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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} UO_2. 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. 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 facture 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 et al. [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

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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. 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 Ref. [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.

[1] All units of W g^{-1} relate to mass of UO_2. 1 W g^{-1} is equal to 1.069 × 107 W m^{-3} 7.25 mm radius fuel at 11 W g^{-1} is equivalent to 16.5 kW m^{-1} linear power.