INL/JOU-16-38537
Accepted Manuscript

PolyPole1: An accurate numerical algorithm for intragranular fission gas release

D. Pizzocri, C. Rabiti, L. Luzzi, T. Barani, P. Van Uffelen, G. Pastore

September 2016

The INL is a
U.S. Department of Energy
National Laboratory
operated by
Battelle Energy Alliance

Prepared for the U.S. Department of Energy
Office of Nuclear Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

Journal of Nuclear Materials xxx (2016) xxx-xxx

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com

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

D. Pizzocri,[a] C. Rabiti,[b] L. Luzzi,[a] T. Barani,[a] P. Van Uffelen,[c] G. Pastore [b, *]

[a] Politecnico di Milano, Department of Energy, Nuclear Engineering Division, Via La Masa 34, 20156 Milano, Italy
[b] Idaho National Laboratory, P.O. Box 1625, Idaho Falls, ID 83415-3840, United States
[c] European Commission, Joint Research Centre, Institute for Transuranium Elements, P.O. Box 2340, 76125 Karlsruhe, Germany

ARTICLE INFO

Article history:
Received 27 April 2016
Received in revised form 15 June 2016
Accepted 16 June 2016
Available online xxx

Keywords:
Diffusion
Nuclear fuel modelling
Intra-granular fission gas release
Numerical algorithms
Modal methods
FORMAS
URGAS
PolyPole

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.

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 inter-linkage 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 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.

* Corresponding author.
Email address: giovanni.pastore@inl.gov (G. Pastore)

http://dx.doi.org/10.1016/j.jnucmat.2016.06.028
0022-3115/

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

$$\begin{cases} \frac{\partial c}{\partial t} = \mathrm{D}\nabla^2 c - gc + bm + \beta \\ \frac{\partial m}{\partial t} = gc - bm \end{cases} \quad (1)$$

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})

$$\frac{\partial c_t}{\partial t} = \beta + \mathrm{D}_{\mathrm{eff}}\nabla^2 c_t \quad (2)$$

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), $\mathrm{D}_{\mathrm{eff}}$ (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 $\mathrm{D}_{\mathrm{eff}}$ to account for the contribution of Brownian bubble motion while preserving the form of Eq. (2).

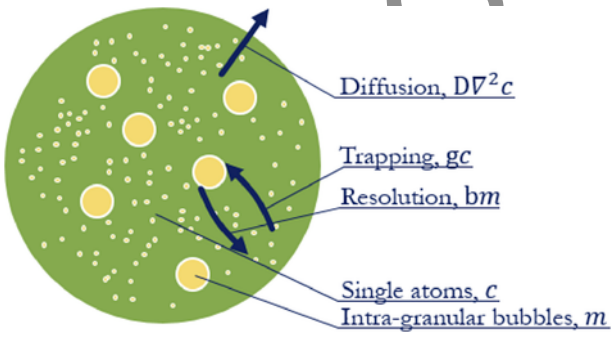

Fig. 1. Sketch representing the main mechanisms of intra-granular fission gas release.

The analytic solution of Eq. (2) for constant conditions (constant β and $\mathrm{D}_{\mathrm{eff}}$) 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

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

The full derivation of Eq. (3) is reported in the Appendix. This solution is not directly applicable to realistic problems, for which time-varying conditions need to be considered. Therefore, the mathematical problem of intra-granular fission gas release of interest for fuel performance analysis and considered in the present work is

$$\frac{\partial c_t}{\partial t} = \beta(t) + \mathrm{D}_{\mathrm{eff}}(t)\nabla^2 c_t \quad (4)$$

with Dirichlet boundary condition $c_t(a,t) = 0$ and the symmetry condition $\left[\partial c_t/\partial r\right]_0 = 0$. Eq. (4) needs to be solved numerically with dedicated algorithms.

3. Overview of numerical algorithms

In computational problems of interest here, time is discretised in time-steps, dt ($t_{i+1} = t_i + dt$), with the initial conditions known at t_i. With reference to Eq. (4), a numerical solution algorithm is defined as (a) *incremental* if it determines an (average) approximate solution, $\bar{c}_t^*(t_{i+1})$, given the initial condition $\bar{c}_t^*(t_i)$, or (b) *non-incremental* if it requires the knowledge of the entire previous history. Generally, non-incremental algorithms require higher computer storage and time.

As mentioned, numerical algorithms used in fuel performance codes need to be applicable to time-varying conditions and to allow for low computational cost. Also, these algorithms need to be verified for accuracy as stand-alone against reference solutions. In this Section, we therefore delineate the background of the present research through an overview of existing numerical algorithms for the solution of Eq. (4). Both algorithms used as reference and used in fuel performance codes are included. In particular, we consider:

- The ANS-5.4 algorithm [34], which has been applied as reference solution in several numerical experiments (Section 3.1.1).
- A finite difference algorithm that we developed and used as reference solution in this work (Section 3.1.2).
- Two state-of-the-art algorithms for fuel performance codes, i.e., the URGAS algorithm developed in [28,29] and the FORMAS algorithm from [26,31] (Sections 3.2.1, 3.2.2). We refer to these methods as URGAS and FORMAS following the nomenclature in [29]. These two algorithms are widely used in modern fuel

performance codes (e.g., [18,20–22]) and will be compared to our new algorithm PolyPole-1 later in this paper.

3.1. Reference algorithms

3.1.1. ANS-5.4 quasi-exact algorithm

The ANS-5.4 algorithm [34] is derived directly from the analytic solution of the diffusion equation for constant conditions (Eq. (3)). The main drawback of this algorithm is that it is non-incremental, thus it requires a computational effort exponentially increasing with the number of time steps. Nevertheless, the ANS-5.4 solution is exact for piecewise-constant conditions. The ANS-5.4 algorithm is thus only affected by errors due to discretization of a real operation history into piecewise-constant conditions. For this reason, it has been used as reference solution in several numerical experiments based on piecewise-constant operation histories [29,30,32].

3.1.2. Finite difference reference algorithm

In this work, a finite difference (FD) algorithm is developed to provide a reference numerical solution of Eq. (4). Such reference solution will be used to evaluate the accuracy of alternative algorithms that are intended to allow for lower computational effort.

The developed FD algorithm is fully implicit first order in time and second order in space. An adaptive time step control is included, as illustrated in Fig. 2. The output solution is calculated with a fully implicit scheme (backward Euler, $\varphi_{i+1}^{\mathrm{B}}$). At each time step, also the explicit solution (forward Euler, $\varphi_{i+1}^{\mathrm{F}}$) is calculated, and the absolute difference between the explicit and the implicit solutions is used to obtain an estimation of the second-order error, ε_{i+1}. The next time step, dt_{i+1}, is then computed based on this estimation. This time step criterion ensures that the second-order error of the FD solution is kept below a fixed tolerance, tol. Details of this method can be found in [35].

This algorithm can be applied to obtain a reference solution of Eq. (4) (in principle, up to any tolerance) for piecewise-linear operation histories, for which algorithms such as ANS-5.4 are not applicable. As further discussed in Section 4, piecewise-linear histories are considered in this work.

3.2. State-of-the-art algorithms used in fuel performance codes

3.2.1. URGAS algorithm

The URGAS algorithm was originally proposed by Elton and Lassmann [28], and considerably improved by Lassmann and Benk [29]. The algorithm is based on the assumption that the spatially averaged concentration at previous time step, $\bar{c}_t^*\left(t_i\right)$, derives from a fictitious irradiation for a time $t_{\mathrm{fic},i}$ with constant conditions, equal to the conditions during the time-step under consideration. Then, based on the analytic solution for constant conditions (Eq. (3)), the fictitious time is determined by solving

$$\begin{aligned}\bar{c}_t^*\left(t_i\right) &= \bar{c}_0 \frac{6}{\pi^2}\sum_{n=1}^{+\infty}\frac{1}{n^2}\exp\left(-\frac{n^2\pi^2 \mathrm{D}_{\mathrm{eff}}\left(t_i\right) t_{\mathrm{fic},i}}{a^2}\right) \\ &\quad + \frac{\beta\left(t_i\right) a^2}{15\mathrm{D}_{\mathrm{eff}}\left(t_i\right)}\left\{1 \right. \\ &\quad \left. - \frac{90}{\pi^4}\sum_{n=1}^{+\infty}\frac{1}{n^4}\exp\left(-\frac{n^2\pi^2 \mathrm{D}_{\mathrm{eff}}\left(t_i\right) t_{\mathrm{fic},i}}{a^2}\right)\right\} \\ &= \bar{c}_0 f_a\left(t_{\mathrm{fic},i}\right) + \bar{c}_\infty f_d\left(t_{\mathrm{fic},i}\right)\end{aligned}$$

$$\bar{c}_0 = \bar{c}_{created}\left(t_i\right) - \beta\left(t_i\right) t_{\mathrm{fic},i} \geq 0 \tag{5}$$

In Eq. (5), $\bar{c}_\infty = \beta\left(t_i\right) a^2 / 15\mathrm{D}_{\mathrm{eff}}\left(t_i\right)$, and f_a and f_d are approximations for the series with a relative error less than $6{\cdot}10^{-7}$ [29]. The system is solved by the Newton method. The average concentration at current time step is then calculated as

$$\bar{c}_t^*\left(t_{i+1}\right) = \bar{c}_0 f_a\left(t_{\mathrm{fic},i+1}\right) + \bar{c}_\infty f_d\left(t_{\mathrm{fic},i+1}\right) \tag{6}$$

where $t_{\mathrm{fic},i+1} = t_{\mathrm{fic},i} + dt$.

The URGAS algorithm is stable and fast, and is used in current fuel performance codes, e.g., TRANSURANUS [20].

3.2.2. FORMAS algorithm

The FORMAS algorithm has been developed by Forsberg and Massih [26], then revised by Lassmann and Benk [29] and later by Hermansonn and Massih [31]. A variant of the algorithm, which is not reviewed here for brevity, considers also the resolution of gas from the grain boundaries by applying a different boundary condition to Eq. (4) [27].

The first step in the derivation of the FORMAS algorithm is the coordinate transformation

$$\tau = \int_{t_i}^{t_{i+1}} \mathrm{D}_{\mathrm{eff}}\left(t\right) \mathrm{d}t \tag{7}$$

Writing Eq. (4) in terms of τ, and expanding it in terms of the eigenfunctions of the Laplacian operator, for the perfect sink boundary condition, one obtains

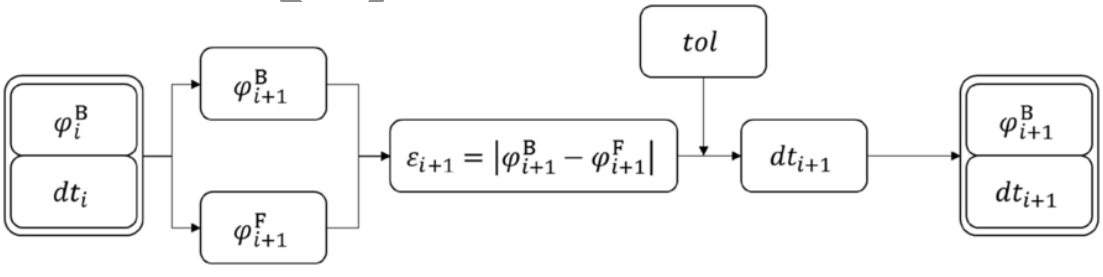

Fig. 2. Schematic of the adaptive time step criterion for the finite difference reference algorithm [35].

$$\bar{c}(\tau) = \frac{3}{4\pi}\int_0^{\tau} K\left(\frac{\tau-\tau'}{a^2}\right) S(\tau')\,\mathrm{d}\tau' \tag{8}$$

where $S(\tau') = \beta\left(t(\tau')\right)/\mathrm{D}_{\mathrm{eff}}\left(t(\tau')\right)$. The kernel $K(x)$ is approximated by

$$K(x) \approx \sum_{i=1}^{I} A_i^k \exp\left(-B_i^k x\right) \tag{9}$$

Various approximations (i.e., various sets of values for the coefficients A_i^k and B_i^k) have been proposed, considering different number of terms, I [26,29,31,36]. Inserting the approximate kernel (Eq. (9)) into Eq. (8) and assuming $S(\tau') =$ constant, one gets the incremental algorithm

$$\bar{c}_t^{\,*}\left(t_{i+1}\right) = \frac{3}{4\pi}\sum_{i=1}^{I}\left[\frac{A_i^k}{B_i^k}\frac{\beta a^2}{\mathrm{D}_{\mathrm{eff}}} + \left(\frac{4\pi}{3}\bar{c}_t^{\,*}\left(t_i\right) - \frac{A_i^k}{B_i^k}\frac{\beta a^2}{\mathrm{D}_{\mathrm{eff}}}\right)\exp\left(-\frac{B_i^k \mathrm{D}_{\mathrm{eff}} dt}{a^2}\right)\right] \tag{10}$$

The FORMAS algorithm is stable and fast, and is implemented in several fuel performance codes, e.g., FALCON [18], TRANSURANUS [20], BISON [21], FRAPCON [22]. In the last two instances, correction for grain-boundary resolution [27] is also considered.

4. PolyPole-1 algorithm

In this Section, we present the new numerical algorithm for the solution of Eq. (4) in fuel performance codes, called PolyPole-1. The objective of the PolyPole-1 development is twofold and comprises (1) the obtainment of improved accuracy and similar computational cost relative to state-of-the-art algorithms, and (2) the construction of a solution concept that is not inherently limited to the quasi-stationary approach, but in perspective can be potentially applied to more general formulations. The importance of such a further development has been pointed out in, e.g., [7,37].

Applying a modal expansion, we write the sought approximated solution of Eq. (4) in the form

$$c_t^*(r,t) = \sum_{n=1}^{+\infty} z_n^*(t)\,\psi_n(r) \tag{11}$$

where $z_n^*(t)$ are the time coefficients and $\psi_n(r)$ are the spatial modes. The form of Eq. (11) is analogous to the analytic solution for constant conditions (see the Appendix, Eq. (A.1)). The time coefficients contain the information about the time dependency of the approximated solution (i.e., the characteristic poles of the system). The spatial modes are the same of the analytic solution for constant conditions and are the orthonormal eigenfunctions of the radial part of the spherical Laplacian (i.e., normalized cardinal sins, with the *ansatz* that they are basis for the solution). A complete derivation of the analytic solution for constant conditions is given in the Appendix.

The other fundamental assumption of the proposed method is that the time coefficients, $z_n^*(t)$, may be expressed as the time coefficients of the analytic solution for constant conditions, $z_n(t)$ (Eq. (A.10)), multiplied by an appropriate polynomial factor. Thus, we write

$$z_n^*\left(t_{i+1}\right) = z_n\left(t_{i+1}\right) P_J\left(t_{i+1}, dt\right) \tag{12}$$

where P_J is a polynomial factor of degree J

$$P_J = 1 + \ldots + a_j dt^j + \ldots + a_J dt^J \tag{13}$$

The time dependency of the diffusion coefficient and of the source term is thus addressed by the polynomial factor. To calculate the coefficients a_j of $P_J\left(t_{i+1}, dt\right)$, J equations are needed. This set of equations is obtained by sampling the time-varying parameters, $\mathrm{D}_{\mathrm{eff}}(t)$ and $\beta(t)$, at J uniformly distributed instants along the time-step dt. The sets of sampled values, $\mathrm{D}_{\mathrm{eff}}[j]$ and $\beta[j]$, contain the information on the variation of the parameters along the time step and are used to calculate the corrective polynomial, as follows.

The time coefficients defined by Eq. (12) are assumed to satisfy Eq. (A.6) at the sampling times $t[j]$, $t_i \le t[j] \le t_{i+1}$

$$\left.\frac{\partial z_n^*}{\partial t}\right|_{t[j]} = \beta_n[j] - \delta_n[j]\, z_n^*(t[j]) \tag{14}$$

$$\left.\frac{\partial\left(z_n P_J\right)}{\partial t}\right|_{t[j]} = \beta_n[j] - \delta_n[j]\, z_n(t[j])\, P_J(t[j]) \tag{15}$$

with $\beta_n[j] = \langle\psi_n|\beta[j]\rangle$ and $\delta_n[j] = \mathrm{D}_{\mathrm{eff}}[j]\left(n^2\pi^2\right)/a^2$. Eq. (15) defines a linear system of J equations for the polynomial coefficients, a_j, and is used to determine the polynomial, $P_J\left(t_{i+1}, dt\right)$. The time coefficients of the analytic solution for constant conditions, z_n, are calculated through Eq. (A.10), for which the parameters β_m and δ_m are needed (see the Appendix). These are taken as the time averages along the time step of the sampled values, $\mathrm{D}_{\mathrm{eff}}[j]$ and $\beta[j]$. Then, the polynomial corrective factor is calculated (through Eq. (15)) and applied to each time coefficient (through Eq. (12)). For time-varying conditions, the accuracy of the approximated (PolyPole-1) solution increases with the degree of the corrective polynomial, J.

The spatial modes, $\psi_n(r)$, are calculated as per Eq. (A.3). The PolyPole-1 solution is then reconstructed as a linear combination of the spatial modes with the corrected time coefficients using Eq. (11). The series is approximated by a finite number of terms (number of modes), N. The value of N is determined based on the D'Alembert remainder criterion, bounded by an a priori limiting value, l

$$\frac{\left|z_N^*\psi_N - z_{N-1}^*\psi_{N-1}\right|}{z_N^*\psi_N} \le l \tag{16}$$

To summarize, the steps of the PolyPole-1 algorithm to find the approximate solution of Eq. (4) are:

1. Sample the time-varying effective diffusion coefficient, $\mathrm{D}_{\mathrm{eff}}(t)$, and source term, $\beta(t)$, at J sampling times $t[j]$ along the

time-step length dt. This gives the set of values $\mathrm{D}_{\mathrm{eff}}[j]$ and $\beta[j]$.

2. Calculate the time coefficients of the analytic solution for constant conditions at each sampling time, $z_n(t[j])$, using Eq. (A.10) and the time averages of $\mathrm{D}_{\mathrm{eff}}[j]$ and $\beta[j]$ along the time step.
3. Solve the system of equations defined by Eq. (15) to obtain the coefficients a_j of the corrective polynomial $P_J(t_{i+1}, dt)$.
4. Evaluate the corrective polynomial and calculate the approximate time coefficients as $z_n^*(t_{i+1}) = z_n(t_{i+1})\, P_J(t_{i+1}, dt)$.
5. Reconstruct the volume-averaged solution, $\bar{c}_t^*(t_{i+1})$, using Eqs. 11, A.12. The infinite series is approximated with a finite number of modes based on the criterion defined by Eq. (16).

The newly developed PolyPole-1 algorithm thus combines the physical poles of the analytic solution with a corrective polynomial to account for the time dependency of the coefficients. In short, the idea behind the PolyPole-1 approach is that the spatial dependency of the solution for time-varying conditions can be approximated by the spatial dependency of the solution for constant conditions, which is known analytically. The deviation from constant conditions is fully embodied in the time-dependent part of the solution and approximated by the time coefficients of the solution for constant conditions multiplied by an appropriate correction. Exploiting an analytic representation of the spatial dependency avoids using spatial discretization and is therefore expected to allow for significantly lower computational time compared to spatial discretization methods. In view of this concept, the algorithm may be labelled as semi-analytic, as opposed to spatial discretization methods such as FD schemes. The URGAS and FORMAS algorithms may also be considered as semi-analytic methods.

It is worth comparing the PolyPole-1 approach to the problem of time-varying conditions to other semi-analytic algorithms':

- The URGAS algorithm addresses the problem of time-varying conditions using a single parameter, i.e., the fictitious time $t_{\mathrm{fic},i}$ (Eq. (5)).
- The FORMAS algorithm relies on I terms to approximate the series (thus, $2I$ parameters, Eq. (9)).
- The PolyPole-1 algorithm relies on a variable number of parameters to satisfy the condition expressed by Eq. (16) (more precisely, a variable number N of modes times a fixed number J of polynomial coefficients). In other words, PolyPole-1 adapts the number of parameters at each time step according to the current conditions. This is a major inherent advantage of PolyPole-1 compared to other algorithms such as FORMAS and URGAS. In particular, it is expected that PolyPole-1 would maintain a more consistent level of accuracy over different conditions. This will be further discussed in Section 5.

Note that, differently from other algorithms considered here, the solution concept of PolyPole-1 is not inherently limited to the single diffusion equation and thus the quasi-stationary approach. Extension of the method to the general problem of intra-granular fission gas diffusion during non-equilibrium trapping and resolution, whose significance has been discussed in, e.g., [7,37], is in principle possible and will be the subject of future work.

The comparison between the approach of the PolyPole-1 algorithm and the ANS-5.4 algorithm provides further insight. As mentioned in Section 3.1.1, the ANS-5.4 algorithm is derived directly from the analytic solution of the diffusion equation for constant conditions. Clearly, for constant (or piecewise-constant) conditions, the corrective polynomial is identically $P_J = 1$, and the PolyPole-1 solution (Eq. (11)) reduces to Eq. (A.1), hence, to the analytic solution for constant conditions (see the Appendix). This implies that for constant (or piecewise-constant) conditions, the solution of the ANS-5.4 algorithm and of the PolyPole-1 algorithm are both exact and equal, within the approximations in representing infinite series with a finite number of terms. Minor differences arising from specific approximations of the series can always be removed by setting an appropriate remainder limiting value in Eq. (16). As mentioned in Section 3.1.1, the ANS-5.4 algorithm has been used as a reference solution in several numerical experiments based on piecewise-constant operation histories [29,30,32]. The intrinsic equivalence between the ANS-5.4 and PolyPole-1 solutions in constant (or piecewise-constant) conditions implies that a comparison between the two algorithms for piecewise-constant operation histories would not be meaningful. It follows that the ANS-5.4 algorithm cannot be used as reference solution for verifying the accuracy of PolyPole-1. Furthermore, piecewise-linear (as opposed to piecewise-constant) conditions are those of interest for fuel performance code calculations. These are the fundamental motivations for the development of the FD algorithm (Section 3.1.2) as a reference solution and the choice to verify PolyPole-1 through a numerical experiment based on piecewise-linear operation histories.

5. Verification

In this Section, we present a numerical experiment aimed to (i) verify the PolyPole-1 solution and (ii) compare the accuracy of the PolyPole-1 solution to other state-of-the-art algorithms currently used in fuel performance codes.

5.1. Set-up of numerical experiment

The numerical experiment is applied to three semi-analytic algorithms for the solution of Eq. (4), namely, (1) URGAS [29], (2) FORMAS[1] [31], and (3) PolyPole-1.[2] The numerical experiment consists of application of each algorithm to the numerical solution of Eq. (4) for 1000 randomly generated operation histories. Results from the three semi-analytic algorithms are compared to the reference FD solution[3].

The considered operation histories are in terms of temperature and fission rate, from which the time-dependent parameters of Eq. (4), i.e., $\mathrm{D}_{\mathrm{eff}}(t)$ and $\beta(t)$, are calculated[4] and applied to the numerical algorithms by the program. The figure of merit for testing and comparing the algorithms is the fractional intra-granular fission gas release at the end of the considered operation history, defined as

$$f := \frac{\bar{c}_{created}(t_{end}) - \bar{c}_t(t_{end})}{\bar{c}_{created}(t_{end})} \tag{17}$$

where $\bar{c}_{created}$ (at. m^{-3}) is the concentration of gas created (i.e., the time integral of $\beta(t)$) and t_{end} (s) is the final time of the operation history. The randomly generated operation histories have the follow-

[1] Among the various versions of the FORMAS algorithm, we use the FORMAS algorithm with four exponential terms from [31].

[2] For this numerical experiment, we consider a second-order corrective polynomial (Eq. (13)) and a limiting value of 10^{-7} for the D'Alembert remainder (Eq. (16)).

[3] For this numerical experiment, we set the tolerance of the FD algorithm to 10^{-6} (Section 3.1.2).

[4] The temperature and fission rate dependent diffusion coefficient from [11] is used as $\mathrm{D}_{\mathrm{eff}}(t)$. $\beta(t)$ is calculated as the fission rate times the yield of fission gas atoms (~0.3). For the purpose of this numerical experiment, as long as dependencies are realistic, the specific choices are arbitrary.

ing characteristics:

- Each individual history is piecewise-linear with varying temperature and fission rate.
- In each individual history, the following quantities are considered as random variables (sampled from uniform distributions):
  - number of linear steps (1–11);
  - time duration of each linear step (0–100 h);
  - temperature (500–2000 K);
  - fission rate (0–$3{\cdot}10^{19}$ fiss m^{-3} s^{-1}).

With these principles, the numerical experiment approximately covers the whole range of intra-granular fission gas release ($0 \leq f \leq 1$). This is demonstrated in Section 5.2.

For calculations with URGAS, FORMAS, PolyPole-1, each linear step is subdivided into 100 time steps. For the FD calculations, the adaptive time step control described in Section 3.1.2 is used (along with a lower bound of 10^4 time steps per linear step). The spatial 1D mesh for the FD algorithm is comprised of 500 points along the grain radius, concentrated towards the grain boundary (where steeper gas concentration gradients are expected) according to a fourth power law.

5.2. Results and discussion

The results of the numerical experiment are presented in Figs. 3–5 for the URGAS, FORMAS, and PolyPole-1 algorithms. Each data point in these figures corresponds to one of 1000 randomly generated operation histories and represents the intra-granular fission gas release (Eq. (17)) obtained by the considered semi-analytic algorithm versus the reference FD algorithm. The deviation from the 45° line is a measure of the accuracy. Results of the numerical experiment indicate that all the three semi-analytic algorithms may be considered as sufficient to be used in a fuel performance code, also in view of the uncertainties involved in the modelling of intra-granular fission gas diffusion [29,38].

To investigate in finer detail the accuracy of the three semi-analytic algorithms, in Fig. 6 we show the relative error of the solution obtained with each algorithm with respect to the FD reference solution. The efficiency and accuracy of the URGAS and FORMAS algorithms were previously analysed by Lassmann and Benk [29]. Although a more recent version of FORMAS is considered here, the results in Fig. 6 are consistent with the conclusions of Lassmann and Benk [29] that (i) the FORMAS algorithm is superior to the URGAS algorithm at fission gas release above $f \approx 0.05$, and (ii) the FORMAS algorithm presents a deficiency for low values of f, which is ascribed to an approximation (i.e., Eq. (9)) involved in the method. Although both algorithms were evaluated as sufficient to be used in a fuel performance code, drawbacks were attributed to each of them in line with the conclusions above. Choice of one of the two algorithms based on the specific application was recommended.

The results in Fig. 6 indicate that the PolyPole-1 algorithm represents a significant path forward in this respect. First, it is evident that the overall accuracy of PolyPole-1 is vastly superior to both FORMAS and URGAS. This is in agreement with the theoretical considerations made in Section 4. Indeed, the accuracy of the FORMAS algorithm may be improved by an increase in the number of parameters [31,36]. However, the accuracy of the PolyPole-1 algorithm can also

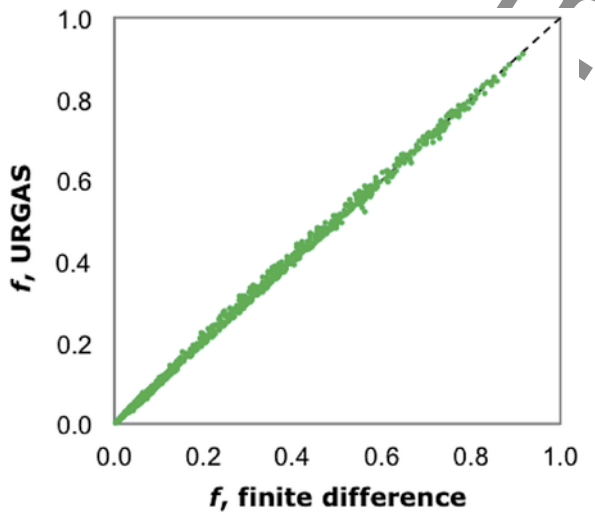

Fig. 3. Comparison between the values of intra-granular fission gas release calculated

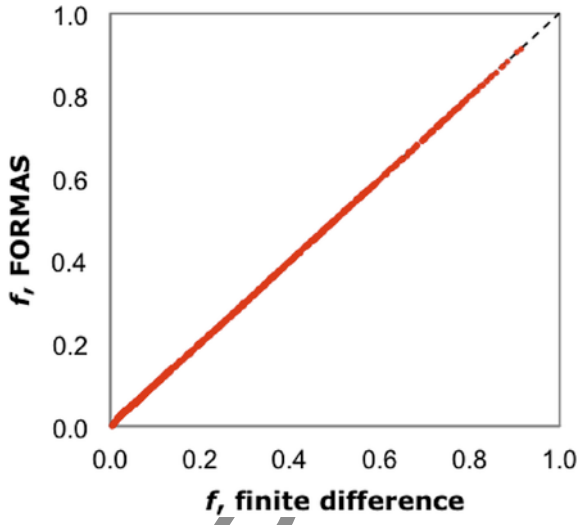

Fig. 4. Comparison between the values of intra-granular fission gas release calculated by the FORMAS algorithm and by the reference finite difference algorithm. Each data point corresponds to a calculation with randomly generated conditions.

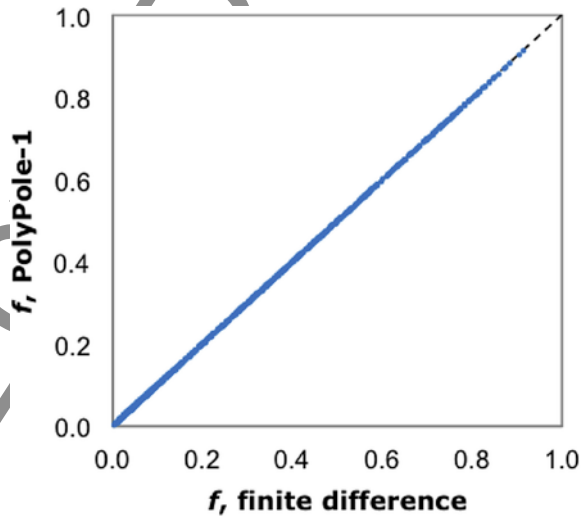

Fig. 5. Comparison between the values of intra-granular fission gas release calculated by the PolyPole-1 algorithm and by the reference finite difference algorithm. Each data point corresponds to a calculation with randomly generated conditions.

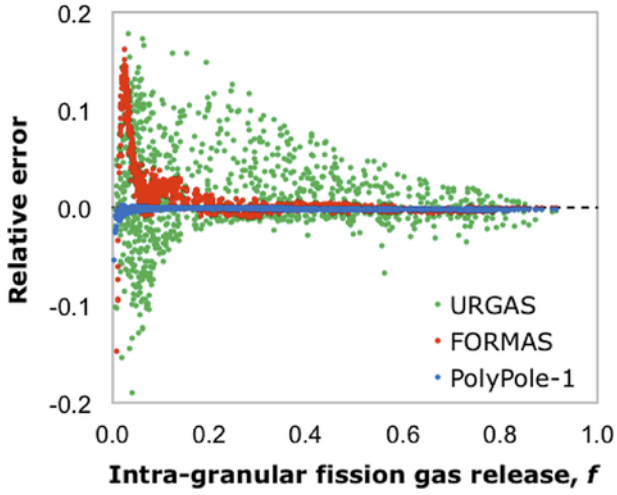

Fig. 6. Comparison between the URGAS, FORMAS and PolyPole-1 algorithms in terms of relative error with respect to the reference finite difference algorithm. Each data point corresponds to a calculation with randomly generated conditions.

be further improved by increasing the order of the polynomial corrective term (Eq. (13)) and/or by decreasing the limiting value for the approximation of the series (Eq. (16)). Furthermore, PolyPole-1 overcomes the deficiency at low FGR that characterizes the FORMAS algorithm. Remarkably, the relative error associated with PolyPole-1 is highly consistent over the whole range of intra-granular fission gas release. This also confirms practically the theoretical considerations made in Section 4 on the inherent capability of PolyPole-1 to allow for a more consistent level of accuracy over different conditions through automatic adaptation of the number of considered series terms.

Besides accuracy, speed of computation is an essential feature for an algorithm to be effectively employed in a fuel performance code. The computational time (i.e., the time took for the analysis of a single operation history) for the three semi-analytic algorithms and all histories considered in the numerical experiment is illustrated in Fig. 7. PolyPole-1 requires a computational time similar to the other algorithms, which are successfully used in fuel performance codes. Such efficiency of computation, combined with the demonstrated accuracy, makes PolyPole-1 suitable for implementation in any fuel performance code. The computational time for the finite difference solution is also shown. Clearly, if a spatial discretization method such as a FD method is used to solve the intra-granular fission gas release problem in a fuel performance code, the associated higher computational time can result in significantly decreased speed of computation of the fuel rod analysis, even with modern computational resources. This highlights the value of developing numerical algorithms that allow for a faster computation while preserving accuracy, such as PolyPole-1.

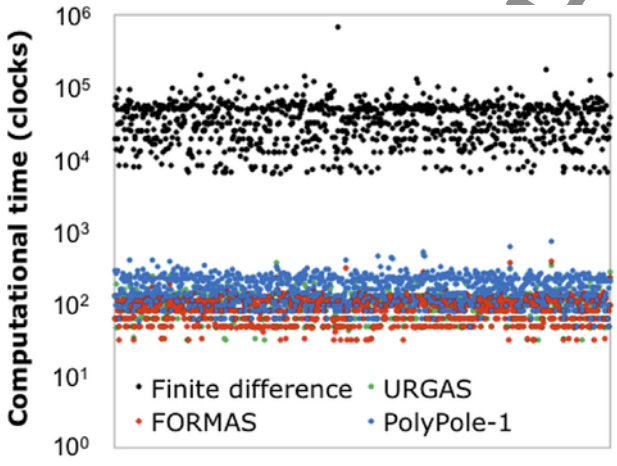

Fig. 7. Comparison between the computational times associated with the finite difference, URGAS, FORMAS and PolyPole-1 algorithms. Each data point corresponds to a calculation with randomly generated conditions.

6. Conclusions and perspectives

In this research, a new algorithm (PolyPole-1) was developed for the numerical solution of the problem of intra-granular fission gas release in time-varying conditions. The development was aimed at obtaining an accurate solution at low computational cost for application in fuel performance codes.

The PolyPole-1 algorithm is based on the analytic modal solution of the diffusion equation for constant conditions, with the addition of polynomial corrective terms that embody the information on the deviation from constant conditions. This semi-analytic concept is intended to allow for significantly lower computational time than spatial discretization methods, such as finite difference schemes. The stand-alone PolyPole-1 algorithm was verified by comparing the results to a finite difference reference solution for a large number of randomly generated operation histories. Also, the performance of PolyPole-1 was compared to two state-of-the-art algorithms widely used in modern fuel performance codes, i.e., the URGAS [29] and FORMAS [31] algorithms. Results demonstrated that:

- The accuracy of the PolyPole-1 solution is high and superior to other algorithms.
- The computational time associated with PolyPole-1 is similar to other algorithms.
- Differently from other algorithms, the accuracy of the PolyPole-1 solution is highly consistent over the whole range of intra-granular fission gas release.

Hence, PolyPole-1 offers a more accurate solution than currently used algorithms, with no significant increase in computational time. In addition, PolyPole-1 features a more flexible strategy for both the time and the space approximations. In particular, the PolyPole-1 concept involves automatic adaptation of the number of considered parameters at each time step in order to satisfy a remainder criterion, which allows for the observed consistency of the solution accuracy over widely different conditions.

The PolyPole-1 algorithm can be implemented in any fuel performance code. PolyPole-1 is being implemented in the fuel performance code BISON [21] of Idaho National Laboratory (INL, USA).

For this work, we considered the mathematical formulation of the intra-granular fission gas release problem based on the hypothesis of equilibrium between bubble trapping and resolution (quasi-stationary approach) [17]. This formulation reduces the problem to a single diffusion equation and is the one considered for models incorporated in fuel performance codes. However, some inherent deficiencies are associated with Speight's formulation, as the quasi-stationary assumption does not hold during situations such as rapid temperature transients. Indeed, the solution of the single diffusion equation is considered as a first step of the development of the new algorithm. 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. Furthermore, a similar numerical approach may be applied to other problems of interest. Significant examples may be the modelling of intra-granular helium release (which

fuels in fast reactors (for which the approach would be extended to cylindrical coordinates).

Besides the numerical problem, calculations of intra-granular fission gas release involve the physical problem of characterizing the intra-granular bubble population, in order to determine the values of the parameters in Eqs. (1)–(4) [3,8,17]. Clearly, a physical model for bubble evolution would need to be validated against experimental data along with the overall fission gas behaviour model to demonstrate the fidelity of calculations to reality, with the prerequisite that the numerical solution is accurate. While the present paper focused only on the numerical problem, the development of a new physical model for intra-granular bubble evolution is also of interest in perspective. This would be combined with an algorithm providing numerical solution of the diffusion problem (such as PolyPole-1 or an extended one) to further improve modelling of intra-granular fission gas release, as well as the coupled intra-granular bubble swelling, in fuel performance calculations.

These further developments will be the subject of future work.

Acknowledgements

This work was funded by the DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program at Idaho National Laboratory (INL, USA), the GENTLE Project 198236 at Institute for Transuranium Elements (JRC-ITU, Germany), and the Doctoral Program in "Energy and Nuclear Science and Technology" at Politecnico di Milano (POLIMI, Italy).

This research contributes to the Joint Programme on Nuclear Materials (JPNM) of the European Energy Research Alliance (EERA), in the specific framework of the COMBATFUEL Project.

The work is also part of the R&D activities carried out by POLIMI in the framework of the IAEA Coordinated Research Programme FUMAC.

The authors are grateful Dr. Andrea Alfonsi (INL) for his help with calculations, Dr. Valentino Di Marcello (KIT, Germany) for his careful review of the manuscript, and Prof. Klaus Lassmann for his kind availability and valuable insights.

The submitted manuscript has been authored by a contractor of the U.S. Government under Contract DE-AC07-05ID14517. Accordingly, the U.S. Government retains a non-exclusive, royalty free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

Appendix

Analytic solution of the effective diffusion equation for constant conditions

Hereinafter, the well-known analytic solution of the diffusion equation for constant conditions, Eq. (2), is derived. The source term, β, and the effective diffusion coefficient, D_{eff}, are assumed as constant in time and uniform in space.

First, the total concentration of fission gas atoms per unit volume, c_t, is written as a linear combination of spatial modes

$$c_t(r,t) = \sum_{k=1}^{+\infty} z_k(t)\,\psi_k(r) \tag{A.1}$$

where r is the spatial coordinate in the grain, t is the time, $\psi_k(r)$ are the spatial modes, and $z_k(t)$ are the time coefficients (in the following, the dependences on t and r are omitted). Substituting Eq. (A.1) into Eq. (2) and using Einstein notation (i.e., implicitly summing over repeated indices) leads to

$$\psi_k \frac{\partial z_k}{\partial t} = \beta + z_k D_{eff} \nabla^2 \psi_k \tag{A.2}$$

From now on, the hypothesis of spherical grain is made, with r representing the radial position and a being the grain radius. The spatial modes are chosen as the eigenfunctions of the spherical Laplacian [17], considering the Dirichlet boundary condition, $c_t(a,t) = 0$, and the symmetry condition at the centre of the grain, $\left[\partial c_t / \partial r\right]_0 = 0$. Thus

$$\psi_k = \frac{1}{\sqrt{2\pi a}} \frac{sin\lambda_k r}{r} \tag{A.3}$$

with the eigenvalues

$$\lambda_k^2 = \frac{k^2\pi^2}{a^2} \tag{A.4}$$

and the *ansatz* that the eigenfunctions (Eq. (A.3)) represent an orthonormal basis for the scalar product defined as

$$\langle \psi_n | \psi_k \rangle = \int_0^a 4\pi r^2 \psi_n \psi_k \mathrm{d}r \tag{A.5}$$

Then, projecting Eq. (A.2) on the spatial modes defined by Eq. (A.3), one obtains

$$\frac{\partial z_n}{\partial t} = \beta_n - \delta_n z_n \tag{A.6}$$

with $\beta_n = \langle \psi_n | \beta \rangle$, and $\delta_n = D_{eff}\left(n^2\pi^2\right)/a^2$. Eq. (A.6) is a linear first order ordinary differential equation in time. Projecting initial conditions $c_t(r,0) = \bar{c}_0$ on the spatial modes

$$z_{0,n} = \langle \psi_n | \bar{c}_0 \rangle \tag{A.7}$$

and Laplace-transforming, $\mathscr{L}(\cdot)$, Eq. (A.6), one obtains

$$sZ_n - z_{0,n} = \frac{\beta_n}{s} - \delta_n Z_n \tag{A.8}$$

where $Z_n = \mathscr{L}\left(z_n\right)$. Eq. (A.8) is solved for

$$Z_n = \frac{s\, z_{0,n} + \beta_n}{s\left(s + \delta_n\right)} \tag{A.9}$$

The inverse transform of Eq. (A.9) is

$$z_n(t) = \frac{\beta_n}{\delta_n}\left[1 - \left(1 - z_{0,n}\frac{\delta_n}{\beta_n}\right)\exp\left(-\delta_n t\right)\right] \tag{A.10}$$

Note that in Eq. (A.10), the term β_n/δ_n is the asymptotic solution of the time coefficient, and that δ_n is the pole governing the time-evolution of the mode. Combining Eqs. A.1, A.3 and A.10, the solution $c_t(r,t)$ results

$$c_t(r,t) = \sum_{n=1}^{+\infty} z_n \psi_n = \sum_{n=1}^{+\infty} \frac{1}{\sqrt{2\pi a}} \frac{sin\frac{n\pi r}{a}}{r} \frac{\beta_n}{\delta_n} \left[1 - \left(1 - z_{0,n}\frac{\delta_n}{\beta_n}\right)\exp\left(-\delta_n t\right)\right] \quad (A.11)$$

which is the solution in spherical geometry of the diffusion equation for constant conditions. Eq. (A.11) can be written in terms of the volume average of the fission gas atom concentration inside a spherical grain, namely

$$\bar{c}_t(t) = \frac{\int_0^a 4\pi r^2 c_t(r,t)\mathrm{d}r}{\frac{4}{3}\pi a^3} \quad (A.12)$$

Combining Eqs. A.11 and A.12 leads to

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

which is the spatially-averaged solution in spherical geometry of the diffusion equation for constant conditions.

References

[1] D.R. Olander, Fundamental Aspects of Nuclear Reactor Fuel Elements, Technical Information Center – Energy Research and Development Administration, University of California, Berkeley, CA, USA, 1976.

[2] Hj. Matzke, Gas release mechanism in UO_2–a critical review, Radiat. Eff. 53 (1980) 219–242.

[3] R.J. White, M.O. Tucker, A new fission-gas release model, J. Nucl. Mater. 118 (1983) 1–38.

[4] R.J. White, The development of grain-face porosity in irradiated oxide fuel, J. Nucl. Mater. 325 (2004) 61–77.

[5] P. Van Uffelen, R.J.M. Konings, C. Vitanza, J. Tulenko, Analysis of reactor fuel rod behavior, In: D.G. Cacuci (Ed.), Handbook of Nuclear Engineering, 13, Springer Science + Business Media, LLC, New York, NY, USA, 2010, pp. 1519–1627.

[6] G. Pastore, L. Luzzi, V. Di Marcello, P. Van Uffelen, Physics-based modelling of fission gas swelling and release in UO_2 applied to integral fuel rod analysis, Nucl. Eng. Des. 256 (2013) 75–86.

[7] P. Lösönen, On the behaviour of intragranular fission gas in UO_2 fuel, J. Nucl. Mater. 280 (2000) 56–72.

[8] F.S. Ham, Theory of diffusion-limited precipitation, J. Phys. Chem. Solids 6 (1958) 335–351.

[9] R.S. Nelson, The stability of gas bubbles in an irradiation environment, J. Nucl. Mater. 31 (1969) 153–161.

[10] J.A. Turnbull, The distribution of intragranular fission gas bubbles in UO_2 during irradiation, J. Nucl. Mater. 38 (1971) 203–212.

[11] J.A. Turnbull, C.A. Friskney, J.R. Findlay, F.A. Johnson, A.J. Walter, The diffusion coefficients of gaseous and volatile species during the irradiation of uranium dioxide, J. Nucl. Mater. 107 (1982) 168–184.

[12] P. Lösönen, Modelling intragranular fission gas release in irradiation of sintered LWR UO_2 fuel, J. Nucl. Mater. 304 (2002) 29–49.

[13] K. Govers, S. Lemehov, M. Verwerft, In-pile Xe diffusion coefficient in UO_2 determined from the modeling of intragranular bubble growth and destruction under irradiation, J. Nucl. Mater. 374 (2008) 461–472.

[14] D.C. Parfitt, R.W. Grimes, Predicting the probability for fission gas resolution into uranium dioxide, J. Nucl. Mater. 392 (2009) 28–34.

[15] D. Schwen, M. Huang, P. Bellon, R.S. Averback, Molecular dynamics simulation of intragranular Xe bubble re-solution in UO_2, J. Nucl. Mater. 392 (2009) 35–39.

[16] D.A. Andersson, P. Garcia, X.-Y. Liu, G. Pastore, M. Tonks, P. Millett, B. Dorado, D.R. Gaston, D. Andrs, R.L. Williamson, R.C. Martineau, B.P. Uberuaga, C.R. Stanek, Atomistic modeling of intrinsic and radiation-enhanced fission gas (Xe) diffusion in $UO_{2\pm x}$: implications for nuclear fuel performance modeling, J. Nucl. Mater. 451 (2014) 225–242.

[17] M.V. Speight, A calculation on the migration of fission gas in material exhibiting precipitation and re-solution of gas atoms under irradiation, Nucl. Sci. Eng. 37 (1969) 180–185.

[18] Y. Rashid, R. Dunham, R. Montgomery, Fuel Analysis and Licensing Code: FALCON MOD01, Technical Report EPRI 1011307, Electric Power Research Institute, 2004.

[19] M. Suzuki, H. Saitou, Y. Udagawa, F. Nagase, Light Water Reactor Fuel Analysis Code FEMAXI-7; Model and Structure. JAEA-data/code 2013-005, Japan Atomic Energy Agency, 2013.

[20] K. Lassmann, A. Schubert, P. Van Uffelen, C. Györi, J. van de Laar, TRANSURANUS Handbook, Copyright © 1975-2014, Institute for Transuranium Elements, Karlsruhe, Germany, 2014.

[21] J.D. Hales, R.L. Williamson, S.R. Novascone, G. Pastore, B.W. Spencer, D.S. Stafford, K.A. Gamble, D.M. Perez, R.J. Gardner, W. Liu, BISON Theory Manual: The Equations behind Nuclear Fuel Analysis, Technical Report INL/EXT-13–29930, Rev. 1, Idaho National Laboratory, ID, USA, 2014.

[22] K.J. Geelhood, W.G. Luscher, P.A. Raynaud, I.E. Porter, FRAPCON-4.0: A Computer Code for the Calculation of Steady-state, Thermal-Mechanical Behavior of Oxide Fuel Rods for High Burnup, Technical Report PNNL-19418 , Vol. 1, Rev. 2, Pacific Northwest National Laboratory, USA, 2015.

[23] A.H. Booth, A Method for Calculating Fission Gas Diffusion from UO_2 Fuel and its Application to the X-2-f Loop Test, Report CRDC-721, 1957, Atomic Energy of Canada Ltd.

[24] J.R. Matthews, M.H. Wood, An efficient method for calculating diffusive flow to a spherical boundary, Nucl. Eng. Des. 56 (1980) 439–443.

[25] L. Väth, Approximate treatment of the grain-boundary loss term in fission gas release models, J. Nucl. Mater. 99 (1981) 324–325.

[26] K. Forsberg, A.R. Massih, Fission gas release under time-varying conditions, J. Nucl. Mater. 127 (1985) 141–145.

[27] K. Forsberg, A.R. Massih, Diffusion theory of fission gas migration in irradiated nuclear fuel UO_2, J. Nucl. Mater. 135 (1985) 140–148.

[28] P.T. Elton, K. Lassmann, Calculational methods for diffusional gas release, Nucl. Eng. Des. 101 (1987) 259–265.

[29] K. Lassmann, H. Benk, Numerical algorithms for intragranular fission gas release, J. Nucl. Mater. 280 (2000) 127–135.

[30] P. Lösönen, Methods for calculating diffusional gas release from spherical grains, Nucl. Eng. Des. 196 (2000) 161–173.

[31] P. Hermansonn, A.R. Massih, An effective method for calculation of diffusive flow in spherical grains, J. Nucl. Mater. 304 (2002) 204–211.

[32] J.-S. Cheon, Y.-H. Koo, B.-H. Lee, J.-Y. Oh, D.-S. Sohn, A two-zone method with an enhanced accuracy for a numerical solution of the diffusion equation, J. Nucl. Mater. 359 (2006) 139–149.

[33] P. Van Uffelen, G. Pastore, V. Di Marcello, L. Luzzi, Multiscale modelling for the fission gas behaviour in the TRANSURANUS code, Nucl. Eng. Technol. 43 (6) (2011) 477–488.

[34] W.N. Rausch, F.E. Panisko, ANS54: a Computer Subroutine for Predicting Fission Gas Release, Technical Report NUREG/CR-0497, 1979, Pacific Northwest Laboratory, USA.

[35] C. Rabiti, Modelling of Fast Neutron Transients in an Accelerator Driven System, PhD thesis, Institut für Kernenergetik und Energiesysteme der Universität Stuttgart, Germany, 2007.

[36] K. Lassmann, Numerical algorithms for intragranular diffusional fission gas release incorporated in the Transuranus code, In: Seminar Proceedings of Fission Gas Behaviour in Water Reactor Fuels, Cadarache, France, 26–29 September, 2000.

[37] M.S. Veshchunov, V.I. Tarasov, Modelling of irradiated UO_2 fuel behaviour under transient conditions, J. Nucl. Mater. 437 (2013) 250–260.

[38] G. Pastore, L.P. Swiler, J.D. Hales, S.R. Novascone, D.M. Perez, B.W. Spencer, L. Luzzi, P. Van Uffelen, R.L. Williamson, Uncertainty and sensitivity analysis

of fission gas behaviour in engineering-scale fuel modeling, J. Nucl.
Mater. 465 (2015) 398–408.