Journal of Nuclear Materials 478 (2016) 322–332

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

Discrete element method study of fuel relocation and dispersal during loss-of-coolant accidents

K. Govers*, M. Verwerft

Institute for Nuclear Material Science, Belgian Nuclear Research Centre (SCK·CEN), Boeretang 200, B-2400 Mol, Belgium

HIGHLIGHTS

- We performed Discrete Element Methods simulation for fuel relocation and dispersal during LOCA transients.
- The approach provides a mechanistic description of these phenomena.
- The approach shows the ability of the technique to reproduce experimental observations.
- The packing fraction in the balloon is shown to stabilize at 50–60%.

ARTICLE INFO

Article history:
Received 14 March 2016
Received in revised form
18 May 2016
Accepted 20 May 2016
Available online 26 May 2016

ABSTRACT

The fuel fragmentation, relocation and dispersal (FFRD) during LOCA transients today retain the attention of the nuclear safety community. The fine fragmentation observed at high burnup may, indeed, affect the Emergency Core Cooling System performance: accumulation of fuel debris in the cladding ballooned zone leads to a redistribution of the temperature profile, while dispersal of debris might lead to coolant blockage or to debris circulation through the primary circuit. This work presents a contribution, by discrete element method, towards a mechanistic description of the various stages of FFRD. The fuel fragments are described as a set of interacting particles, behaving as a granular medium. The model shows qualitative and quantitative agreement with experimental observations, such as the packing efficiency in the balloon, which is shown to stabilize at about 55%. The model is then applied to study fuel dispersal, for which experimental parametric studies are both difficult and expensive.

1. Introduction

In order to bring a reactor to a safe state following to a Loss-of-Coolant Accident (LOCA), acceptance criteria have been defined for the design of the Emergency Core Cooling System, see e.g. the provisions of US NRC 10.CFR.50, §46 [1]. Similar considerations drive other national regulations [2]. According to US regulation, four main criteria directly address the behaviour of the fuel during the accident:

- A limit on cladding oxidation (17% Equivalent Cladding Reacted), to keep a sufficient ductility of the cladding to sustain quench and post-quench loads.
- A limit on the peak cladding temperature (1204 °C) to avoid entering into conditions propitious to runaway oxidation and to limit the oxygen uptake of the zirconium metal.
- A limit on the total amount of generated hydrogen: 1% of the total amount that would be generated if all of the cladding contained in the core was to react with water or steam, except for the material surrounding the plenum.
- A limit on the changes of the core geometry: "*Calculated changes in core geometry shall be such that the core remains amenable to cooling*".

Since their definition in 1973, these criteria were slightly adapted to reflect the changes in design, materials and operating conditions. The major changes are driven by the progressive increase of fuel discharge burnup, and are related to the accompanying issue of hydrogen uptake by the cladding as oxidation proceeds during irradiation [3,4]. It has also led to an industrial response in the form of the development of novel cladding alloys

* Corresponding author.
E-mail address: kgovers@sckcen.be (K. Govers).

http://dx.doi.org/10.1016/j.jnucmat.2016.05.031
0022-3115/

that show better performances with regard to oxidation and hydrogen uptake.

More recently, the attention of the safety community shifted from the cladding to the fuel itself: recent LOCA tests at the Halden reactor (IFA-650 series [5]) have shown the occurrence of severe fragmentation of the fuel into fine particles at high to very high burnup, accompanied for some of the tests by extensive relocation of the fuel stack into the balloon region, as well as by dispersal of fuel fragments through the burst opening. Similar observations were obtained from the US NRC out-of-pile tests performed at Studsvik [6].

Indeed, the smaller size of the fuel fragments at high burnup makes them more mobile, compared to low or medium burnup fuel: while at moderate burnup, up to 38 MWd/kg_{HM}, Siefken [7] reports loss of tightening of the fragments at cladding hoop strain larger than 17%, the threshold decreases to the range 2–5% at high to very high burnup in the Halden experiments [8–10]. Axial relocation of the fuel within the balloon will affect the temperature profile as well as the oxidation level of the cladding, with a potential impact on the design of the Emergency Core Cooling Systems (ECCS). A fraction of the fragments may also escape through the burst opening directly into the primary circuit; the impact of such debris particles, flowing through the primary circuit, on flow blockage, criticality or on the mechanical integrity of components (like the primary pumps) remains an open question.

The importance and safety significance of fuel relocation and dispersal during LOCA transients has been recognized worldwide [9–12]. Efforts are still on-going today through integral tests at Halden and Studsvik, while the physical mechanisms at play are also under investigations, for example within the NFIR program of EPRI [13,14]. Efforts are also undertaken in the field of modelling. While engineering models have been developed for fuel fragmentation [14] and pragmatic approaches followed for relocation and dispersal [8,15], a true mechanistic description of these phenomena is still at an early stage of development.

In this paper, we propose to complement the existing experimental investigations with an insight into the *dynamics* of relocation and dispersal. Computer simulations of granular material flow enable one to track the trajectory of the various fuel fragments during their free fall into the ballooned zone. Several approaches to the study of granular material flow exist according to the way the particles are described: as individual particles – discrete element methods, DEM – or as a continuous medium; or to the way the time-evolution algorithm proceeds – with constant timesteps or event-based discretization [16].

Although their use for nuclear applications is not new – e.g. pebble flow calculations in pebble-bed nuclear reactor [17], development of a scram system for liquid metal cooled reactors [18] –, the work of Martin [16] is, to the best of our knowledge, the only work based on granular material simulations that treats the relocation of fuel fragments into the balloon zone. His work focuses on the one hand on the flow instability and on the jamming phenomenon for a 2D system with circular particles and on the other hand to the coupling of this system to a description of the surrounding gas flow. The work makes use of non-smooth contact dynamics [19], which enables using larger timesteps than in conventional soft spheres DEM.

Still, a soft spheres DEM approach is considered here to address fuel relocation and dispersal. We are indeed convinced that some of the early limitations, such as the timestep length and the particle number issues, are overcome by today's computer capabilities and by the possibility to build rigid bodies with complex shapes.

In the DEM approach, the trajectory of each particle of the fuel column is calculated while all interactions between particles are accounted for. One can then obtain insight into the elementary mechanism by performing parametric studies on safety-relevant parameters related to relocation such as, for example, the cladding strain threshold from which relocation becomes important and the packing fraction of the fuel fragments in the balloon. One can also study the role of the fragment size distribution in the relocation process, or explore dispersal through the burst opening as a function of fragment size. Such investigations are reported in this manuscript. Section 2 describes the computational technique and the model developed to simulate a fuel rod experiencing fuel fragmentation as well as clad ballooning and burst. Section 3 presents the results of parametric studies of the relocation phenomenon. Dispersal is addressed in Section 4. The performance of our model is finally discussed in Section 5, and we conclude the manuscript with possible further developments.

2. Methodology

2.1. Computational technique

Granular matter is often distinguished from other states of matter as it sometimes behaves as a solid, a liquid or a gas, depending on the density and the velocity of the individual particles. It is therefore not surprising that several, distinct modelling techniques exist to treat granular systems [16]. Some of them, similar to fluid dynamics, describe the average behaviour of a large system thereby neglecting the behaviour of the separate particles. Other approaches pay much more attention to the individual behaviour of each particle: one speaks of discrete element methods or DEM. The latter methods are more limited in space (number of particles) and time.

In this work, discrete element methods are used. The material is discretized as a set of particles whose motions are computed, including the interactions between particles when collisions occur. Such a description of the particle interactions is, from the point of view of the algorithm, very close to atomistic simulations. Therefore, the implementation of a granular model on a platform that originally was developed to perform atomistic simulations is not surprising; for example, in view of the high flexibility of the code, this was implemented in the LAMMPS code [20], which is used here. The simplest particle shape is spherical and more complex shaped bodies can be described as rigid agglomerates of spheres.

While interactions between two granular particles are typically pairwise, some specificity has to be included that is usually not present in atomic-scale simulations: friction forces, which depend not only on the particle positions, but also on their velocities. The Hertz model is used in this work. It is based on elastic theory of deformation, so that the force $\boldsymbol{F}_{ij}$ between spherical particle i and j is not simply a linear function of the 'overlap' (like a spring) but depends on the overlap area, while also accounting for possible radius difference between two interacting particles [21,22]:

$$\boldsymbol{F}_{ij} = \sqrt{\delta}\cdot\sqrt{\frac{R_i R_j}{R_i+R_j}}\cdot\left\{\left(k_n\delta \;-\; m_{\text{eff}}\;\gamma_n\;v_n\right)\mathbf{e}_{ij} - \left(k_t\boldsymbol{\Delta s_t} + m_{\text{eff}}\;\gamma_t\;v_t\boldsymbol{e}_t\right)\right\} \tag{1}$$

where δ is the overlap distance of two particles; R_i (respectively R_j), the radius of particle i (resp. j) and m_{eff}, the effective mass of the binary system. Subscripts n and t stand for the normal and tangential components of the following parameters: k, the stiffness constant; γ, the viscoelastic damping constant and $\boldsymbol{v}$, the velocity vector. The unit vector $\boldsymbol{e}_{ij}$ follows the line passing through the centre of both spherical particles and $\boldsymbol{e}_t$ follows the tangential component of the velocity; $\boldsymbol{\Delta s_t}$ is the tangential displacement vector (not necessarily in the same plane formed by $\boldsymbol{e}_{ij}$ and $\boldsymbol{e}_t$) [21].