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Abstract

This report documents recent work to improve the accuracy and robustness of the mechanical constitutive models used in the BISON fuel performance code. These developments include migration of the fuel mechanics models to be based on the MOOSE Tensor Mechanics module, improving the robustness of the smeared cracking model, implementing a capability to limit the time step size based on material model response, and improving the robustness of the return mapping iterations used in creep and plasticity models.

The work described in this report was performed under funding from the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. This report is issued in satisfaction of the Level 3 milestone M3MS-17IN0201015 on Oxide Fuel Mechanics in 3D for the INL Engineering-Scale Fuel Performance (BISON) Work Package.

Contents

Introduction

The mechanical response of oxide nuclear fuel during irradiation is complex, and is affected by multiple physical phenomena including fracture, relocation, creep, hot pressing, thermal expansion, and swelling. Accounting for the combined effects of these phenomena is important in fuel performance simulations, as the mechanical response of the fuel significantly affects the size of the fuel/cladding gap and the mechanical response of the cladding after it comes in contact with the fuel. These in turn significantly affect other aspects of fuel performance such as the temperature profile.

BISON has included models for all of these phenomena for some time, although the use of mechanical constitutive models including the effects of cracking, creep, and hot pressing in practice has been very limited because of solver robustness problems when using those models. Solver robustness has been particularly challenging with the smeared cracking model because of its strain-softening behavior. To obtain realistic predictions of stresses within the fuel, it is critical to use a cracking model. Since the creep and hot-pressing models are highly dependent on the stress state, the standard practice in BISON has been to not include those models either, because the response predicted by those models is not particularly meaningful in the absence of a cracking model.

This report documents robustness improvements made to the mechanical constitutive models used for oxide fuel in the BISON code. These developments are in the following areas:

- Transition of mechanical models to be based on the MOOSE Tensor Mechanics module
- Smeared cracking model improvements
- Time step control for plasticity and creep models
- Robustness improvements to the return mapping algorithm used by creep and plasticity models

These developments and their implications are summarized in the following sections of this report. Following that discussion, these improved models are demonstrated in a representative 3D simulation of a fuel rodlet.

1 Tensor Mechanics Transition

The open-source MOOSE software that BISON is based on consists of both the core framework, which provides the core functionality of the MOOSE solution environment, and the MOOSE modules, which provide a set of physics capabilities that are shared by applications that are built on MOOSE. Since the early development of BISON, the models for the mechanical response of solids have been based on the `solid_mechanics` module in MOOSE.

As more applications have been build on MOOSE, the requirements of those applications on the MOOSE modules have evolved. There is a need for material science models to have more general functionality for modeling mechanical response than is provided by the `solid_mechanics` (Solid Mechanics) module. In particular, there arose a need for a more general representation of the elasticity, stress, and strain tensors than what was provided in the Solid Mechanics module. To address that need, a separate module, named `tensor_mechanics` (Tensor Mechanics), was developed alongside the existing Solid Mechanics module, and provides these more general capabilities. In addition to providing more generality, the Tensor Mechanics models are based on a modular architecture that permits the various aspects of the stress computation (elasticity tensor, strain, stress, volumetric strains, etc.) to be computed by separate code objects, which allows for a broader set of models with minimal code duplication.

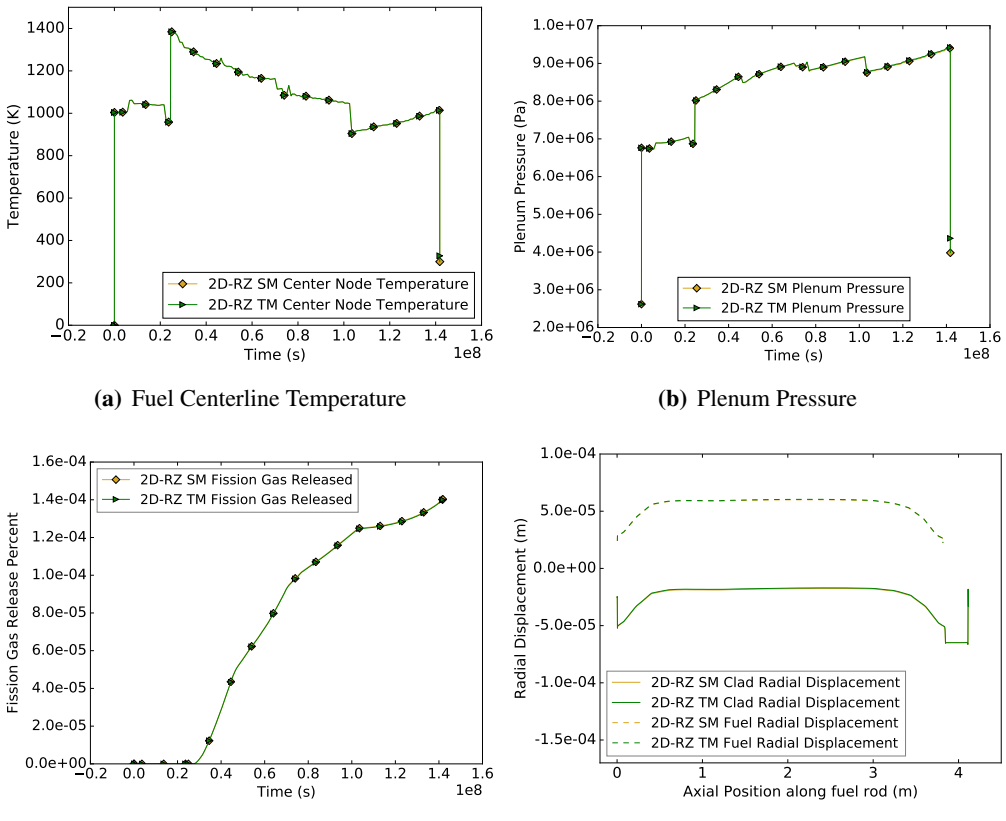
Maintaining parallel implementations of these mechanics capabilities is a significant burden on the code development teams, so there has been a significant effort to move all of the mechanics models used by BISON, as well as other applications, to be based on the more modern Tensor Mechanics module.

The implementation of BISON's models into new versions based on Tensor Mechanics is nearly complete. The majority of material models and related components for modeling oxide fuels have been converted. The major fuel and cladding material models that have been completed are listed below:

- Fuel
  - Fission Product Swelling
  - Thermal and Irradiation Creep
  - Hotpressing
  - Relocation
  - Smeared Cracking

- Cladding
  - Plasticity
  - Thermal and Irradiation Creep
  - Oxidation
  - Irradiation Growth
  - Damage/Failure

To test these new implementations, several examples of oxide fuel pin models have been converted to be based on Tensor Mechanics. The results have been compared to the Solid Mechanics solutions and are in good agreement. Comparisons of quantities of interest on one of the BISON 2D assessment case problems are shown in Figure 1.1, and show very good agreement between the two models.



(a) Fuel Centerline Temperature

(b) Plenum Pressure

(c) Fission Gas Release

(d) Radial Displacement at EOL

Figure 1.1: Comparison of the BISON Solid Mechanics (SM) and Tensor Mechanics (TM) results for the 2D axisymmetric simulation of the TSQ002 assessment case

Further examples of solution comparisons between Solid Mechanics and Tensor Mechanics can be found in a recent CASL letter report [1].

2 Smeared Cracking Model Improvements

The smeared cracking model used by BISON is based on the fixed smeared cracking approach originally proposed by [2]. The smeared cracking approach represents the effects of cracking through a strain-softening constitutive model run at the standard finite element integration points. When one of the principal stresses exceeds a tensile failure limit, the model converts to an orthotropic model that has a softening response in the direction of cracking. The orientation of the first crack is fixed, and up to two additional cracks are allowed to form at a given material point in directions orthogonal to the pre-existing cracks.

The softening response is obtained in the material model by making two key modifications to the material response. First, the elasticity tensor in the coordinate system of the crack is modified so that the stiffness is reduced in the direction of cracks. This damaged elasticity tensor, based on the maximum strain in the previous time step, is used to compute an updated stress during each material evaluation. The second modification made to the response is that the predicted stresses in the direction of cracking are adjusted to follow a defined softening function.

The nonlinear softening behavior of smeared cracking models makes solution convergence notoriously difficult, and the MOOSE/BISON implementation of the model is no exception. The implementation of the model in Solid Mechanics is full-featured, but has seen very limited use because of difficulties in obtaining convergence.

Prior to the work documented here, a limited version of the smeared cracking model had been implemented in Tensor Mechanics. To improve BISON's abilities to model oxide fuel behavior, as well as to migrate from the legacy Solid Mechanics model, the following modifications were made to that model:

- Multiple changes were made to the model to correct code issues and bring its behavior more in line with that of the Solid Mechanics implementation.
- The model originally only permitted the uncracked continuum to behave as elastic material, and did not permit the incorporation of creep and plasticity models. The model was modified to permit creep and plasticity models to be active before cracking, but once cracking initiates, the inelastic strains from creep and plasticity are frozen, and those models are de-activated.

  Creep and plasticity are de-activated at that point for two reasons: Because the material response is no longer isotropic, the techniques used for computing the creep and plastic response (which are based on assumptions of an isotropic elasticity tensor) are no longer applicable. Also, including both effects simultaneously at a material point can increase the likelihood of encountering problems with solution convergence.

In the future, ways to reliably include creep and plasticity simultaneously with cracking will be considered. However, it is believed that the current approach is a reasonable compromise between the competing demands of solution robustness and accurate modeling of the important physics. In oxide nuclear fuel, creep and plasticity typically have the most effect in the center of the pellet, whereas cracking is more important in the peripheral regions of the pellet.

- When cracking occurs, the original smeared cracking model abruptly dropped the shear stiffness between the crack plane and the two orthogonal directions to zero. This causes convergence issues because if multiple neighboring elements are cracked, the solution is ill-defined. An option was added for a user-supplied shear-retention factor, which defines how much that component of the shear stiffness should be reduced. When that factor (controlled using the `shear_retention_factor` parameter in the input file) is set to 0.0, the original behavior is recovered, and there is no stiffness in that direction. When set to 1.0, the full shear stiffness is retained. In our testing, setting this factor to a small number in the vicinity of 0.1 results in much-improved convergence behavior, while not resulting in significant spurious stresses due to excessively high shear stiffness.

- The solution difficulties in the smeared cracking model have been found to stem primarily from the update to the stress to follow the softening curve, rather than from the use of the damaged elasticity tensor. An option was added to the smeared cracking model to limit the change in stress due to the stress correction. The newly introduced `max_stress_correction` parameter defines the maximum allowable change in the stress from the elastic stress predicted using the damage state from the previous step. If that parameter is set to 1.0 (the default behavior), the full correction is made to the stress to follow the desired softening curve. If set to 0.0, no correction is made.

  It is common practice in damage mechanics models to use the damage from the previous step, and setting `max_stress_correction` to 0.0 mimics that behavior. When the model is run this way, its response in a given step is linear, so convergence is quite robust. This robustness comes at the sacrifice of some accuracy, and the model does over-estimate the stress in the post-peak softening curve somewhat, but that has a negligible effect on the quantities of interest in a nuclear fuel simulation. The model still limits the tensile stresses on the periphery of the pellet, and results in reasonable stresses in the center of the pellet, where creep is the most important mechanism.

Using a combination of the modifications to the numerical algorithms described here has permitted a robust solution of the 3D rodlet model presented in Section 5. This model was run with far more success than has been achieved in previous attempts to include smeared cracking in 3D fuel models.

3 Time Step Control for Plasticity/Creep

It was recently observed that the plasticity and creep material models implemented in MOOSE and BISON may be susceptible to the accumulation of numerical error due to a time step size dependence on the solution. Figure 3.1 plots the creep strain in the y-direction as a function of time for a series of single-element models run with various time step sizes. The baseline solution uses $\Delta t = 100.0$ and is shown as the blue dashed line. Using a larger time step of $\Delta t = 200.0$ results in a different solution seen as the dashed red line. Reducing the time step size should eventually result in a stable solution, and the results for $\Delta t = 10.0$ and $\Delta t = 5.0$ overlap, which indicates that the solution has converged.

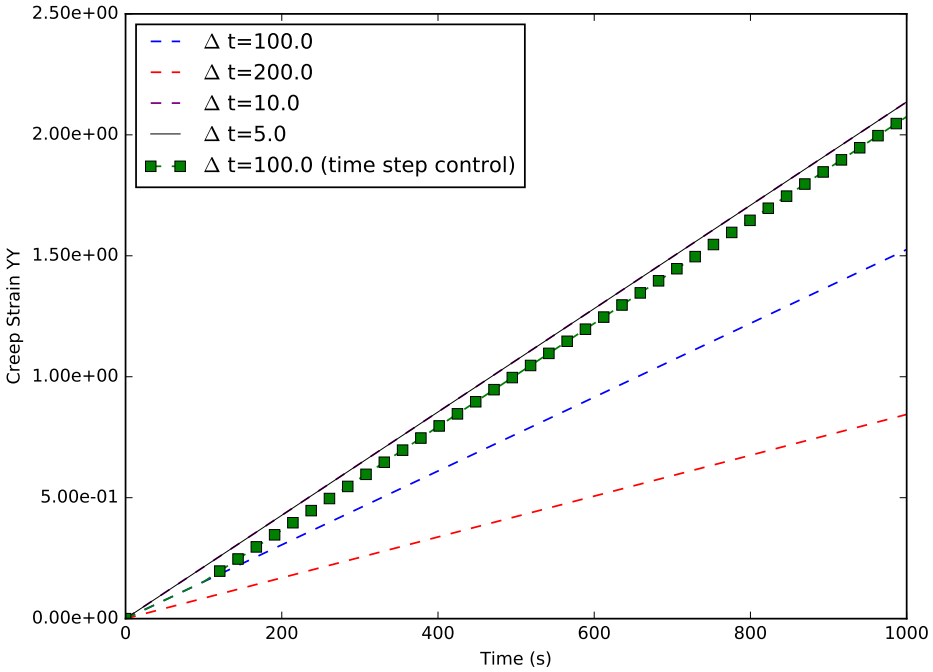


Figure 3.1: Creep Strain Time Step Size Dependence

To address this issue and ensure that the time steps taken are small enough to avoid time-integration errors, a material-based time step control feature has been developed. The maximum inelastic strain increment allowed in a given time step is specified for the material in the input file. During the analysis the time step size corresponding to the maximum inelastic strain increment is computed for every element. A postprocessor then finds the minimum time step size for

all material points in the model, which is then used to limit the size of the next time step taken. The solid green squares in Figure 3.1 are the results from an analysis in which the time step is controlled using this feature. The model takes an initial (user-prescribed) step of $\Delta t = 100.0$. After the initial time step, the subsequent time steps are limited in size based on a maximum inelastic strain increment set to 0.01. This model matches the "converged" solution much better than one that takes a constant step size of 100.0.

4 Robustness Improvements to Return Mapping Algorithm

There have been longstanding issues with poor convergence of the Newton return mapping iterations in the creep and plasticity materials, which are used for both fuel and cladding. This has led some users to set loose tolerances for those iterations to be able to obtain solutions.

A recent set of code changes adds a combination of line searches and bisection to that iteration procedure, which has drastically improved the ability of those models to converge to tighter tolerances. It also modifies all creep and plasticity models to compute a residual in terms of the inelastic strain increment. Previously, some of those models computed residuals in terms of the inelastic strain rate, while others computed the residual in stress units.

Now that residuals are computed in consistent units, the same tolerances are applicable for all models. They also all use the elastic strain as the quantity to compare against for relative convergence, which is much more broadly applicable than the initial residual, which was used previously.

These models have now been found to converge much more robustly than previously, and the default tolerances have been changed to values that in our experience work much better: `relative_tolerance = 1e-8`, and `absolute_tolerance = 1e-11`. Because the models are being forced to converge much more tightly in many cases, it occasionally takes a large number of iterations to converge the material model when the trial stress is large. To avoid failed solves, we now allow more iterations, and we have changed the default: `max_its = 300`. If a solve ever fails, it is repeated so that we can capture the iteration history, which gets printed out automatically, so the `output_iteration_info` and `output_iteration_info_on_error` parameters are no longer necessary. Because of these changes, it is recommended that anyone using these models simply remove all usage of any of these commands from the creep or plasticity model blocks, and use the default options.

This change was first made in Solid Mechanics, and the Tensor Mechanics materials were subsequently modified to use the same return-mapping code as well.

5 3D Model Demonstration and Summary

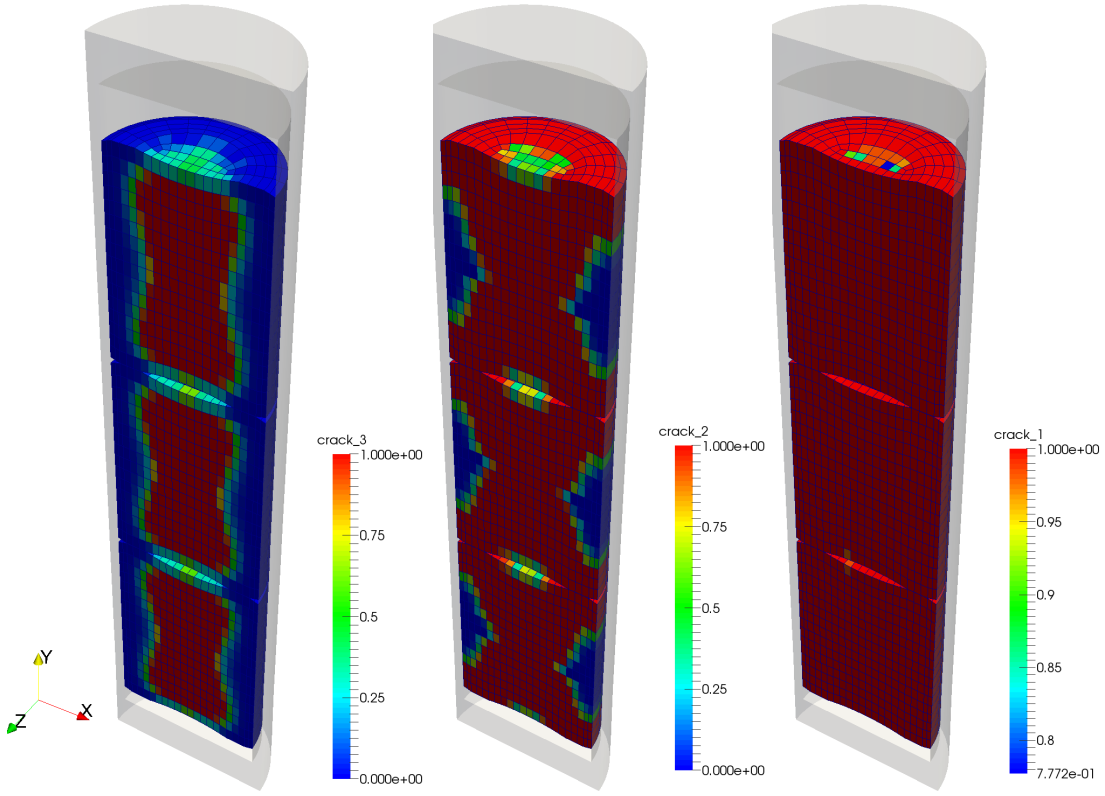
To demonstrate the capabilities documented here, a representative 3D model of a 3-pellet oxide light water reactor fuel rodlet was created and run using appropriate Tensor Mechanics-based models for fuel and cladding mechanical response. This rodlet is based on geometry for an upcoming experiment to be run in the Halden reactor, which has typical pellet geometry, but has a smaller than normal initial fuel/cladding radial gap of 80 μm. The smaller gap was used to induce contact earlier than usual. In this model, the power is ramped up to a level of 30 kW/m, and held at that level.

This model was run using a shear retention factor of 0.1, and with `max_stress_correction = 0.002`, which allowed for a correction of up to 0.2% to be made from the stress computed using the previous step's damaged elasticity tensor for a given step. The creep models in the fuel and cladding used the new return mapping algorithm described here, and the material-based time step limiter was also used.

Results are shown with various contours to highlight the mechanical response in Figures 5.1 and 5.2. These are shown after 204 days of irradiation, a point in time after which the major radial cracks have fully developed, and the cladding is in full contact with the fuel. Figures 5.1 shows the extent of cracking in the directions of the first, second, and third cracks. It can be seen that the most extensive damage is in the direction of the first crack, which is primarily in the radial direction, and occurs around the entire outer rim of the pellet. There is some localization of the cracking into bands of elements. There is also significant cracking in the second direction (axial) at the pellet mid-height, and almost no formation of cracks in a third direction.

Figure 5.2 shows contours of stresses and effective creep strains for this same model at the same irradiation time. On the symmetry plane, σ_{zz} is equal to the hoop stress. The smeared cracking model is very effective at representing softening behavior of the material once it cracks, and these hoop stress are far below the fracture stress, which was set to be 130 MPa in this case. The creep model is active only in the center of the pellet, as evident by the fact that that region has lower von Mises stresses and much higher effective creep strains than the periphery, where cracking is active.

The combination of the model developments summarized in this report has enabled this 3D simulation with a combination of oxide fuel models. The fact that this model is able to converge robustly is a significant development, because lack of solution robustness has previously prevented any significant validation testing of the previous smeared cracking model. These are initial results, and more testing on a variety of problems is needed to validate this modeling approach, but the solutions appear quite reasonable.

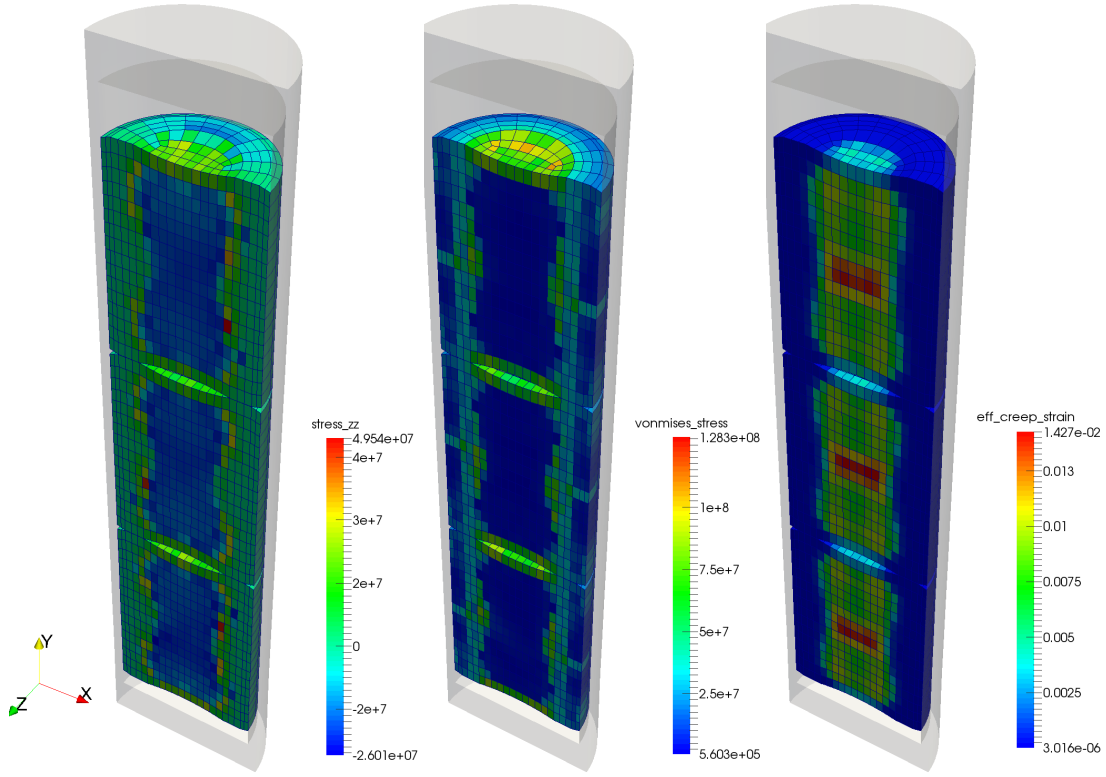


(a) 1st crack **(b)** 2nd crack **(c)** 3nd crack

Figure 5.1: Extent of cracking in directions of first, second, and third cracks in 3-pellet model after 204 days of irradiation. Values of 1.0 indicate un-damaged material, while 0.0 indicates complete loss of strength in cracking direction. Note that the labels correspond to the principal stresses when the cracks formed, so "crack_3" is the first crack to initiate since it is in the direction with the highest tension.

It is important to note that while the demonstration shown here uses a 3D model, these constitutive models are ed for all BISON models, regardless of dimensionality, so these improvements are also applicable to 2D axisymmetric, 2d cross-section, and layered 1D models.

The current set of BISON validation problems does not yet use these constitutive models due to historical issues with solution robustness. Now that these constitutive models are more robust, those validation cases can be modified to include them. Comparison of those results with experimental data will help assess the accuracy of these constitutive models.



(a) Stress in zz direction (Pa) **(b)** von Mises Stress (Pa) **(c)** Effective creep strain

Figure 5.2: Stresses and creep strains in 3-pellet model after 204 days of irradiaiton.

Acknowledgments

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