.

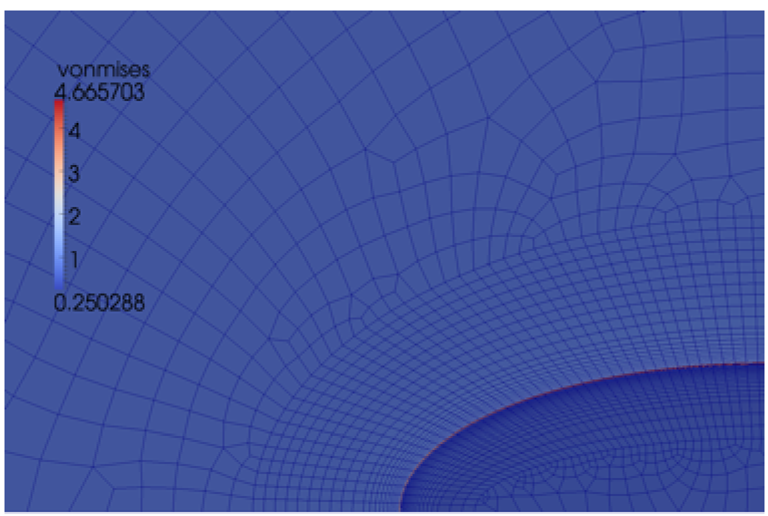


Figure 2: Close-up showing the crack front region of the semi-elliptical flaw mesh. The bottom edge is a free surface ($\Phi = 0°$) and the right hand edge is a symmetry plane ($\Phi = 90°$).

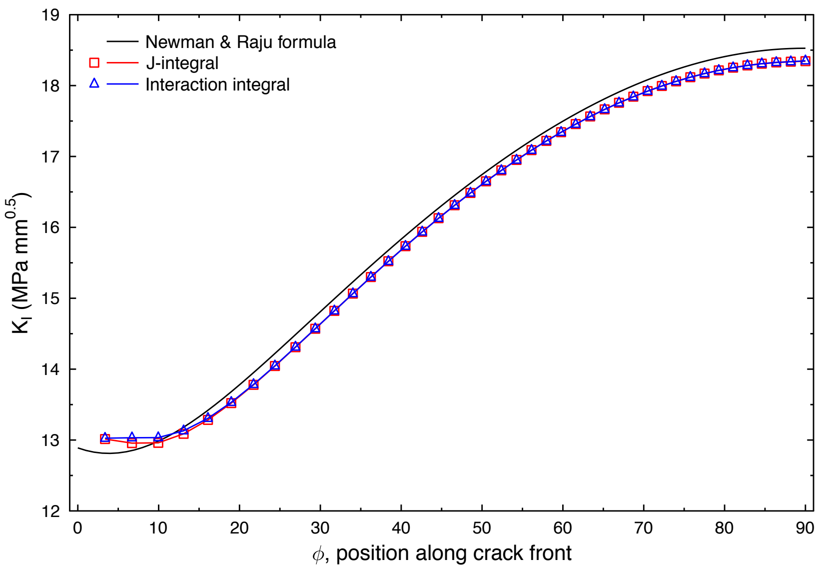


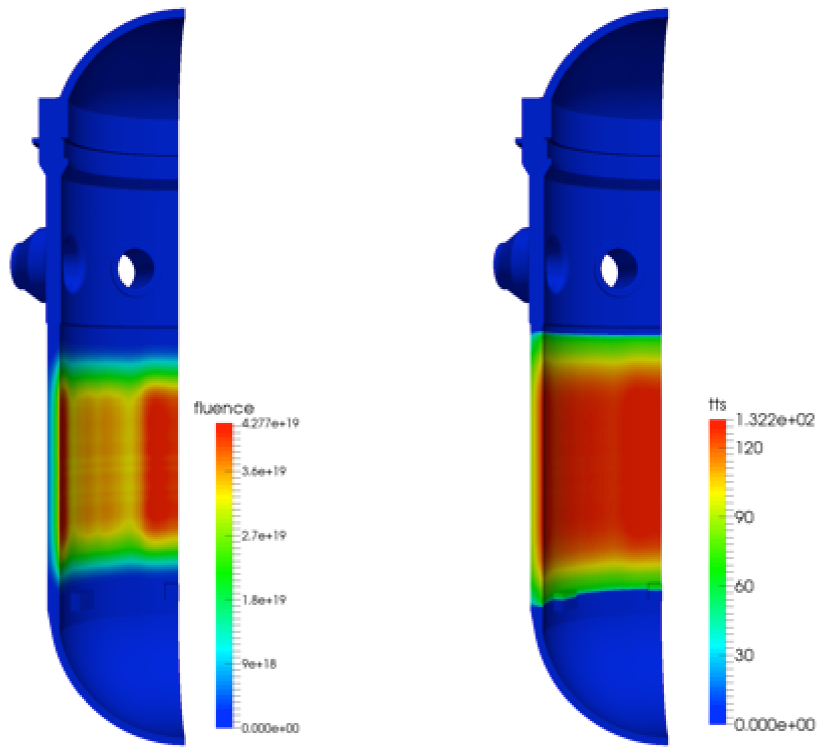
Figure 3: Mode I stress intensity factor along the crack front of a semi-elliptical surface-breaking flaw compared with the formula of Newman and Raju (1981).

DEMONSTRATION GRIZZLY RPV SIMULATION

To demonstrate the use of Grizzly in addressing ageing issues in nuclear power plants, an analysis of a flaw in an embrittled RPV during a PTS accident scenario was performed. A full-scale RPV model was used to determine the global thermomechanical response and the stresses on a postulated flaw was simulated in a submodel containing an axial flaw with boundary conditions driven by the global model. Embrittlement of the RPV steel was estimated by the EONY model at a neutron fluence corresponding to 32 effective full power years of operation. Figure 4 shows a map of the accumulated neutron fluence in the core region as well as the transition temperature shift calculated using the EONY model for this neutron fluence distribution.

A pressurized thermal shock (PTS) loading history was chosen as an accident scenario relevant for assessing the risk of failure in ageing pressure vessels. The pressure and temperature histories plotted in Figure 5 were applied as boundary conditions on the inner wall of the global RPV model. This transient is representative of an event during which a pressure release valve was stuck open, resulting in depressurization and significant decrease in temperature followed by a rapid repressurization and slow temperature increase once the valve was closed again. Figure 6 shows the temperature and stress distribution in the RPV model at the pressure spike 4800s into the PTS event. The temperature and pressure boundary conditions are spatially uniform in this case, but the 3D model permits local variations.

A submodel containing a surface-breaking, semi-elliptical flaw with a depth of 2.54 cm and a width of 15.24 cm was positioned in the core region at one of the symmetry planes of the global model and run with boundary conditions resulting from the PTS transient. The Mode I stress intensity factor K_I along the crack front was calculated using an interaction integral. The transition temperature shift from the EONY model was input into the Master Curve method, by which the fracture toughness K_{Ic}, given a failure probability, can be calculated. The time history of K_I at the deepest position of the flaw is plotted in Figure 7 and compared with K_{Ic} from the master curve. The master curve method is valid only in the lower shelf to transition region of the curve of fracture toughness as a function of temperature, which is why values of K_{Ic} are shown only during the period of low temperature. For this simulated accident scenario and postulated flaw, the load on the flaw K_I does not exceed the material fracture toughness K_{Ic} at any point during the transient.



(a) Neutron fluence (n/cm^2) (b) Transition temperature shift (^{o}F)
Figure 4: Neutron fluence and transition temperature shift calculated by EONY model after 32 effective full power years of reactor operation

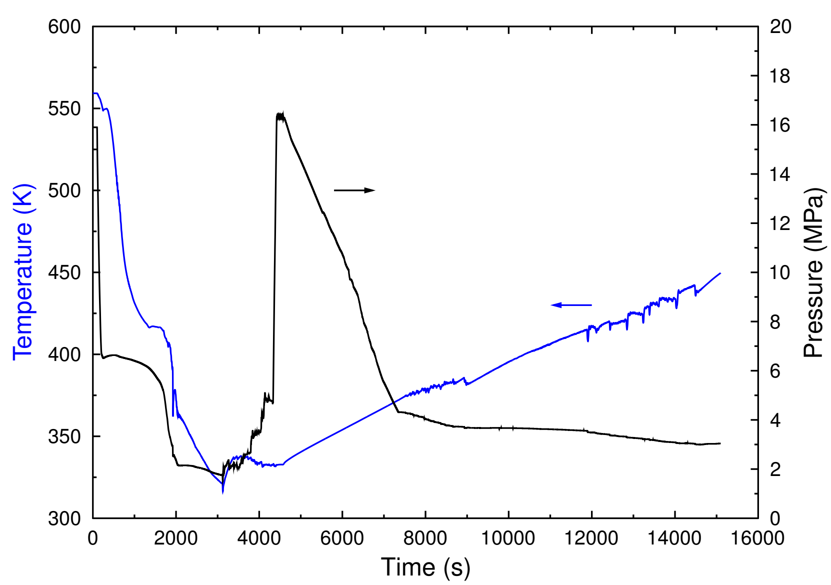


Figure 5: Time histories of temperature and pressure in demonstration PTS loading scenario

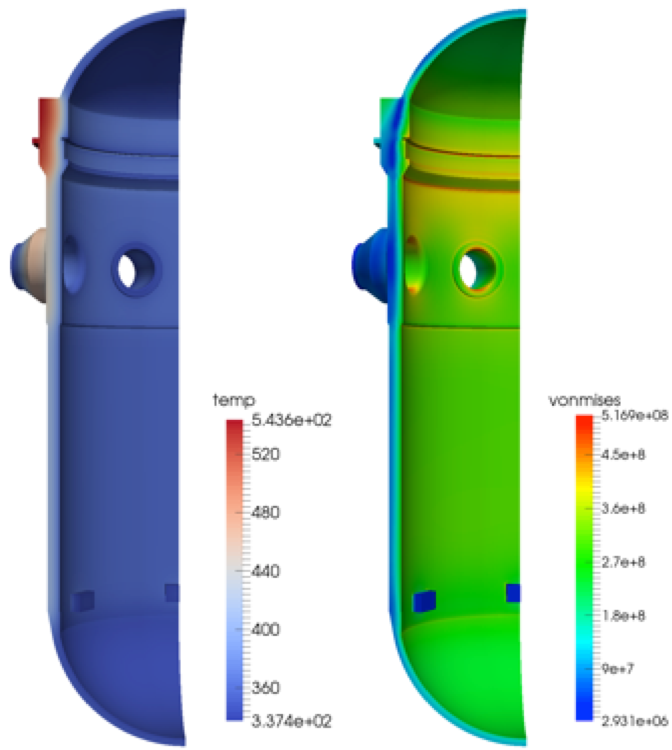


Figure 6: Temperature and von Mises stress in the global RPV model at the pressure spike 4800s into the PTS event.

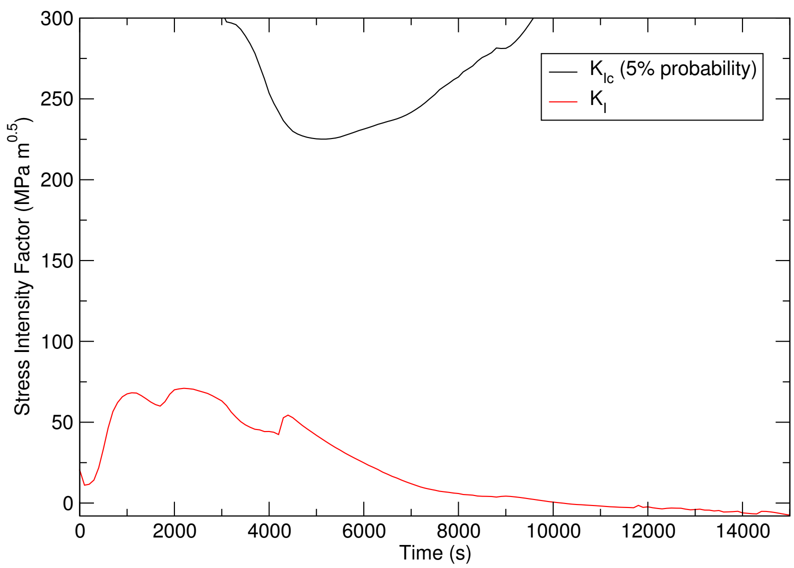


Figure 7: Time history of computed Mode I stress intensity factor and fracture toughness (5% probability)

CONCLUSION

Grizzly is under development at Idaho National Laboratory as a tool for safety assessment of age-related degradation of systems, components, and structures in nuclear power plants. Current capabilities of Grizzly include domain integral postprocessors for calculating stress intensity factors at flaws as well as implementations of the EONY model and master curve method to provide estimates of fracture toughness of an embrittled RPV. Mode I domain integrals (J-integral and interaction integral) have been verified and agree well with known benchmark solutions. The paper demonstrates the use of Grizzly to assess brittle failure of a pre-existing flaw in an RPV during a PTS accident scenario.

ACKNOWLEDGEMENT

This work was supported by the US Department of Energy's Light Water Reactor Sustainability (LDRD) program. The submitted manuscript has been authored by a contractor of the U.S. Government under Contract DE-AC07-05ID14517. Accordingly, the U.S. Government retains a non-exclusive, royalty free license to publish or reproduce the pub- lished form of this contribution, or allow others to do so, for U.S. Government purposes.

REFERENCES

ASTM E1921-14a (2014), *Standard Test Method for Determination of Reference Temperature, To, for Ferritic Steels in the Transition Range*. ASTM International, West Conshohocken, PA.

Benthem, J. P. (1977). "State of stress at the vertex of a quarter-infinite crack in a half-space." *International Journal of Solids and Structures*, 13(5): 479–492.

Dickson, T., Williams, P. T., and Yin, S. (2012). *Fracture Analysis of Vessels – Oak Ridge, FAVOR, v12.1, computer code: User's guide*. ORNL/TM-2012/566, USNRC Adams number ML13008A016, Oak Ridge National Laboratory, Oak Ridge, TN.

Eason, E., Odette, G., Nanstad, R., and Yamamoto, T. (2013). "A physically-based correlation of irradiation-induced transition temperature shifts for RPV steels." *Journal of Nuclear Materials*, 433(1-3):240–254.

Gaston, D., Newman, C., Hansen, G., and Lebrun-Grandié, D. (2009). "MOOSE: A parallel computational framework for coupled systems of nonlinear equations", *Nuclear Engineering and Design*, Vol. 239, Issue 10, pp. 1768-1778.

Newman, J. C. and Raju, I. S. (1981). "An empirical stress-intensity factor equation for the surface crack." *Engineering Fracture Mechanics*, 15(1-2): 185–192.

Niffenegger, M. and Reichlin, K. (2012). "The proper use of thermal expansion coefficients in finite element calculations." *Nuclear Engineering and Design*, 243:356–359.

Odette, G. R. and Lucas, G. E. (2001). "Embrittlement of nuclear reactor pressure vessels." *JOM*, 53(7):18–22.

Rice, J. R. (1968). "A path independent integral and the approximate analysis of strain concentration by notches and cracks." *Journal of Applied Mechanics* 35:379-386.

Shih, C. F., Moran, B. and Nakamura, T. (1986). "Energy release rate along a three-dimensional crack front in a thermally stressed body", *International Journal of Fracture*, 30(2):79-102.

Tada, H. (2000). *The stress analysis of cracks handbook, 3rd ed*. ASME Press, New York.

Walters, M. C., Paulino, G. H., and Dodds, R. H. (2005). "Interaction integral procedures for 3-D curved cracks including surface tractions." *Engineering Fracture Mechanics*, 72(11):1635–1663.

Yau, J. F., Wang, S. S., and Corten, H. T. (1980). "A mixed-mode crack analysis of isotropic solids using conservation laws of elasticity." *Journal of Applied Mechanics* 47(2):335-341.