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Joint modeling of thermal creep and radiation damage interaction with gas permeability and release dynamics: The role of percolation

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HIGHLIGHTS

- Dynamical percolation leads to a time-dependent gas flux in a percolating pore system.
- The roles of various damage mechanisms can be assessed.
- We study the effect of microcrack healing on percolation and gas release.

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ABSTRACT

Nuclear fuel material is an example of a sintered, porous ceramic material. We formulate a two-dimensional model which couples three physical mechanisms in the material: (scalar) damage accumulation by thermal creep and radiation effects, porosity changes due to the damage, and the time-dependent diffusion of (radiation-induced) gases in the pore system thus created. The most important effect in the dynamics arises from the process where the pore system is swept through the percolation transition. The main conclusions that can be drawn concern the fractional gas release and its dependence on the three effects present in the damage dynamics: creep, radiation-induced bubble formation, and recovery due to bubble closure. In the main, the model reproduces the experimentally observed quick gas release phenomenon qualitatively.

1. Introduction

Joint or multiphysics modeling is becoming a necessity for the treatment and understanding of many physicochemical phenomena. One particular example of this kind of approach concerns the transport properties of porous media, of importance in applications from geophysics to materials science to biology [1–3]. A more focused case is that of the time-dependent permeability of materials, where the medium can be rocks – and the pores consist of fault or crack systems – or porous composites like ceramics, whose barrier and thermal insulation characteristics are often of interest. In geophysics, the joint evolution of damage and permeability is an important issue [4–9], and these days such issues appear in the context of dealing with carbon dioxide by storage [10].

Another materials science field where such questions are of importance is found in the nuclear industry. Fuel pellets making up the fuel rods are sintered together from micron-scale particles. During the life-time of the fuel, the irradiation and the mechanical loading will change the material properties [11]. Indeed, the burn-up of the fuel leads to the presence

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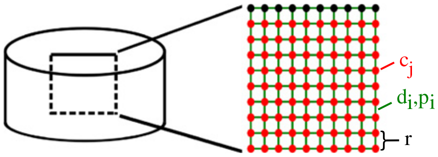

Fig. 1. Schematic of the simulation system: A rectangular cross-section is taken from a pellet. Gas nodes (red, gas concentrations c_j) are interconnected through bonds (green, damage d_i and porosity p_i). The gas nodes are set in a regular square lattice with a distance r between neighboring nodes. Fission gas is released through the top boundary, where the gas concentrations are set to zero (black nodes). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

of daughter gas concentrations in the fuel. Such gases are of importance not only since they are a diagnostic of the life-time history of the fuel, but since they change the thermal response of fuel rod setups in the case such gases are able to accumulate [12]. The most interesting phenomenon is that of "quick gas release" when the evolution of the pore network allows the accumulated gases to escape after a time threshold, related to the fundamental physical mechanisms, has been reached [13–15].

The release or, simply diffusion, of fission induced gases has thus received quite some attention in the nuclear materials engineering context. Studies of this problem are complicated by the multiphysics aspects. The material microstructure depends on the past (fuel burnup and temperature histories) and the presence of fission gases confined in bubbles. Since in the context of reactor operations thermal transients are of major importance so called "out-of-pile" experiments are the most frequent [16]. There, already radiated samples are tested under temperature rise protocols. Such studies however do not measure simultaneously sample mechanical properties and gas release. Ideas have been circulated from the modeling of pore systems from a percolation perspective [17]. The presence of a percolation threshold indicates that the pore system evolution or damage accumulation can be thought to be able to lead to the observed gas dynamics due to the rapid permeability changes in the proximity of the percolation threshold.

The purpose of this work is to combine the three issues: damage evolution due to the creation of cracks, the subsequent changes in system porosity, and the resulting gas dynamics. The study is done in a simplified form. As explained below, we resort to a two-dimensional simulation geometry instead of a 3D one. This simplification is not essential but is of very large help in reducing the numerical challenge of the computations. The damage mechanics modeling is done using the scalar damage accumulation laws. We include two crack growth mechanisms. The first is due to thermal creep fracture; the fuel pellets are in realistic conditions under constant thermal stresses at temperatures which do not vary much under time. Moreover, the formation of localized fission gas bubbles presents another, additive mechanism. The relative importance of these two is then one interesting question. The bubbles are also known to be able to be removed over time, that is there is a recovery mechanism that needs to be studied and could be of interest when the damage dynamics is not controlled mainly by creep. Behind the physics of the gas dynamics or release is the question of when and how the pore system reaches its percolation threshold.

For the joint modeling of gas dynamics we resort to a time-dependent simulation of gas dynamics in a system with a permeability or diffusion coefficient which varies both in time and space. The solution of the diffusion equation could be done with a discretization scale different from that of the damage mechanics, but we instead for simplicity resort to the same. The local diffusion properties are then found from a percolation-style description. The caveat of this approach is that it is known that the percolation threshold (in 2d or 3d) depends to a degree on the shape (e.g. spheres vs. narrow ellipsoids) of the objects that percolate; given the number of details in the multiphysics modeling here we do not think this is important (but see e.g. Ref. [18]).

The final model thus gives estimates of the time-dependent gas release under a number of assumptions of the dynamics (fracture, gas diffusion) and simplifications. It is tuned for the particular nuclear fuel application, but is also more generally a description of the gas barrier properties of porous media which accumulate creep damage. Below, in Section 2 we explain in detail the model developed. Section 3 contains an account of the various scenarios studied with an emphasis on the effects of the damage dynamics mechanisms taken to be present. Section 4 finishes the paper with conclusions and discussion.

2. Model

2.1. Damage

Our model combines the evolution of porosity caused by creep and radiation damage to gas diffusion, where the diffusion coefficient varies locally with porosity. A cross-section of the pellet is discretized into a 2D square lattice, with N_{gas} equidistant gas nodes connected to neighboring nodes via N_{bonds} bonds. This is taken to be slice of a 3D system, with the parameters chosen accordingly. A schematic of the simulation system is shown in Fig. 1. Gas diffuses between neighboring nodes with diffusion coefficients determined for each connecting bond according to its porosity.

The microstructural state of a fuel pellet is modeled as a 2D scalar network of discrete bonds, which are characterized by the amount of damage they have sustained due to creep fracture and radiation induced fission gas buildup. Damage [19] d is defined as the reduction of the Young's modulus E of a bond: $E \rightarrow E(1-d)$. We use here a scalar approach instead of dealing