Modelling explicit fracture of nuclear fuel pellets using peridynamics

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Abstract

Three dimensional models of explicit cracking of nuclear fuel pellets for a variety of power ratings have been explored with peridynamics, a non-local, mesh free, fracture mechanics method. These models were implemented in the explicitly integrated molecular dynamics code LAMMPS, which was modified to include thermal strains in solid bodies. The models of fuel fracture, during initial power transients, are shown to correlate with the mean number of cracks observed on the inner and outer edges of the pellet, by experimental post irradiation examination of fuel, for power ratings of 10 and 15 W g⁻¹ UO₂. The models of the pellet show the ability to predict expected features such as the mid-height pellet crack, the correct number of radial cracks and initiation and coalescence of radial cracks. This work presents a modelling alternative to empirical fracture data found in many fuel performance codes and requires just one parameter of fracture strain. Weibull distributions of crack numbers were fitted to both numerical and experimental data using maximum likelihood estimation so that statistical comparison could be made. The findings show P-values of less than 0.5% suggesting an excellent agreement between model and experimental distributions.

1.0 Introduction

1.1. Fuel crack modelling in fuel performance codes

Nuclear fuel modelling has been carried out for many decades in support of fuel management in many reactor systems. Recent work in the US using the BISON code now has many new capabilities of solver technology, high performance computing and multi-physics modelling [1]. PLEIADES [2] in France is also able to model pellet segments and missing pellet parts. Most of this modelling has centred on standard finite element methods (FEM) meaning the explicit introduction of cracks and defects is difficult and limited to approaches such as smeared crack models and cohesive zones where cracks paths are specified in advance.

There have been several previous attempts to incorporate pellet failure in fuel performance modelling. Many of these follow the approaches taken in LIFE-II [3] where pellet damage was represented by a modification of the pellet material properties (most commonly: the pellet's Young's modulus, Poisson's ratio and creep behaviour). Many of these models used empirical data from post irradiation examination (PIE) to obtain pellet crack densities. However, using PIE data limits the understanding of the cracks to the final cooled down, ex-situ and sectioned states meaning there is no guarantee this accurately represents the cracked pellet in reactor. This also does not show us when the cracks formed or which power transients caused them. Despite this PIE based models still produces accurate models for fuel under known operational conditions [4].

Attempts to remedy this have been made by Marchal [5] through the incorporation of smeared cracking models. While smeared crack models can capture some stress concentrations on surrounding components such as the cladding it lacks the accuracy of explicit crack modelling. Additionally strain localisations [6], in smeared crack models, can lead to finite but non-convergent pellet stresses. Smeared crack models were themselves predated by models which accommodate cracking and pellet fragment relocation as a pellet plastic strain [7]. These strains also reduced as

the pellet fragment cracks healed, which can occur when two hot fuel fragments are pressed together for a sufficient time at high temperature. While these models required fewer experimental parameters to gain a relatively accurate estimate of pellet radial displacements for pressurised water reactor fuel and good estimates of crack densities, they still lead to strain localisation problems and lack the ability to capture concentrated stresses imparted onto the cladding by pellet fragment cladding interactions.

To further enhance the ability to model pellet cracking, in a fuel performance context, there have been recent applications of the commercial code ABAQUS to model the explicit cracking of the pellet, along predetermined paths, through the use of cohesive zones [8]. While capable of modelling explicit fracture patterns, with an accurate stress state, and also capable of precise stress concentration studies on the cladding, these cohesive zone models lack the ability to capture crack branching or coalescence. What appear to be branches of radial pellet cracks are commonly observed towards the outer edges of pellets in PIE [9]. Additionally, and very recently, there has been an attempt to model early life pellet fracture using the discrete element method in 2D [10]. This study did not include a comparison with experimental data but showed, for the first time, that explicit crack models represented a potential way forward for fuel performance modelling. The crack prediction abilities of peridynamics, in 3D, will be applied in this paper and are shown to correlate very well with experimental data from PIE.

1.2 Non-local modelling

To date modelling of stresses in solid bodies has largely been dominated by the finite element method (FEM) or, more recently, the extended finite element method (XFEM). Modelling brittle solids or brittle solids on ductile substrates can be difficult using the FEM as incorporating cracks requires damage criteria for crack nucleation and crack branching, as well as a prior decision on how many branches are allowed to form [11]. Experimentally observed crack growth is often due to irregularities on a micro scale, far below that of the continuum model so predetermining branching criteria severely limits the use of FEM for realistic modelling of crack growth.

Thus far XFEM has produced some of the best results for crack growth in FEM as it has less mesh dependence as crack paths can pass through elements instead of being limited to element boundaries. However, XFEM crack growth speeds do not match observed experimental data without significant scaling of the fracture energies and branching angles tend to be smaller than experimental results [12]. Other FEM methods for crack growth modelling include the non-local FEM. This uses non-local damage to simulate crack growth but does not include a non-local evaluation of the stress state. The non-local approach was traditionally applied to suppress the strain and the damage localization found in continuum damage mechanics, through the application of a non-local damage theory [13-15]. Within the non-local framework, the evolution of inelastic strain and/or damage is governed not only by the state/solution variables at a particular point but also by the state/solution at neighbouring points. For these non-local continuum damage approaches the stress is still treated locally, only creep and damage are non-local, which makes strain localization problems possible at the tips of cracks in brittle materials [16].

The difficulties with FEM, in modelling defects in brittle solids, occur because the spatial derivatives necessary to calculate the deformed state cannot be evaluated at the discontinuities present in a damaged material. This occurs because of the use of classical partial differential equations, which leads to singularities at crack surfaces and crack tips. To circumvent this problem, peridynamics modelling, as proposed by Silling [17], relies on an integral formulation of constitutive models and so does not include spatial derivatives. Therefore, the peridynamic description is applicable throughout the solid, even across singularities such as cracks and voids. Peridynamics is related to other non-local theories, for example the ones developed by Eringen [18-19], Kröner [20] and Edelen [21-23].

Peridynamics has great potential for application to many difficult problems in the nuclear industry. Previous work has shown that it can be applied to bonded dissimilar materials [24]. The study of a bonded bi-material strip of a brittle material, attached to a pseudo-ductile substrate, was the first step towards a set of tools to describe and predict the formation of slivers of fuel, bonded to cladding, as seen in advanced gas-cooled reactor (AGR) fuel PIE studies.

This paper applies the bond-based peridynamics method to issues related to fuel pellet fracture. Statistical information from over 170 PIE studies of crack patterns of AGR fuel were compared to a similar number of peridynamics models. This paper describes a model that is able to reproduce fracture patterns created by the first heat-up of fuel pellets. The model's predictions are then compared to Central Electricity Generating Board (CEGB) studies [9] of the same uniform heat-up procedure to full power heat-ups of ratings of 10, 15 and 20 W g⁻¹.¹ It is shown that the branched radial cracks observed in PIE are not formed by the growth and branching of one crack but are actually independently nucleated inner and outer surface radial cracks that coalesce.

2.0 Method

2.1 LAMMPS implementation

This study used the peridynamics implementation available in the molecular dynamics code LAMMPS [25]. This was due to the ease by which a system with hundreds of thousands of material points could be modelled. However, it could equally well be implemented in a FE code such as ABAQUS [24,26]. The modification to LAMMPS came in the form of a modified pair potential describing the bond-based form of peridynamics. Tabulated data from a previous FE model of AGR fuel [4] was used to produce a time and space dependent modification of the forces between two points to represent the addition of thermal strain. The fuel pellet model was subjected to a uniform temperature change per time-step as shown in Fig. 1 and the calculated thermal strain of the bonds were used to load the peridynamic model. As the temperature changes are taken from pre-computed thermal profiles, from [4], heat flow was not implemented in the constitutive equations. Heat flow, in peridynamics, is a focus of on-going and future work.

Detailed methods on the implementation of peridynamics are given elsewhere [27-28]. Here we describe only the most necessary aspects of the modelling procedure. In this work a micro-elastic material was used, in which the pairwise interaction force varies as a linear function of the bond stretch. Bond stretch is identical to the one-dimensional definition of strain. The bond at equilibrium has a stretch of zero and a stretch of one at twice the original length. An advantage to the peridynamics description of material is the possibility of bonds breaking when stretched beyond a given limit. This allows for the evolution of damage within a material to be observed without producing a stress singularity. When a bond fails it remains failed for the remainder of the simulation. Peridynamics is very well suited to investigating crack growth and damage problems, especially under thermal loading as it does not require a pre-crack. Instead, cracks can nucleate naturally anywhere when a simple fracture criterion is met [29]. This fracture strain (s_0) is easily verified in studies of brittle materials as it can be checked with tensile tests. It can also be directly compared with experimental fracture strains.

Fracture and damage is controlled by a history function μ (defined between 0 for zero damage and 1 for a failed bond), which controls the bond failure when the stretch exceeds a critical stretch value, s_0 . A zeroth order failure behaviour was used where the bond strength is reduced to zero,

¹ All units of W g⁻¹ relate to mass of UO₂. 1 W g⁻¹ is equal to 1.069×10⁷ W m⁻³. 7.25 mm radius fuel at 11 W/g is equivalent to 16.5 kW m⁻¹ linear power.

with no further strain, when the critical value s_0 is reached. Considering all the bonds connected to a single point $\mathbf{x}$, damage can be defined as,

$$\Psi(\mathbf{x}, t) = 1 - \frac{\int_{\delta} \mu(t, \boldsymbol{\eta}, \boldsymbol{\xi}) dV_{\mathbf{x}'}}{\int_{\delta} dV_{\mathbf{x}'}} \quad (1)$$

where $\Psi(\mathbf{x}, t)$ is a scalar value of damage at each material point found from the summation of all the bond failures within a volume, V , defined by a horizon, δ , surrounding that material point, where $\Psi(\mathbf{x}, t) = 1$ defines undamaged material and this surrounding region defined by a horizon parameter is the source of non-locality. This is the same definition of damage found in traditional continuum mechanics [6]. In equation 1 we define $\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$ as the relative position of two points in the undeformed configuration and $\boldsymbol{\eta} = \mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t) = \mathbf{u}' - \mathbf{u}$ as the relative displacement of the two points at time $t \geq 0$. To form the discrete peridynamics model we use the equation of motion

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{F}_T^n = \mathbf{F}_s^n. \quad (2)$$

In the simplified form $\mathbf{M}$ is the lumped mass matrix; $\ddot{\mathbf{u}}$ is the acceleration; $\mathbf{F}_s^n$ is the external force vector, and $\mathbf{F}_T^n$ is the internal force vector. Each diagonal term of $\mathbf{M}$ is ρV_i (where ρ and V_i is the density and volume of particle i respectively) and each component of $\mathbf{F}_s^n$ is $\mathbf{b}_i^n V_i$ ($\mathbf{b}_i^n$ is a body force vector), leaving $\mathbf{F}_T^n$ to represent the sum of all the forces from the trusses connected to material point i , which is defined as $\sum_p \mathbf{f}(\mathbf{u}_p^n - \mathbf{u}_i^n, \mathbf{x}_p - \mathbf{x}_i) V_i V_p$. Once the element matrix has been defined, what remains is to create a mesh for the peridynamics material. It is straightforward to generate peridynamic truss meshes, this entails: placing all the material points that define your material and connecting each material point to each other material point within a sphere with a radius equal to the user-defined distance (the horizon here denoted by δ). Such a mesh in 3D can produce millions of trusses, even for a moderately-sized problem.

$$\rho \ddot{\mathbf{y}}_i^n V_i = \sum_{p \in F_i} \left(\frac{\|\mathbf{y}_p - \mathbf{y}_i\| - \|\mathbf{x}_p - \mathbf{x}_i\|}{\|\mathbf{x}_p - \mathbf{x}_i\|} \right) \mu(t, \boldsymbol{\eta}, \boldsymbol{\xi}) \mathbf{v}(\mathbf{x}_p - \mathbf{x}_i) V_p \frac{\mathbf{y}_p - \mathbf{y}_i}{\|\mathbf{y}_p - \mathbf{y}_i\|} \times (s - \alpha\theta + \varepsilon) + \sum_{p \in F_i^s} \min \left(0, \frac{c_s}{\delta} (\|\mathbf{y}_p - \mathbf{y}_i\| - d_{pi}) \right) V_p \frac{\mathbf{y}_p - \mathbf{y}_i}{\|\mathbf{y}_p - \mathbf{y}_i\|} + \mathbf{b}_i^n \quad (3)$$

Equation 3 is an expanded application of Newton's second law, where $\mathbf{y}$ and $\mathbf{x}$ are the current and initial coordinate vectors respectively. It is expanded to cover material points, which interact with a finite radius force field. There is a force that increases linearly with stretch between each pair of material points within the given horizon. When the critical stretch of a bond is reached, however, the force goes to zero in order to represent bond breaking. The force on the bond then remains at zero for the remainder of the simulation and this history dependent damage state is held by μ . The second summation in equation 3 is representative of a short range contact force where c_s is a force constant to prevent material point overlap (as discussed in-depth in [27-28]).

In the modified equations of motion s is the current stretch of the bond, α in this context is the thermal expansion coefficient and ε is the viscous damping term. With a pre-calculated temperature field (from [4], and represented in Fig 1), the peridynamics model can undergo damage from thermal events similar to that in nuclear fuel during heat-up and cool-down.

The bond-based peridynamics method limits the number of free elastic constants and hence forces the Poisson's ratio to 1/4 in 3D or 1/3 in 2D and also fixes the shear modulus i.e. this only allows isotropic materials to be modelled. This limitation can be removed by the use of a state-based formulation.

It is not trivial to extract the stress tensor from peridynamic models as it is for FE models and hence many works do not present stresses. The hoop stresses were calculated by extraction of bond

strains associated to material points, the stress tensor was then constructed and transformed to cylindrical coordinates. The stresses were then projected back onto the material points and these were then used to produce hoop stress contour plots. The theory and detailed method for the stress calculation procedure is outlined in [30].

2.2 Model parameters

Table 1 presents the parameters used in these simulations. The bond-based material properties were typical of uranium dioxide. The Young's modulus was 194 GPa; Poisson's ratio was 0.25 and density of 10690 Kg m⁻³. The time-step chosen was 1.0×10^{-8} s, well below the von Neumann stability criterion. In this first model the properties were neither burn-up, nor temperature dependent, for simplicity. The fracture strain s_0 is specified as a single value for the bond fracture strain and the macroscopic material fracture strain this is because the definition of strain between peridynamics and continuum mechanics is the same. All bonds have the same fracture strain and heterogeneity that may induce nucleation of cracks would originate from numerical rounding in regions where the material is approaching the fracture strain. The geometry of the model was of an annular fuel pellet (geometry in Table 1), a material point spacing of 2.0×10^{-4} m and a horizon distance, δ , three times larger than that. Despite the use of an explicit time stepping method the loading step was quasi-static through the use of dynamic relaxation. This is a process by which the material is loaded and then allowed to relax fully before taking the next time increment. The size of each dynamic relaxation step is chosen as a length of time it takes for a sound wave to move through (farthest distance) the specimen and return.

The peridynamic models are more computationally expensive than traditional FEM. Models of just over 100,000 nodes require 3 seconds per explicit time step on a single 3.0 GHz Intel Xeon (2014) processor core. Parallel computation was not used despite LAMMPS ability to scale due to the modifications to the code involving thermal strain. These initial modifications were written with simplicity and not parallelism in mind and would require further development and testing to ensure correct parallel functionality. This leads to over one hour per dynamic relaxation step; however, parametric studies were conducted in parallel as each model was independent of all others.

Seventy simulations were made per power level and the statistics compared with PIE data from [9] provided by EDF Energy. Early simulations showed that under the smallest thermal strains all the bonds would break and all material points would escape the simulation domain at high velocity. This required the inclusion of a damping term, introduced through a spring like construct, connecting the material point to its starting position with a small stiffness (50 N m⁻¹). For small strains this emulates the viscous damping for thermal problems presented in equation 3. The inclusion of a damping term removes the continuous oscillation of the material points, which occurs when load was applied. When these oscillations reached an amplitude with sufficient energy to break bonds the material disintegrated. The imposed damping prevented pellet disintegration but combined with positional variation, in the 6th decimal place, also made the model non-deterministic. Therefore results for a particular thermal load may sample many possible different fracture states. This damping term is possibly physically representative of internal frictions (to sound wave propagation) within the materials such as structural deviations from perfect crystals (e.g. grains). The damping term was chosen, as the smallest possible damping coefficient required to prevent pellet disintegration. The minimum resistive force was found through trial and error.

Fig. 2 shows the mechanical deformation of a single pellet modelled by simple FEM, extracted from previous studies of AGR fuel [4,30]. The previous studies lack an accurate expression of pellet fracture. Fig. 2 has a region of high tension, greater than a typical UO₂ fracture stress (See Table 1), on the outer rim of the pellets and fracture was therefore expected to nucleate at these positions. Such models are applied in the current study as a precomputed thermal field on the pellet for

fracture studies. Additionally the noted models are used as for comparison for pellet thermal expansion without fracture with an alternate mechanical modelling approach.

Fig. 1 shows 10 quasi-static thermal strains applied to the pellet model during the thermal ramp for 10 W g⁻¹ final power rating. When the pellet is loaded the fracture strain is taken as the total bond strain minus thermal strain [31]. This ensures fracture is from the mechanical deformation of the pellet and not from pure thermal expansion, which is not physical.

2.3 PIE data

The experimental data used in this study were crack measurements in irradiated AGR fuel pellets from PIE metallographic cross-sections of the fuel. Within the report describing the dataset a FORTRAN program (FUELCRAK) was used to analyse radial crack distributions [24]. However, in this work only the number of cracks counted at each power rating were used. The datasets had the purpose of identifying stress concentration effects on the cladding, which leads to creep fatigue cracks. The stress concentration imposed onto the fuel cladding is strongly influenced by the number of regions in tension and compression formed by an impinging fuel pellet crack. The data set represents 177 specimens covering a period from September 1977 to May 1986. Of the specimens 135 were initial charge fuel and 37 were feed fuel and 5 were instrumented pin fuel (with thicker cladding and a thermocouple included). These pins were only taken to a low burn-up of 7000 MW d tU⁻¹. The initial charge and feed fuel pellets have an inner pellet surface radius of approximately 2.5 and 3 mm respectively and an outer radius of 7.25 mm. The data set notes there was no significant difference between the initial charge and feed fuel. The crack count data were given with respect to the maximum fuel power rating and a similar range of ratings was also selected for modelling. Because of the absence of exact loading history a slow increase in power of 30 minutes was assumed for the ramp to full power in the modelling.

2.4 Statistical analysis

This section describes the parameter estimation for the experimental data and simulations for an assumed Weibull distribution. Included is the process of data conditioning to produce a goodness of fit to determine whether peridynamics modelling of early life fuel heat-up is representative of the available PIE data.

In the case of brittle fracture a Weibull distribution is traditionally assumed. As the pellets contain no cracks, before first loading, there is no need for a minimum parameter suggesting a two parameter Weibull was appropriate. The 2-parameter Weibull probability density function is given in equation 4 where the random variable is x ; a is the scale parameter and b is the shape parameter. To determine the two parameters in equation 4 the method of maximum likelihood for the two parameter Weibull distribution is applied.

$$y = f(x|a, b) = ba^{-b}x^{b-1}e^{-\left(\frac{x}{a}\right)^b} \quad (4)$$

The maximum likelihood method can be used for parameter estimation when there are insufficient results to make an accurate goodness of fit [32]. Typically there should be at least 5 counts in each bin for a Pearson-Chi squared analysis to be probability distribution independent. However, the bins cannot be condensed to meet this condition as it would severely reduce the quality of the analysis. The maximum likelihood estimator for a 2-parameter Weibull was found using MATLAB

by taking the logarithm and differentiating with respect to the shape and scale factor and eliminating the scale factor to find

$$\frac{\sum_{i=1}^n x_i^b \ln(x_i)}{\sum_{i=1}^n x_i^b} - \frac{1}{b} - \frac{1}{n} \sum_{i=1}^n \ln(x_i) = 0 \quad (5)$$

Where n is the number of data points available, which may be solved for an estimate of b via procedures such as Newton-Raphson. Once b is known it can be introduced into the derivative of the log likelihood with respect to the scale parameter to find the estimate for a :

$$a = \frac{\sum_{i=1}^n x_i^b}{n} \quad (6)$$

To enhance the current dataset, due to the limits on the amount of data per bin described above, the estimated probability distribution were each subjected to a 1000 Monte Carlo samplings to produce a distribution appropriate for a goodness of fit test and still representative of the original data. A goodness of fit test may be applied to the conditioned data and the peridynamics models applicability was characterised by the use of a P-value of the fitted distributions, where a significance threshold of 5 % is usually considered a good fit and 1% an excellent fit.

3.0 Results and discussion

3.1 Initial heat-up studies and statistical analysis

As a verification of the peridynamics method the displacements from the peridynamic pellet, deforming under thermal strain, without fracture, at 5, 10, 15, 20 W g⁻¹ were compared to an equivalent ABAQUS FE model with identical material properties. The FE model was composed of a uniform mesh of 50 μm 3D reduced integration continuum elements (C3D8R). The results are presented in Table 2. These show excellent agreement for this verification test case with no differences observed greater than a fraction of a per cent. The difference between the FE and peridynamic models was expected to be quite small as the peridynamic bond strain was identical to macroscopic strain and the additional of thermal strain was the same for both models.

Fig. 3 shows the material points (mesh) of a typical fuel pellet fracture pattern, taken from a slice at quarter-axial pellet height. The colour scale depicts damage fraction (see equation 1). Fig. 4 then shows the resulting hoop stress at increasing time steps during heat-up. Fig. 4a shows the pellet just at the point where damage was nucleating on the inner surface but as yet none has formed on the outer surface. Fig. 4b-d then show snapshots of hoop stress as time increases during crack evolution. The individual cracks are difficult to see in both figures, due to mesh resolution, but schematic indicator lines have been placed on both Fig. 3 and Fig. 4 to show the crack locations. Difficulty in seeing explicit cracks, on the edges, is probably due to a coalescence of a great number of small cracks not distinguished by this mesh compounded by the peridynamics surface softening effect mentioned in [33]. The effect is usually only noticeable for a distance of the first horizon diameter in from the surface.

The radial centre of the pellet and the upper and lower ridges of the pellet experience a high density of damage due to the tensile stresses generated in these regions as shown in Fig. 2d (outer edge) and Fig. 4a (inner edge). Fig. 4a depicts the stress state in the hoop direction. Interestingly damage initiates on the inner surface first. This was due to the geometric distortions depicted in Fig. 2, which generates regions of initial tension on the inner surface skin. These can just be seen as yellow/green regions in Fig. 4a. However, shortly after this event the tension on the outer surface

nucleates a series of cracks there as well and the tensile fields at the crack tips can clearly be seen in Fig. 4b-c. At the same time the inner cracks very quickly arrest due to growth into regions of compressive hoop stress, again clearly visible in Fig. 4b-c. Finally, Fig. 4d shows how the outer radial cracks coalesce with the inner radial cracks. Perhaps this is the most interesting feature of the work as it shows that radial cracks do not grow from the inner surface and then branch, as might be inferred by studying their final state from PIE alone, but in fact grow as independent inner and outer cracks which coalesce presumably because the stress fields interact and draw them together. The reason they appear branched was a consequence of the fact there were always more outer cracks than inner ones to join up with.

Fig. 5 and Fig. 6 shows the distributions of cracks compared to the experimentally measured crack distribution from PIE, for 15 W g^{-1} peak power. Line plots were added for the predicted distributions found during maximum likelihood estimation. The parameters for which are given in Table 3. Fig. 5 shows a mean inner surface crack count of around 8 for both distributions and Fig. 6 an outer surface crack count of 10 (PIE) and 11 (model). Inner crack count has an almost identical predicted crack distribution while the outer cracking simulation data was similar but with small differences. The peridynamics models predict a slightly wider spread of outer crack number. Outer crack count is considered a very important parameter when studying PCI stress concentrations [5]. The simulations were repeated for 10 W g^{-1} and 20 W g^{-1} maximum power and the results are compared to the fit made to PIE data (Table 4). The 20 W g^{-1} entry shows the only discrepancy between the model and PIE for the outer crack count.

A detailed statistical analysis was carried out for the 15 W g^{-1} peak power rating. For this power the maximum likelihood method was used to fit Weibull distributions to both model results and PIE data. The fitted inner crack distributions were found to have a mean and variance that differ by less than 6 and 7 % respectively. Whilst the shape parameters differ by 4.6 % and the scale parameters differ by 6.2 %. For the outer crack distributions the mean and variance of the distribution differ by 1.3 % and 44 % respectively. The outer distribution fits give shape parameters that differ by 28 % and scale parameters that differ by only 0.7 %. From these comparisons we can see excellent agreement for inner crack count with only some differences for the outer crack count. Fig. 6 shows the peridynamics model distribution has its peak at the same position as the experimental data, however, it has a narrower distribution, which impacts the fit of the shape function. The fact that the means are very similar but the variance of the fits differs is plausibly due to the resolution of the model mesh, which may not capture all the small peripheral cracks on the pellet edges. However, the model results still serve as a lower bound for cracking at different power ratings.

Despite the differences in the Weibull distribution shape parameter the crack surface statistics, for 15 W g^{-1} maximum power, show a P-value of 0.05 %, for inner cracks, and a P-value of 0.47 % for outer cracks. These P-values show that both the experimental and peridynamic model show a very strong statistical correlation. The P-values give some confidence that modelling of fuel for early life, through peridynamics, is appropriate and reasonably accurate noting the fact the mesh resolution may need increasing to better represent the variance in outer crack distributions.

3.2 Mid-height crack formation

There are experimental data available from PIE studies of crack distributions, however this data does not provide a complete picture of how the fuel has fractured. It is known that the fuel cracks normal to the pin axis at mid-height [9,34]. It is expected in early life for the pellet to halve in height and later at higher burn-ups to axially divide several times further [8]. The study in [8] includes these pin normal cracks in the form of cohesive zones. In this case the user has had to predetermine the path of the crack and the simulation allows it to open when a fracture criterion is met. If peridynamics is a predictive method of fracture these mid-height normal cracks should appear after the initial heat up without requiring specific user input. Although not described in considerable

detail (primarily due to lack of PIE data), the peridynamic models did produce these axial mid-height cracks through bisection of the pellet through to the end of heat-up (see Figs. 7-9).

From analysis of the peridynamics fracture simulation all pellets fracture in a similar manner. Whilst the number of radial cracks changed the order of damage evolved was the same. Mid-height (pin normal) cracks initiated earlier than radial cracks. The time evolution of the crack fronts for both axial and radial cracks are shown in Fig. 8 (schematically) and Fig. 9 (actual simulation). Both radial and pin normal mid-height cracks stop growing at roughly the same time, in the simulation, despite the earlier initiation of mid-height cracks. This is because normal cracking was quickly suppressed between 15 and 45% full power by the compressive stress region within the pellet centre, which was later relaxed by the radial crack growth from the outer surfaces. This radial crack growth starts at about 30% power. The axial pellet halving happens very much like previous delamination peridynamics studies [35] except in this case it is not two bound materials that separate but one pellet fragment splitting into two. This shows peridynamics, even in the quasi-static approximation, can offer a great deal of insight into mechanisms of fuel pellet crack behaviour.

3.3 Implications for future fuel modelling

Looking to the future of fuel performance modelling, this work has shown the ability to produce accurate predictions in crack density, which can feed into other models of pellet expansion and relocation, which previously depended on PIE data. Although computationally expensive it was capable of reproducing findings from PIE of early fuel life. The notable limitations for whole life fuel fracture modelling are the absence of crack healing and plastic behaviour (inclusive of irradiation; thermal creep; fuel swelling and densification) of the pellet and variation in fracture stress with changing fuel material microstructure. It is notable that we chose to use a single value for the fracture strain and this gives a good representation of the PIE data but a more accurate description could incorporate a distribution of fracture strains. This addition might also lead to the broader crack number distributions observed in PIE compared to simulated fracture patterns. Additionally, the simplification of neglecting cross crack heat conduction is acceptable when radial cracking dominates, however later in life the fuel circumferential cracking will impact the thermal profile further modifying cracking behaviour. Ideally all these extra factors should be included in future models, however, it is noted that despite the presence of some of these missing features in the current work, on low-burn-up fuel ($7000 \text{ MW d tU}^{-1}$), the results were surprisingly good. This work, while initially targeted at studying stress concentration sources on AGR cladding would be useful in a light water reactor (LWR) fuel context. In LWR fuel a cracked pellet may also cause increased local clad strains and a pellet fracture model, such as the one presented here, may offer insights into pellet relocation and pellet-cladding interactions. Both of these features are thus far hard to model but have a big impact on fuel performance and lead to operational fuel restrictions in LWRs and in some cases fuel failures.

4.0 Conclusions

With respect to pellet fracture studies there is a great deal of similarity between the results found with the peridynamics simulations and those found from an analysis of low burn-up irradiated fuel.

1. The peridynamics predictions of crack counts were good for what appears to be the domain where the damaged volume was far less than un-damaged volume. The predictions of outer crack count were better for the 10 W g^{-1} than the 20 W g^{-1} power ratings because of this effect. The inner crack counts were more similar.

2. The models make very reasonable estimates of crack distributions and morphologies given that the models are not parameterised by the PIE data; the only experimental data used was the single fracture strain value of UO_2 .

3. All the results correlate well with peak power rating and this is something that needs to be tested as the fuel burn-up increases and operational history becomes more important.

4. Mid-height pin normal cracks were found to form and initiated before radial pellet cracks. The normal cracks were arrested on the inner surface by the strong compressive stresses there.

5. Radial pellet cracks nucleate first on the inner surface, quickly arrest, due to the compressive hoop stress, whilst outer surface cracks nucleate independently and grow. Eventually the inner and outer radial cracks coalesce in a manner that resembles the growth of a single branched crack.

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Figure Captions

Fig. 1: a) Typical temperature profile for early life fuel for (10 W g^{-1} power rating). b) The extracted thermal strains, which were used to load the pellet fracture model, these thermal strains have a radial dependency and changes in each dynamic relaxation step.

Fig. 2: Finite element evaluation analysis of AGR fuel pellet with no cracks allowed. a) Shows the radial component of displacement (m). b) Shows the internal pressure in the pellet (Pa). c) Shows the temperature profile that is driving the mechanical deformation (C). d) The maximum principal stress where the higher tension can be seen on the outer ridges of the pellet (Pa).

Fig. 3: r- θ slice showing damage fraction from pellet quarter-height showing radial and branching cracks for 15 W g^{-1} peak power rating. Black lines are added to show approximate location of cracks.

Fig. 4: r- θ slice showing hoop stress evolution from pellet quarter-height showing radial and branching cracks for 15 W g^{-1} peak power rating. Blue lines are drawn by hand to show approximate location of cracks. Black Lines show the edges of the pellet. a) $<5 \%$ power. (b-d) show the evolution and eventual coalescence of radial cracks at increasing times.

Fig. 5: Comparison of pellet fracture between PIE and peridynamics predictions on the number of inner surface cracks for 15 W g^{-1} peak power rating. The bars represent simulation and experimental data while lines represent Weibull fits from maximum likelihood estimates.

Fig. 6: Comparison of pellet fracture between PIE and peridynamics predictions on the number of outer surface cracks for 15 W g^{-1} peak power rating. The bars represent simulation and experimental data while lines represent Weibull fits from maximum likelihood estimates.

Fig. 7: View of outside of pellet quarter showing mid-height crack. Scale shows damage at 15% of full power for 10 W g^{-1} power rating.

Fig. 8: a) Sketch of half pellet. b) Schematic radial crack front evolution with time during ramp to full power). c) Crack front evolution with time for pin normal cracks shown on cut away of pellet at half height position. Scale shows damage and approximate powers of events are noted.

Fig. 9: Half height slice normal to pin axis, showing crack surface (green, red and yellow) and still bonded (blue). The increasing weight of the overlaid contours are approximations of the crack front position in order from light weight (early crack position at 35%, medium at 40% and heavy 50% full power). Scale shows damage at 50 % power for 10 W g⁻¹ power rating.

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Table 1: Peridynamics simulation parameters for fuel fracture simulations.

Parameter	Value
Inner pellet radius	0.003 m
Outer pellet radius	0.007 m
Dishing/chamfering	None
Pellet height	0.015 m
Lattice size	2×10^{-5} m
Max power	15 W g^{-1}
Time increment size	< 10 ns
Size of dynamic relaxation step	15.0×10^{-6} s
Density	10690 Kg m^{-3}
Thermal expansion (isotropic)	9.67×10^{-6}
Material point volume	$8.0 \times 10^{-12} \text{ m}^3$
Horizon size	3.1 times lattice spacing
UO ₂ Young's modulus	194 GPa [4]
UO ₂ fracture strain (s_0)	0.0007 [8]

Table 2: Comparison of displacements between a peridynamics pellet and a finite element pellet, both modelled without fracture.

	Finite Element Model			Peridynamics Model		
W g^{-1}	Inner Radius (m)	Outer Radius (m)	Mid-height Outer Radius (m)	Inner Radius (m)	Outer Radius (m)	Mid-height Outer Radius (m)
5	3.72E-05	4.21E-05	2.85E-05	3.71E-05	4.21E-05	2.85E-05
10	4.61E-05	4.86E-05	3.25E-05	4.60E-05	4.85E-05	3.25E-05
15	5.50E-05	5.51E-05	3.65E-05	5.50E-05	5.51E-05	3.65E-05
20	6.39E-05	6.18E-05	4.04E-05	6.39E-05	6.17E-05	4.04E-05

Table 3: Distribution fits for PIE and peridynamic models describing the inner and outer surface cracks for a peak power rating of 15 W g^{-1} .

	Inner Surface PIE Fit	Inner Surface Model Fit	Outer Surface PIE Fit	Outer Surface Model Fit
Distribution	Weibull	Weibull	Weibull	Weibull
Mean	7.09	7.55	9.54	9.66
Variance	3.32	3.52	8.16	4.63
Parameter (Std. Err.)				
<i>a</i>	7.78(0.14)	8.27(0.19)	10.57(0.19)	10.51 (0.19)
<i>b</i>	4.41(0.24)	4.58 (0.35)	3.72 (0.17)	5.16(0.38)

Table 4: Comparison of mean crack numbers between PIE and peridynamics for different full power ratings.

Peak Rating (W g ⁻¹)	Inner Surface PIE	Inner Surface Peridynamics	Outer Surface PIE	Outer Surface Peridynamics
10	6	6	7	7
15	8	8	11	11
20	8	8	11	15

a)

b)

a)

b)

c)

d)

a)

b)

c)