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

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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 work, 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, demonstrating a high accuracy. 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.

Keywords: Diffusion, nuclear fuel modelling, intra-granular fission gas release, numerical algorithms, modal methods, FORMAS, URGAS, PolyPole.

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 to the grain boundaries. It follows that modelling of this process is a fundamental component of any fission gas behaviour model in a fuel performance code. Intra-granular fission gas transport occurs by thermal and irradiation-enhanced diffusion of single gas atoms, coupled to trapping in and irradiation-induced resolution from intra-granular bubbles. Diffusion of intra-granular bubbles becomes relevant at high temperatures, above $\sim 1800^{\circ}\text{C}$ [2,7]. Thus, modelling the process of gas transport to the grain boundaries calls for the treatment of different concomitant processes, 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 to fuel performance analysis, which calls for the

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

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. Clearly, 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 high associated 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 critical comparison with the characteristics of 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 bubble trapping and resolution can be stated mathematically with a system of partial differential equations

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

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 ($\text{m}^2 \text{s}^{-1}$) is the single gas atom diffusion coefficient, g (s^{-1}) is the trapping rate, b (s^{-1}) is the resolution rate, and β (at $\text{m}^{-3} \text{s}^{-1}$) is the gas production term. Intra-granular bubbles are considered as immobile. The processes described by Eqs. 1 are represented in Fig. 1.

Speight [17] solved Eqs. 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 Eqs. 1 into a single diffusion equation for the total concentration of gas in the grain $c_t = c + m$ (at m^{-3})

$$\frac{\partial c_t}{\partial t} = \beta + D_{\text{eff}} \nabla^2 c_t \quad (2)$$

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, D_{eff} ($\text{m}^2 \text{s}^{-1}$), 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 approximation with 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

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

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

$$\frac{\partial c_t}{\partial t} = \beta(t) + D_{\text{eff}}(t) \nabla^2 c_t \quad (4)$$

with Dirichlet boundary condition $c_t(a, t) = 0$ and the symmetry condition $[\partial c_t / \partial r]_0 = 0$. 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).

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

• 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 algorithms 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 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 discretisation 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, φ_{i+1}^B). At each time step, also the explicit solution (forward Euler, φ_{i+1}^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].

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

161 3.2. State-of-the-art algorithms used in fuel performance codes

162 3.2.1 URGAS algorithm

163 The URGAS algorithm was originally proposed by Elton and Lassmann [28], and considerably
 164 improved by Lassmann and Benk [29]. The algorithm is based on the assumption that the spatially
 165 averaged concentration at previous time step, $\bar{c}_t^*(t_i)$, derives from a fictitious irradiation for a time
 166 $t_{\text{fic},i}$ with constant conditions, equal to the conditions during the time-step under consideration.
 167 Then, based on the analytic solution for constant conditions (Eq. 3), the fictitious time is determined
 168 by solving

$$\begin{aligned}\bar{c}_t^*(t_i) &= \bar{c}_0 \frac{6}{\pi^2} \sum_{n=1}^{+\infty} \frac{1}{n^2} \exp\left(-\frac{n^2 \pi^2 D_{\text{eff}}(t_i) t_{\text{fic},i}}{a^2}\right) + \frac{\beta(t_i) a^2}{15 D_{\text{eff}}(t_i)} \left\{ 1 - \frac{90}{\pi^4} \sum_{n=1}^{+\infty} \frac{1}{n^4} \exp\left(-\frac{n^2 \pi^2 D_{\text{eff}}(t_i) t_{\text{fic},i}}{a^2}\right) \right\} = \\ &= \bar{c}_0 f_a(t_{\text{fic},i}) + \bar{c}_\infty f_d(t_{\text{fic},i}) \\ \bar{c}_0 &= \bar{c}_{\text{created}}(t_i) - \beta(t_i) t_{\text{fic},i} \geq 0\end{aligned}\tag{5}$$

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

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

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

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

175 3.2.2 FORMAS algorithm

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

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

$$\tau = \int_{t_i}^{t_{i+1}} D_{\text{eff}}(t) dt \quad (7)$$

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

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

183 where $S(\tau') = \beta(t(\tau')) / D_{\text{eff}}(t(\tau'))$. The kernel $K(x)$ is approximated by

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

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

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

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

190 4. PolyPole-1 algorithm

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

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

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

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

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

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

208 where P_J is a polynomial factor of degree J

$$P_J = 1 + \dots + a_j dt^j + \dots + a_J dt^J \quad (13)$$

209 The time dependency of the diffusion coefficient and of the source term is thus addressed by the
 210 polynomial factor. To calculate the coefficients a_j of $P_J(t_{i+1}, dt)$, J equations are needed. This set
 211 of equations is obtained by sampling the time-varying parameters, $D_{\text{eff}}(t)$ and $\beta(t)$, at J
 212 uniformly distributed instants along the time-step dt . The sets of sampled values, $D_{\text{eff}}[j]$ and
 213 $\beta[j]$, contain the information on the variation of the parameters along the time step and are used to
 214 calculate the corrective polynomial, as follows.

215 The time coefficients defined by Eq. 12 are assumed to satisfy Eq. A.6 at the sampling times $t[j]$,
 216 $t_i \leq t[j] \leq t_{i+1}$

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

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

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

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

$$\frac{|z_N^* \psi_N - z_{N-1}^* \psi_{N-1}|}{z_N^* \psi_N} \leq l \quad (16)$$

230 To summarize, the steps of the PolyPole-1 algorithm to find the approximate solution of Eq. 4 are:
 231 1. Sample the time-varying effective diffusion coefficient, $D_{\text{eff}}(t)$, and source term, $\beta(t)$, at J
 232 sampling times $t[j]$ along the time-step length dt . This gives the set of values $D_{\text{eff}}[j]$ and
 233 $\beta[j]$.
 234 2. Calculate the time coefficients of the analytic solution for constant conditions at each sampling
 235 time, $z_n(t[j])$, using Eq. A.10 and the averages of $D_{\text{eff}}[j]$ and $\beta[j]$ along the time step.
 236 3. Solve the system of equations defined by Eq. 15 to obtain the coefficients a_j of the corrective
 237 polynomial $P_j(t_{i+1}, dt)$.
 238 4. Evaluate the corrective polynomial and calculate the approximate time coefficients as
 239 $z_n^*(t_{i+1}) = z_n(t_{i+1}) P_j(t_{i+1}, dt)$.
 240 5. Reconstruct the volume-averaged solution, $\bar{c}_t^*(t_{i+1})$, using Eqs. 11, A.12. The infinite series is
 241 approximated with a finite number of modes based on the criterion defined by Eq. 16.
 242 The newly developed PolyPole-1 algorithm thus combines the physical poles of the analytic
 243 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 $t_{\text{fic},i}$ (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 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) FORMAS¹ [31], and (3) PolyPole-1². 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 solution³.

The considered operation histories are in terms of temperature and fission rate, from which the time-dependent parameters of Eq. 4, i.e., $D_{\text{eff}}(t)$ and $\beta(t)$, are calculated⁴ and applied to the

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 10^{-7} limiting value for the D'Alembert remainder (Eq. 16).

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

⁴ The temperature- and fission rate dependent diffusion coefficient from [11] is used as $D_{\text{eff}}(t)$. $\beta(t)$ 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.

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

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

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 following 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 hours);
 - temperature (500–2000 K);
 - fission rate ($0\text{--}3 \cdot 10^{19}$ fiss $\text{m}^{-3} \text{s}^{-1}$).

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].

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

343 The results in Fig. 6 indicate that the PolyPole-1 algorithm represents a significant path forward in
344 this respect. First, it is evident that the overall accuracy of PolyPole-1 is vastly superior to both
345 FORMAS and URGAS. This is in agreement with the theoretical considerations made in Section 4.
346 Indeed, the accuracy of the FORMAS algorithm may be improved by an increase in the number of
347 parameters [31,36]. However, the accuracy of the PolyPole-1 algorithm can also be further
348 improved by increasing the order of the polynomial corrective term (Eq. 13) and/or by decreasing
349 the limiting value for the approximation of the series (Eq. 16). Furthermore, PolyPole-1 overcomes
350 the deficiency at low FGR that characterizes the FORMAS algorithm. Remarkably, the relative
351 error associated with PolyPole-1 is highly consistent over the whole range of intra-granular fission
352 gas release. This also confirms practically the theoretical considerations made in Section 4 on the
353 inherent capability of PolyPole-1 to allow for a more consistent level of accuracy over different
354 conditions through automatic adaptation of the number of considered series terms.

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

366 numerical algorithms that allow for a faster computation while preserving accuracy, such as
367 PolyPole-1.

368

369

370 Figure 3. Comparison between the values of intra-granular fission gas release calculated by the
371 URGAS algorithm and by the reference finite difference algorithm. Each data point corresponds to
372 a calculation with randomly generated conditions.

373

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

377
378 Figure 5. Comparison between the values of intra-granular fission gas release calculated by the
379 PolyPole-1 algorithm and by the reference finite difference algorithm. Each data point corresponds
380 to a calculation with randomly generated conditions.

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

385
 386 Figure 7. Comparison between the computational times associated with the finite difference,
 387 URGAS, FORMAS and PolyPole-1 algorithms. Each data point corresponds to a calculation with
 388 randomly generated conditions.

389 6. Conclusions and perspectives

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

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

- 403 • The accuracy of the PolyPole-1 solution is high and superior to other algorithms.
- 404 • 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 approach 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 [37]. 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 is governed by similar equations), or intra-granular fission gas release from the columnar grains of the restructured region of mixed oxide 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.

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Appendix

Analytic solution of 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

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

where r is 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

$$\psi_k \frac{\partial z_k}{\partial t} = \beta + z_k D_{\text{eff}} \nabla^2 \psi_k \quad (\text{A.2})$$

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

$$\psi_k = \frac{1}{\sqrt{2\pi a}} \frac{\sin \lambda_k r}{r} \quad (\text{A.3})$$

469 with the eigenvalues

$$\lambda_k^2 = \frac{k^2 \pi^2}{a^2} \quad (\text{A.4})$$

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

$$\langle \psi_n | \psi_k \rangle = \int_0^a 4\pi r^2 \psi_n \psi_k dr \quad (\text{A.5})$$

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

$$\frac{\partial z_n}{\partial t} = \beta_n - \delta_n z_n \quad (\text{A.6})$$

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

$$z_{0,n} = \langle \psi_n | \bar{c}_0 \rangle \quad (\text{A.7})$$

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

$$sZ_n - z_{0,n} = \frac{\beta_n}{s} - \delta_n Z_n \quad (\text{A.8})$$

476 where $Z_n = \mathcal{L}(z_n)$. Eq. A.8 is solved for

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

477 The inverse transform of Eq. A.9 is

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

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

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

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

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

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

$$\bar{c}_t(t) = \bar{c}_0 \frac{6}{\pi^2} \sum_{n=1}^{+\infty} \frac{1}{n^2} \exp\left(-\frac{n^2 \pi^2 D_{\text{eff}} t}{a^2}\right) + \frac{\beta a^2}{15 D_{\text{eff}}} \left\{ 1 - \frac{90}{\pi^4} \sum_{n=1}^{+\infty} \frac{1}{n^4} \exp\left(-\frac{n^2 \pi^2 D_{\text{eff}} t}{a^2}\right) \right\} \quad (\text{A.13})$$

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