# SCIANTIX OPEN-SOURCE CODE FOR FISSION GAS BEHAVIOUR:

# OBJECTIVEs AND FORESEEN DEVELOPMENTS

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Fuel performance codes (FPCs) have been developed and validated for the predictive analysis of the behaviour of nuclear fuel rods under irradiation [1]–[8]. Fission gas behaviour (FGB) represents a potential life-limiting factor for the operation of nuclear, and requires dedicated modelling efforts in the frame of FPCs [5], [8]–[11].

To model FGB, physics-based models (in particular, rate-theory models) offer inherent advantages:

* They can describe with a limited set of governing differential equations different phenomena, hence being applicable to different fuel materials with minor modifications [12]–[15].
* They are naturally applicable for the simulation of a wide range of operational and accidental transient scenarios [16]–[22].
* They benefit directly from the availability of new experimental data, since these data can be used to extend their validation database [12].
* They allow for bridging information arising from lower-length scales (e.g., by definition of specific model parameters [17], [23]–[30]).

To leverage these advantages, different codes dealing with physics-based modelling of FGB have been developed [17], [18], [31]–[42]. Remarkably, none of these codes is open source, hindering their applicability in the frame of multi-scale//multi-physical projects involving different software tools.

Given the importance of FGB modelling in fuel performance simulations, the SCIANTIX FGB code [43], [44] has been developed with the objective of:

* Effectively bridging lower-length scale and the engineering scale of fuel performance simulations, acting as FGB module within the FPCs that translates in the preferential use of physics-based models with a focus on keeping a limited CPU time.
* Being applicable as a stand-alone code for the simulation of separate-effect experiments at the fuel-grain scale involving inert gas behaviour (or in general for samples with uniform conditions), both supporting the design of the experiment itself and the interpretation of the results.

SCIANTIX is available as open source under MIT license [43], greatly easing its usage as FGB module in existing FPCs. Because of this licensing choice, all the models implemented in the currently available version of SCIANTIX are already published and validated.

We herein briefly report the inert gas behaviour models for UO2 available in the current version of SCIANTIX. More detailed information about each model can be found in dedicated publications [18], [22], [32], [45]–[47]. The present abstract is concluded by a description of envisaged developments, targeted in the frame of several research initiatives, and by an outline of the strategy foreseen for the further development of open-source software and documentation.

The basic features of FGB models adopted in SCIANTIX can be divided in two steps; the *intra-granular* and the *inter-granular* behaviour.

The *intra-granular* FGB model currently available in SCIANTIX [45] considers single-gas atom diffusion, gas bubble nucleation, re-solution, and gas atom trapping at bubbles. Intra-granular diffusion is treated by assuming a spherical grain of radius *a* [48], and adopting the approach proposed by Speight [49], i.e., following the evolution of the total intra-granular gas concentration, given by the sum of the single-atom gas concentration *c*1 and the gas concentration trapped in intra-granular bubbles *m*:

|  |  |
| --- | --- |
| $$\left\{\begin{array}{c}\frac{∂}{∂t}\left(c\_{1}+m\right)=\frac{α}{α+β}D\frac{1}{r^{2}}\frac{∂}{∂r}r^{2}\frac{∂}{∂r}\left(c\_{1}+m\right)+yF\\ \\\frac{d}{dt}N\_{ig}=ν-αN\_{ig} \end{array}\right.$$ | (1) |

where *D* is the single-atom diffusion coefficient, *α* is the re-solution rate, *β* is the trapping rate, *y* is the fission yield of fission gas, *F* is the fission rate, *r* is the radial coordinate within the grain, and *t* is time.

The evolution of intra-granular bubble concentration *N*ig assumes that bubbles are formed at a nucleation rate *ν* and destroyed by irradiation induced re-solution.

The intra-granular component of the gaseous swelling is derived as:

|  |  |
| --- | --- |
| $$\left(\frac{ΔV}{V}\right)\_{ig}=\frac{4}{3}πN\_{ig}R\_{ig}^{3}$$ | (2) |

in which the average radius of intra-granular bubbles *R*ig is calculated adopting a hard-sphere equation of state [45].

The *inter-granular* bubble evolution model currently available in SCIANTIX is the one proposed by Pastore et al. [18], [32], extended to consider the micro-cracking of grain boundaries during temperature transients [22], [50]. The evolution of the inter-granular gas concentration *q* is described as:

|  |  |
| --- | --- |
| $$\frac{∂}{∂t}q=-\left[\frac{3}{a}\frac{α}{α+β}D\frac{∂}{∂r}\left(c\_{1}+m\right)\right]\_{r=a}-R$$ | (3) |

The source term for *q* is the flux of single atoms diffusing from inside the fuel grain – from Eq. (1), whereas the release term *R* is modelled accounting for the gas atoms arriving at the grain boundaries and being collected in inter-granular bubbles of lenticular shape. The growth of these bubbles is diffusion-controlled and governed by the over-pressurization due to the presence of fission gases [51]. As bubbles grow, they interconnect, resulting in a decreasing inter-granular bubble concentration *N*gf on grain faces as their projected area on the grain face *A*gf grows. The net result of inter-granular bubble growth and interconnection is the increase of the grain-face fractional coverage *F*gf = *N*gf *A*gf (/). When the fractional coverage reaches a saturation value *F*gf = *F*gf,sat = 0.5, it is assumed that the grain faces are vented, allowing for the release of gas from the grain boundaries.

Paired to this mechanistic description of fission gas release, the inter-granular component of fission gaseous swelling is connected to the evolution of the bubble population by:

|  |  |
| --- | --- |
| $$\left(\frac{ΔV}{V}\right)\_{gf}=\frac{3}{a}\frac{4π}{3}N\_{gf}R\_{gf}^{3}$$ | (4) |

where *R*gf is the radius of inter-granular bubbles and 3/*a* is the surface-to-volume ratio of fuel grains.

The validation strategy applied for SCIANTIX involves both stand-alone validation against available separate-effect experiments, and as well the comparison between the results from integral irradiation experiments and the simulation results of FPCs including SCIANTIX as FGB module [22], [50], [52]. For the sake of brevity, we herein report a summary of the stand-alone validation database of SCIANTIX, focusing on gaseous swelling (Fig. 3), i.e., comparing the predictions on both intra-granular swelling, Eq. (2), and inter-granular swelling, Eq. (4).

The experimental database by Baker [53] is made of irradiation at constant temperatures (from 1273 K to 2073 K) and relatively low burn-up (6.5 GWd/tUO2) of standard uranium dioxide fuels in the UKAEA’s Winfirth SGHWR. The results are in line with those shown in a previous publication of the intra-granular model employed in SCIANTIX [45], and demonstrate an acceptable deviation from the experimental data in terms of gaseous swelling.

As for inter-granular swelling, the considered experimental cases are taken from the database by White and co-workers [54]. The database consists in measurements performed on uranium dioxide AGR (Advanced Gas Reactor) samples of fuel rods irradiated up to burnup between 9 and 21 GWd/tUO2 in the Halden reactor, followed by power ramp tests or power cycle histories.

The comparison shows a satisfactory agreement between calculated and measured data, yet showing an overestimation of the low swelling data.



FIG.1. Comparison of calculated intra- and inter-granular gaseous swelling by SCIANTIX with the experimental data by Baker [53] (swelling due to intra-granular bubbles, blue markers) and by White and co-workers [55] (swelling due to inter-granular bubbles, red markers). This figure is reproduced from [44].

We conclude the description of SCIANTIX by outlining the ongoing model developments and the research initiatives in which these activities are grafted:

* The mechanistic description of helium behaviour is being pursued [56]–[58]. Modelling of helium is important for the simulation of uranium-plutonium mixed oxide fuels and minor-actinide bearing fuels, being a research topic in the frame of the INSPYRE [59] and PATRICIA [60] Projects.
* The inclusion of a depletion module [61], i.e., describing the evolution of a set of nuclide concentrations along burnup [62]–[64]. Tracking of radioactive fission products is relevant in the frame of the R2CA Project [65], whereas the helium production rate is again connected to the activities performed in INSPYRE [59] and PATRICIA [60].
* The mechanistic description of the migration of radioactive fission products from their production within the fuel to the fuel rod gap, relevant for the assessment of radiological consequences of accidents and therefore targeted in the R2CA Project [65].
* The description of intra-granular bubble coarsening, extending the model presented in this abstract by adding an additional growth mechanism of the bubbles close to dislocations [54]. This model will allow a more accurate description of intra-granular bubble swelling during transients and has being targeted in the frame of an I-NERI collaboration between Idaho National Laboratory, Joint Research Centre – Karlsruhe, and Politecnico di Milano.
* The description of a model describing the formation of high burnup structure and the evolution of its local porosity [66], [67], targeted in INSPYRE [59] and R2CA [65].

As for the inclusion of SCIANTIX within fuel performance codes as a FGB module, the current status is that coupling has been demonstrated in TRANSURANUS [68] and GERMINAL [69] in the frame of the INSPYRE Project [59], and in the OFFBEAT opensource fuel performance code [70]. Integration with other codes is being discussed in the frame of the already referred projects.

As the SCIANTIX code is growing in its predictive capabilities, we are planning different actions to support its continuous opensource development:

* The current and future versions of the code are going to always be hosted on the online repository Gitlab.
* The development of an object-oriented version is targeted, to ease the incorporation/coupling in/with other opensource tools and ensure the maintainability of the code itself.
* The documentation of the code is progressively going to be integrated with a video-manual, i.e., a set of recorded short videos detailing the various model capabilities and the respective validation. The goal is to involve the users in the realization of these videos, starting from the MSc/PhD students working on SCIANTIX at Politecnico di Milano.
* The verification strategy of the numerical solvers included in the code, already available based on the method of manufactured solutions is going to be standardized and made available to the users through dedicated routines.
* The inclusion of a set of regression tests is targeted, supporting the robustness of the code as it develops.

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