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PolyPole-1: An accurate numerical algorithm for intra-granular fission gas release

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HIGHLIGHTS

- A new numerical algorithm (PolyPole-1) for intra-granular fission gas release in time-varying conditions is developed.
- The concept combines the modal analytic solution for constant conditions and a polynomial correction.
- PolyPole-1 is extensively verified and compared to other state-of-the-art algorithms.
- PolyPole-1 exhibits a superior accuracy and a similar computational time relative to other algorithms.
- The PolyPole-1 algorithm can be implemented in any fuel performance code.

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ABSTRACT

The transport of fission gas from within the fuel grains to the grain boundaries (intra-granular fission gas release) is a fundamental controlling mechanism of fission gas release and gaseous swelling in nuclear fuel. Hence, accurate numerical solution of the corresponding mathematical problem needs to be included in fission gas behaviour models used in fuel performance codes. Under the assumption of equilibrium between trapping and resolution, the process can be described mathematically by a single diffusion equation for the gas atom concentration in a grain. In this paper, we propose a new numerical algorithm (PolyPole-1) to efficiently solve the fission gas diffusion equation in time-varying conditions. The PolyPole-1 algorithm is based on the analytic modal solution of the diffusion equation for constant conditions, combined with polynomial corrective terms that embody the information on the deviation from constant conditions. The new algorithm is verified by comparing the results to a finite difference solution over a large number of randomly generated operation histories. Furthermore, comparison to state-of-the-art algorithms used in fuel performance codes demonstrates that the accuracy of PolyPole-1 is superior to other algorithms, with similar computational effort. Finally, the concept of PolyPole-1 may be extended to the solution of the general problem of intra-granular fission gas diffusion during non-equilibrium trapping and resolution, which will be the subject of future work.

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1. Introduction

During irradiation of nuclear fuel in the reactor, various isotopes of the noble gases xenon and krypton are directly created inside the fuel grains by fission, but may also originate from decay processes. Fission gas atoms can diffuse to the grain boundaries where they precipitate into inter-granular bubbles contributing to fuel swelling. A fraction of the gas that reaches the grain boundaries can eventually be released to the fuel rod free volume through interlinkage of the inter-granular bubbles [1–6].

Hence, the first and basic step of fission gas release (FGR) and gaseous swelling is gas atom transport from within the grains to the grain boundaries (intra-granular fission gas release). It follows that modelling of this process is a fundamental component of any fission gas behaviour model in a fuel performance code. Fission gas transport to the grain boundaries occurs by thermal and irradiation-enhanced diffusion of single gas atoms, coupled with trapping in and irradiation-induced resolution from intra-granular

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bubbles. Diffusion of intra-granular bubbles becomes relevant at high temperatures, above ~1800 °C [2,7]. Thus, modelling intra-granular fission gas release calls for the treatment of different concomitant mechanisms, namely, diffusion coupled with trapping and resolution of gas atoms. Extensive literature deals with the evaluation of the parameters characterizing these mechanisms, both experimental and theoretical work (e.g., [2,3,8–16]). Rather, in this paper we deal with the numerical problem associated with the computational solution of the equations describing the process. Clearly, this problem has an enormous practical importance for fission gas behaviour calculations in fuel performance analysis.

Speight [17] proposed a simplified mathematical description of intra-granular fission gas release. He lumped the trapping and resolution rates into an effective diffusion coefficient, restating the mathematical problem as purely diffusive. Such simplification implies the assumption of equilibrium between trapping and resolution (quasi-stationary approach). To the best of our knowledge, the formulation of Speight is universally adopted for models employed in fuel performance codes (e.g., [18–22]). In addition, the assumption of spherical grain geometry [23] is applied. The solution of the diffusion equation for constant conditions is well known. Nevertheless, time-varying conditions are involved in realistic problems. Therefore, the solution for time-varying conditions is the issue of interest for applications in fuel performance analysis, which calls for the development of dedicated numerical algorithms. Given the very high number of calls of each local model (such as the fission gas behaviour model) in a fuel performance code during the analysis of a detailed fuel rod irradiation history, in addition to the requirement of suitable accuracy for the numerical solution, there is a requirement of low computational cost. Of course, the numerical solution of the diffusion equation in time-varying conditions may be obtained using a spatial discretization method such as a finite difference scheme. However, the associated high computational effort can make a space-discretization based solution impractical for application in fuel performance codes. Several alternative algorithms that provide approximate solutions at high speed of computation and can be used in fuel performance codes have been developed [24–32]. In this work, we propose a new numerical algorithm for the accurate and fast solution of the diffusion equation in time-varying conditions, which we call PolyPole-1.

The structure of the paper is as follows. In Section 2, we discuss the mathematical formulation of the intra-granular fission gas release problem. In Section 3, we provide an overview of existing numerical algorithms for the solution of the problem. In Section 4, we describe the concept of the PolyPole-1 algorithm and provide a theoretical comparison with other algorithms used in fuel performance codes. In Section 5, we verify the PolyPole-1 algorithm through an extensive numerical analysis. Also, we compare PolyPole-1 to other state-of-the-art algorithms in terms of accuracy and computational efficiency. Conclusions are drawn and suggestions for further development are outlined in Section 6.

2. Mathematical problem

The problem of gas atom diffusion during trapping and resolution can be stated mathematically with a system of partial differential equations

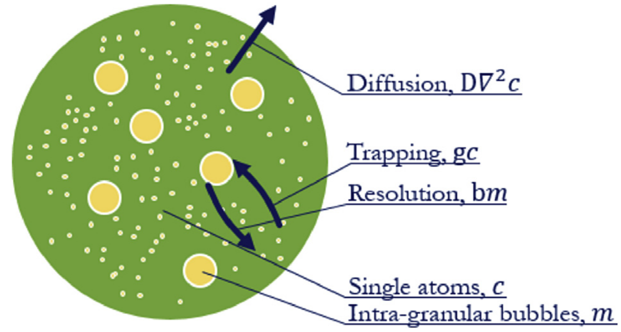

Fig. 1. Sketch representing the main mechanisms of intra-granular fission gas release.

$$\begin{cases} \dfrac{\partial c}{\partial t} = D\nabla^2 c - gc + bm + \beta \\ \dfrac{\partial m}{\partial t} = gc - bm \end{cases} \tag{1}$$

where c (at. m^{-3}) is the concentration of single gas atoms dissolved in the lattice, m (at. m^{-3}) is the concentration of gas atoms in intra-granular bubbles, D (m^2 s^{-1}) is the single gas atom diffusion coefficient, g (s^{-1}) is the trapping rate, b (s^{-1}) is the resolution rate, and β (at. m^{-3} s^{-1}) is the gas production term. Intra-granular bubbles are considered as immobile. The processes described by Eq. (1) are represented in Fig. 1.

Speight [17] solved Eq. (1) in spherical geometry, for constant conditions (i.e., constant D, g, b, β) and with zero initial conditions for c and m. He then simplified the analytic solution assuming that, for times of engineering interest, trapping and resolution are in equilibrium, i.e., $gc - bm = 0$ (quasi-stationary approach). This leads to simplification of Eq. (1) into a single diffusion equation for the total concentration of gas in the grain $c_t = c + m$ (at. m^{-3})

$$\frac{\partial c_t}{\partial t} = \beta + D_{eff}\nabla^2 c_t \tag{2}$$

Eq. (2) is formally identical to the diffusion equation previously derived by Booth [23] for the case of diffusion of single gas atoms in absence of bubbles. The effective diffusion coefficient in Eq. (2), D_{eff} (m^2 s^{-1}), accounts for the reduced diffusion rate of single gas atoms due to the trapping and resolution effects in presence of immobile intra-granular bubbles. Van Uffelen et al. [33] extended Speight's formulation for D_{eff} to account for the contribution of Brownian bubble motion while preserving the form of Eq. (2).

The analytic solution of Eq. (2) for constant conditions (constant β and D_{eff}) in spherical grain geometry is well known (e.g., [29]). For the purpose of modelling intra-granular fission gas release, we focus on the spatial average in the grain of the total gas concentration, $\bar{c}_t(t)$. A perfect sink boundary condition at the grain boundary, i.e., $c_t(a,t) = 0$ with a (m) being the radius of the spherical grain, and initial condition $\bar{c}_t(0) = \bar{c}_0$ are considered. The analytic expression of $\bar{c}_t(t)$ for constant conditions is obtained by integrating the solution of Eq. (2), $c_t(r,t)$, over the spherical domain, and reads

$$\bar{c}_t(t) = \bar{c}_0 \frac{6}{\pi^2}\sum_{n=1}^{+\infty}\frac{1}{n^2}\exp\left(-\frac{n^2\pi^2 D_{eff} t}{a^2}\right) + \frac{\beta a^2}{15 D_{eff}}\left\{1 - \frac{90}{\pi^4}\sum_{n=1}^{+\infty}\frac{1}{n^4}\exp\left(-\frac{n^2\pi^2 D_{eff} t}{a^2}\right)\right\} \tag{3}$$