BISON mesh generation script for analysis of cracked fuel pellets

Authors: Jussi Peltonen

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Summary
This report describes the meshing script developed to facilitate the meshing and modelling of fuel rods containing cracked pellets. The meshes were run with the BISON fuel performance code and its predictions were compared to simulations performed on the same boundary conditions as uncracked meshes. These differences, and the limitations of the meshed cracks are discussed. The built-in cracking models of BISON were tested and reviewed as well.

This work delves into the crack modelling in BISON, examining the possibilities and limitations of mesh-based solutions. The initial attempts at using the built-in cracking models yielded some mixed results, with some of the models working and others remaining obscure to the user.

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Written by Reviewed by Accepted by
Jussi Peltonen, Janne Heikinheimo, Ville Tulkki, Research Scientist Research Scientist Research Team Leader

VTT’s contact address
VTT Technical Research Centre of Finland, P.O. Box 1000, FI-02044 VTT, FINLAND

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1. Introduction

Modelling of cracking and fragmentation of the pellet is important in determining the consequences of a loss-of-coolant accident (LOCA), as more fragmented fuel will be more easily released from within the fuel cladding. Furthermore, fuel cracking is strongly related to FGR as cracks within the fuel can immediately release the fission gas trapped at grain boundaries or within grains. These types of phenomena are often modelled via relocation models and other mathematical formulations that estimate the impact of cracking without considering the cracks as part of the mesh geometry.

PORA project combines SAFIR, KYT and NKS funding to study the pellet cracking via multiscale analysis. The coupling from the mesoscale to macroscale is being developed currently, for example, within the MOOSE (Multiphysics Object-Oriented Simulation Environment) framework between the MARMOT and BISON code packages [1], the latter of which is used in this work to study the macroscopic cracking behaviour. In order to fully utilize the results from mesoscale simulations, fuel behavior analysis at the engineering scale must be performed with traditional fuel performance codes due to high computational cost of more accurate models.

The BISON fuel performance code [2] is being developed at the Idaho National Laboratory (INL) in the USA. The BISON code has been initially taken into use at VTT by Arkoma [3], and was previously used by Loukusa [4] to study the impact of missing pellet surface defects on the cladding stress. The work performed in this report was done with a version in the devel branch (bison-devel-2f8330f67efcda7da04f6890657a92cd0a949e26) in the BISON git repository.

![Figure 1. BISON simulation with a cracked pellet mesh.](image.png)

The aim of this work is to create a meshing script for cracked/deformed pellet geometries, and to study how this type of meshing impacts the fission gas release, temperature and stress field predictions of BISON, such as the one pictured in fig. 1. Additionally, the built-in cracking models of BISON were investigated and tested, to facilitate their application in the future. Lastly, the research topic offered a valuable opportunity for the writer to familiarize himself with the BISON code. This knowledge should be valuable in the future, since BISON is the only fuel performance code at VTT capable of 3D calculations.
2. Mesh generation process

BISON fuel performance code requires an input file (.i) and an exodus mesh file (.e). The former defines the simulation setup, models for pellet and clad thermomechanics, boundary conditions and other necessary input information. The latter contains the meshed geometry of the fuel rod, containing the pellet and rod geometries as separate blocks. Furthermore, the exodus mesh file defines the sidesets (i.e. the surfaces of pellet and cladding which interact via mechanical contact).

These exodus files are produced using a meshing tool, such as Trelis, which uses an user input to define the 2D- and 3D-geometries of the cladding and pellet. For example, a simple 3D-model of cladding is defined by five rectangles, which are volume swept to create a cladding tube consisting of five volume elements. After this, the meshing interval is defined for the boundaries of each volume. Trelis uses this information to generate a mesh of desired density. This is illustrated in fig. 2 below. The degree of volume sweep can be either 90 degrees to create a computationally lighter quarter model of the cladding, or 180/360 degrees for a more complete model.

Figure 2. The stages of generating a meshed 3D quarter model of rodlet clad.
A meshed pellet model can be produced in a similar way. For a non-cracked pellet a circle is defined as the initial surface, which can be volume swept perpendicularly to create a cylindrical pellet. By defining the intervals on the boundaries of the cylinder, a pellet mesh can be produced and exported to the inside volume of a meshed clad. However, for a cracked pellet the first step takes considerably more effort.

Since a cracked pellet has an irregular shape, its initial cross section needs to be defined via individual vertices. These are 0D objects that are linked via lines and arched curves to define the boundaries of the pellet cross section. Once this is finished, the cross section can be volume swept perpendicularly and meshed to produce an axially symmetric cracked pellet mesh. This process is visualized in the fig. 3 below. In order to facilitate the process of BISON mesh generation for the purpose of cracked pellet research, a new script was designed.

The meshing script uses template files to produce a journal file (.jou) that contains all the necessary Trelis syntax to produce either 2D- or 3D-model of a fuel rod geometry with cracked pellets. The cracks can be defined by user in two different ways, depending on whether simple radial cracks or more complex cracks are required. All the models produced by the script are axially symmetric. Axially non-symmetric geometries were tested in the beginning of this research, but due to their vastly higher computational complexity and the limitations BISON presented modelling these, they were omitted from this study. The easiest way to produce these non-symmetric meshes was to modify pre-existing journal files of 3D geometries by subtracting properly positioned prisms from the pellet volume.

Figure 3. The stages of generating a meshed 3D quarter model of radially cracked pellet.
3. Meshing script

Meshing script uses a template file in Trelis journal file format (.jou) to generate a modified journal file. By running the modified journal file in Trelis (Tools -> Play Journal File), Trelis generates a meshed pellet geometry, which can be saved as an exodus file (.e) from File -> Export. This exodus file must be referred to from the bison input file (.i) to use it as the input mesh.

The meshing script consists of an input file, and a few functions. The physical dimensions of the pellet and the meshing density intervals are defined in the input file structure Pellet:

```python
pellet = Pellet()
pellet.pellet_outer_radius = 0.004 # in units m
pellet.pellet_height = 0.01 # in units m
pellet.pellet_circumferential_total_interval = 12
pellet.pellet_radial_interval = 5
pellet.pellet_axial_interval = 5
```

where `pellet_outer_radius` is the pellet outer surface radius in units (m), `pellet_height` is the pellet height in units (m), `pellet_circumferential_total_interval` is the mesh interval for the whole pellet outer surface, `pellet_radial_interval` is the mesh interval for pellet x- and y-axis boundaries, `pellet_axial_interval` is the mesh interval for pellet z-axis boundaries (used in 3D meshing).

The structure Rod defines the physical dimensions of the cladding and the rod, as well as the relevant meshing intervals.

```python
rod = Rod()
rod.clad_wall_thickness = 0.00056
rod.clad_inner_radius = 0.00418
rod.rod_bottom_thickness = 0.00224
rod.rod_top_thickness = 0.00224
rod.active_rod_length = 0.42696
rod.clad_circumferential_interval = 36
rod.clad_radial_interval = 10
```

where `clad_wall_thickness` is the cladding wall thickness in units (m), `clad_inner_radius` is the cladding inner radius in units (m), `rod_bottom_thickness` is the thickness of the cladding layer under the pellet stack (m), `rod_top_thickness` is the thickness of the cladding layer on top of the pellet stack (m), `active_rod_length` is the length of the active part of the rod (m), `clad_circumferential_interval` is the mesh interval for the clad outer surface, `clad_radial_interval` is the mesh interval for the clad x- and y-axis boundaries,
The structure `Options` defines the journal file template and output filename used for the generation of a Trelis journal file.

```
Options.template = 
    "C:/data/PORA/2D_plane_strain_rod_cracked/3D_quarter_rodlet_template"
Options.outputfile = "3D_quarter_rodlet.jou"
```

The `template` string defines the template file in use, while `outputfile` defines the name of the modified journal file output.

Lastly, `Cracks` is an optional struct which is used as an input structure to the optional function `generate_pellet_vertices(pellet, Cracks)` to produce a simple set of vertices that form radial cracks.

```
Cracks.number = 3
Cracks.angle = [pi/6, pi/4, pi/3]
Cracks.length = [0.5, 0.6, 0.3] # relative length to radius < 1
Cracks.width = [pi/300, pi/200, pi/180] # angular width of the crack on the pellet surface
```

Here `number` states the desired number of cracks, `angle` defines the polar coordinates in which the cracks are located, `length` defines the lengths of the cracks relative to the radius of the pellet and `width` defines the angular widths of the cracks. The values of the example on the above result in a journal file that generates the geometry of fig. 4 in Trelis.

![Figure 4. Three radial cracks introduced to a 2D pellet geometry.](image)

Figure 5 demonstrates how the pellet geometry is defined in the edited journal file. The journal file lists the vertices of the cladding and pellet, defines the boundary curves of the cladding and pellet surfaces with them, and creates a mesh for the defined surfaces. After this the blocks (pellet and clad) and sidesets are defined, which are used to set the boundary conditions of the BISON simulation.
Figure 5. Vertices visualized in the geometry of fig. 4.

The vertices have indices progressing from 1 to $N_{\text{vertex}}$ counterclockwise, with $N_{\text{vertex}}$ being determined from the cracks introduced. The vertex 1 is always set at the (0,0) x-y coordinates, whereas the subsequent vertices define the pellet outer surface piecewise. The vertices thus each have three coordinates assigned to them, as well as a string value of either ‘edge’ or ‘inner’. These strings values define whether the vertex is located on the outer radius of the pellet, or inside a crack.

As seen in fig. 6, the vertices 1, 4, 7 and 10 have the identifier ‘inner’ attached to them, whereas the other vertices have the identifier ‘edge’. This information is used to define whether the outer surface boundary between two individual vertices is in shape of an arc centered around the (0,0) coordinate (such as between vertices 2 & 3), or in shape of a straight line (such as between vertices 3 & 4). Essentially, two vertices are connected by an arc if both vertices have the identifier ‘edge’. If either of the vertices has the identifier ‘inner’, the vertices will be connected by a straight line.

Figure 6. The pellet vertex data of fig. 2 geometry in form \{x,y,z,index,’edge’/’inner’\}
Alternatively, the geometry of the cracked pellet can be defined by listing the vertices of the pellet outer surface. This is necessary if circumferential cracks, or cracks and defects of other shapes need to be introduced to the geometry. An example is presented in fig. 7. In this case, the list of pellet vertices was written as such:

```plaintext
pellet_vertices = [[0, 0, 0, 1, 'inner'], [pellet.pellet_outer_radius, 0, 0, 2, 'edge'], [0.0029, 0.00280, 0, 3, 'edge'], [0.0025, 0.0024, 0, 4, 'inner'], [0.0025, 0.0018, 0, 5, 'inner'], [0.0020, 0.0013, 0, 6, 'inner'], [0.0019, 0.0010, 0, 7, 'inner'], [0.0018, 0.0014, 0, 8, 'inner'], [0.0023, 0.0018, 0, 9, 'inner'], [0.0023, 0.0024, 0, 10, 'inner'], [0.00285, 0.00285, 0, 11, 'edge']]
```

Either `generate_3D_quarter_mesh(pellet, rod, Options, pellet_vertices)` or `generate_2D_quarter_mesh(pellet, rod, Options, pellet_vertices)` is called at the end of the mesh generation script. These functions use all the information in the structs other than Cracks, and loop over the list of pellet vertices to create strings which contain the geometry specific Trelis syntax. By substituting these strings in the journal file template, a complete journal file for the mesh generation is created.

![Figure 7. Non-radial crack defined by listing the vertices.](image)
4. BISON simulations with cracked pellet meshes

BISON and MOOSE environment were installed on a virtual version of Ubuntu 16.04, with the size of the whole system being roughly 40GB. The disc image of the system can be found in the BISON-Trelis folder on X, as well as the meshing script files and the BISON inputs and outputs.

The BISON simulations were based on two example test scenarios, one being a 2D plane-train model, and the other being a 3D model of a rodlet with three pellets inside. Initially, the meshes of these test scenarios were replaced with modified ones that had a single crack/defect introduced in them. Since non-convergence has been an issue in the past BISON research at VTT, the complexity of the pellet geometry was increased gradually, to test out the limitations of BISON. Scenarios such as those with strong pellet-cladding contact are likely to require some adjustments in the mechanical model setup of the input file (.i), as well as further knowledge on how these features work in BISON.

BISON simulations were set to create two outputs: a file containing scalar value data (such as FGR) and an exodus output file which can be run with software such as Paraview to view the time-evolution of various field values. All of the test scenarios in this study were straightforward power ramps, and thus most of the relevant phenomena can be observed from mesh plots depicting the last time step of the simulation. The FGR values of the scalar output data, alongside the temperature and von Mises stress fields obtained from simulations run on three different cracked meshes will be analyzed next. Since none of the models had any pellet-cladding mechanical interaction, and the cladding is identical in all scenarios, the focus shall be on the pellet values only.

Four differently cracked meshes were chosen for these comparisons. The first one is un-cracked, the second has a small radial crack at an angle of 45 degrees, the third has three radial cracks of different positions and lengths, and the fourth has a large non-radial crack. All of these simulations converged at each set timestep both in 2D and 3D rods, with the 2D model simulation finishing in about 20 minutes and the 3D rodlet model taking longer than 3 hours to finish. The result comparison, only the 3D simulations are now compared due to higher intricacy.
4.1 Fuel temperature at end-of-simulation

Fuel temperature for a non-cracked pellet peaks at roughly 1600K in the center of the pellet, and decreases to around 850K on the outer surface of the pellet. By introducing a crack to the mesh, these temperatures decrease due to improved heat transfer via gas medium. As seen by comparing figs. 8 and 10, a drop of 15K centerline temperature and 30K outer surface temperature is observed.

Figure 8. Fuel temperature at end-of-simulation for an uncracked pellet.

Figure 9. Fuel temperature at end-of-simulation for a pellet containing a small radial crack.
Furthermore, the shape of the crack can cause uneven distribution of fuel temperature in the pellet for two mesh elements of equal radial distance from the center. The nonradial crack of fig. 11 has noticeably higher temperatures on the top side of crack than on the bottom side, possibly due to how the heat flow is modelled in BISON.

*Figure 10. Fuel temperature at end-of-simulation for a pellet containing three radial cracks.*

*Figure 11. Fuel temperature at end-of-simulation for a pellet containing a large non-radial crack.*
4.2 Von Mises stress at end-of-simulation

Von Mises stress $\sigma_V$ is a useful measure for evaluating whether a material yields under a multi-axial loading. It is calculated based on the components of the stress tensor as:

$$\sigma_V = \sqrt{\left(\sigma_x - \sigma_y\right)^2 + \left(\sigma_y - \sigma_z\right)^2 + \left(\sigma_z - \sigma_x\right)^2}$$ \hspace{1cm} (4.1)

where $\sigma_i$ are the stress components in a 3D space. The impact of the cracks was investigated by studying the stress field evolution in the pellet mesh for the simulations that converged. Von Mises stresses of the pellet were compared between meshes with varying cracks. The stress in uncracked pellet 12 increases steadily as the radial distance from the centre of the pellet increases, similar to the pellet with a small crack in fig. 13. For the pellets of figs 14 and 15 the cracks propagate deeper into the pellet and consequently the stresses on the outer parts of the pellet are lower than in the center. For all cracked pellets, the stresses generally peak in the mesh elements at the bottom of the crack.

Figure 12. Von mises stress at end-of-simulation for an uncracked pellet.

Figure 13. Von mises stress at end-of-simulation for a pellet containing a small radial crack.
Figure 14. Von mises stress at end-of-simulation for a pellet containing three radial crack.

Figure 15. Von mises stress at end-of-simulation for a pellet containing a large non-radial crack.
4.3 Fission gas release at end-of-simulation

The fission gas release of cracked and uncracked pellets was also studied. The simulations were performed using the Simple Integrated Fission Gas Release and Swelling (Sifgrs) model [5]. The model follows the intrinsic pattern of modern day FGR models calculating the fission gas accumulation to the grain boundaries, resolution and other in-material behaviour. These stages of FGR are heavily dependent on the fuel temperature, which in the BISON simulations of this study has been higher for less cracked pellets.

However, another mesh dependent contribution to FGR comes from the athermal gas release portion of FGR. At low temperatures especially, only the gas formed at the external surface of the solid is capable of escape, independent of the material temperature. The athermal contribution to fission gas release originates from the surface-fission release mechanisms caused by high kinetic energy fissions fragments in the outer layer (10 \( \mu \text{m} \) from the surface) of the fuel volume. The rate of fission gas release per unit fuel volume due to surface-level recoil and knock-out, \( R_a \) is calculated as:

\[
R_a = \frac{yF}{4V} \left( S_{g\mu_f} + 2S_{t\mu_{U\text{U}}} \right) \tag{4.2}
\]

where

- \( y \) = Fractional yield of fission gas atoms
- \( F \) = Fission rate density \( (m^{-3}s^{-1}) \)
- \( V \) = Volume of fuel \( (m^3) \)
- \( S_g \) = Geometrical surface area of fuel \( (m^2) \)
- \( S_t \) = Total surface area of fuel including computationally cracked surface \( (m^2) \)
- \( \mu_f \) = Fission fragment range in fuel \( (m) \)
- \( \mu_{U\text{U}} \) = Range of higher order uranium knock-on in UO\(_2\) \( (m) \)

Defects and cracks in the pellet mesh increase the geometrical and total surface area of the fuel. BISON also estimates the impact of non-meshed material cracks to the total surface area by assuming these cracks to propagate radially through the brittle outer area of the pellet at below 1200 \( \text{C} \) temperature. The number of these estimated cracks increases linearly with fuel linear power. The meshed cracks should increase the athermal gas release and this effect was studied by running BISON simulations of a 3D rodlet with a varying amount of cracks.

Regardless, the BISON calculations indicate lower FGR for pellets with meshed cracks. The general decrease in fuel temperature lowers the fission gas release significantly more than the theoretical increase in athermal release increases. The simulation of non-cracked pellet yielded \( 8.325 \times 10^{-6} \% \) FGR, the mesh with a tiny crack yielded \( 8.291 \times 10^{-6} \% \) FGR, the mesh with three cracks yielded \( 7.536 \times 10^{-6} \% \) FGR and the mesh with a large complex crack yielded \( 7.515 \times 10^{-6} \% \).

As it stands, merely introducing crack-shaped deformities in the BISON pellet mesh does not increase the fission gas release. Grain-face separation (micro-cracking) which entails the gas depletion of the impacted grain faces is a phenomenon in fuel temperature transients, during which bursts of fission gas release occur. BISON includes a model that calculates the micro-cracking process as a purely temperature-dependent behaviour.
5. Cracking models in BISON

5.1 Relocation model

As an alternative way to account the cracking in fuel without mesh-based solutions, the fuel relocation model in BISON can be used to apply a radial strain to the fuel pellet, accounting the impact of the free surfaces of the cracks that effectively increase pellet diameter [5]. Relocation strain is defined in the ESCORE relocation model as a function of power, as-fabricated pellet diameter and gap thickness, and burnup:

\[
\left( \frac{\Delta D}{D_0} \right)_{REL} = 0.80Q \left( \frac{G_0}{D_0} \right) (0.005Bu^{0.3} - 0.20D_0 + 0.3)
\]  

(5.1)

where

\[
\left( \frac{\Delta D}{D_0} \right)_{REL} = \text{Diametral relocation strain} \]
\[
D_0 = \text{As-fabricated cold pellet diameter (in)} \]
\[
q' = \text{Pellet average linear heat (kW/ft)} 
\]
\[
Q = \begin{cases} 
0 & \text{for } q' \leq q_1 \\
(q' - 6)^{1/3} & \text{for } q_1 < q' \leq q_2 \\
(q' - 10)/2 & \text{for } q' > q_2 
\end{cases}
\]
\[
G_0 = \text{As-fabricated cold pellet-cladding gap diameter (in)} 
\]
\[
Bu = \text{Pellet average burnup (MWd/MTU)} 
\]
\[
q_1 = 6 \text{ kW/ft} 
\]
\[
q_2 = 14 \text{ kW/ft} 
\]

Relocation strain is applied incrementally between timesteps and its growth is stopped at a set burnup value. The application range of the model is between 8 and 22 kW/ft of linear heat and between 0 and 11500 MWd/MTU of burnup. A modified version of the ESCORE model considers the initiation of relocation to occur in linear heats lower than 6 kW/ft, and is thus suitable for scenarios with low linear heat:

\[
\left( \frac{\Delta D}{D_0} \right)_{REL} = q(0.8)(2) \left( \frac{G_0}{D_0} \right) (0.005Bu^{0.3} - 0.20D_0 + 0.3)/q_2
\]  

(5.2)

GAPCON relocation model is also available in BISON, which uses the following formula:

\[
u^{rel} = (42b/(1 + b) + 0.274q' + 3)G_0/100
\]  

(5.3)

where \(u^{rel}\) is the displacement caused by relocation and \(b = e^{-4+Bu^{0.25}}\). The relocation model was used in all of the simulations performed in this study, with the setup parameters of the original 3D rodlet and 2D plane strain models. Further testing of relocation model was left out of this work.
5.2 Smeared cracking

In ceramic fuel such as UO$_2$, the temperature gradient can induce cracking in the fuel due to the accompanied stress. The cracks reduce the stress in the fuel and increase the effective fuel volume by decreasing the gap size. A smeared cracking model in BISON can be activated to account for this cracking by adjusting the elastic constants at material points. While active, principal stresses are compared to a critical stress. If the material stress exceeds the critical stress, the material point is considered cracked in that direction, and the stress is reduced to zero. From that point on, the material point will have no strength unless the strain becomes compressive.

The orientation of the principal coordinate system is determined from the eigenvectors of the elastic strain tensor. However, once a crack direction is determined, that direction remains fixed and further cracks are considered in directions perpendicular to the original crack direction. A scalar value, $c_i$, is stored for each possible crack direction in a mesh element. A value of 1 indicates the absence of a crack for that direction, whereas lower values indicate the presence of a crack.

The smeared cracking model was tested with a few 2D and 3D geometries, of which a 2D model using the complex crack geometry of fig. 7 calculated some smeared cracking. The pre-existing crack in the mesh resulted in a sufficiently peaked pellet stress in the z-direction to exceed the threshold cracking stress of 1.3e8 Pa. By comparing figs 16 and 17, one can see that crack flag values below 1 have been assigned to the mesh elements which had the higher z-directional stress. 3D simulations generally failed to converge after enough cracking had occurred in them, as seen in a simulation run of fig. 18, during which a single fuel pellet in rodlet was examined. The simulations were performed as power ramps to linear heat of up to 25 kW/m.

![Figure 16. Smeared cracking in a pre-cracked geometry of fig. 7 at the end of simulation.](image)
Figure 17. Z-directional stresses in the geometry of fig. 7 at the end of simulation.

Figure 18. Smeared cracking for a single 3D pellet in a rodlet at the last timestep before divergence.
5.3 Isotropic cracking

Isotropic cracking model describes the cracked fuel in an isotropic mechanical framework. The model assumes that the cracking of the fuel occurs in the elastic regime, the crack spans the full fuel dimension in the considered direction, the description of the cracked material is only dependent on the number of cracks and the principal strain are conserved. Under these assumptions, the elastic constants are scaled based on the number of cracks and calculated stresses are scaled accordingly and isotropically. The model allows for multiple fuel cracking, and an empirical correlation for the number of cracks as function of the rod average linear heat rate is developed.

The pre-existing test scenario of isotropic cracking was found in the BISON test files. It models a single pellet with no clad in RZ-coordinates undergoing a power and pressure ramp. While the solution of the model converges and contains the field parameters for the number of cracks in the pellet, no cracking is calculated for the pellet during the power ramp. The input file of the model gives a general idea of the syntax required for activating the isotropic cracking model. However, importing this syntax to more realistic fuel rod models resulted mostly in non-converging solutions without yielding any fruitful results.
6. Summary and discussion

A meshing script was designed for the generation of 2D and 3D cracked pellet meshes. The script functions as intended for generating axisymmetric quarter models of fuel rod. Should axially non-symmetric pellet deformities, or stacked pellets in a rodlet require a meshing tool in future, the script can be further developed to suit these functions as well. Alternatively, the tool could be developed further by implementing a model which generates random cracks based on experimental data for the meshing, which could then be applied to more statistical modelling.

These meshes were run in BISON power ramp simulations alongside uncracked meshes to study the impact of cracks on the predictions of temperature, stress distribution and fission gas release. The cracked meshes yielded lower temperature predictions, and consequently the fission gas release predictions of these simulations were lower too. The stresses in the pellet were also generally lower for cracked pellets, and the cracks altered the stress distribution in the pellet considerably depending on the size and shape of the crack.

The built-in cracking models of BISON were investigated with syntax from the library of BISON test scenarios. Of these models, the smeared cracking model managed to predict some local cracking in the 2D and 3D simulations. The isotropic cracking model was tested with no success. The relation between pellet cracking and relocation model was briefly investigated. Depending on how the PORA project continues in the future, these models could be revisited to bridge the research interests of higher-fidelity crack modelling.
Bibliography


