SIMULATION OF FISSION GAS RELEASE IN THE 3D FUEL PERFORMANCE CODE OFFBEAT

A. GIANESELLO
Department of Energy and Environmental Engineering, National Institute of Applied Sciences of Lyon
Lyon, France

A. SCOLARO
Laboratory for Reactor Physics and System Behavior, EPFL
Lausanne, Switzerland

C. FIORINA
Laboratory for Reactor Physics and System Behavior, EPFL
Lausanne, Switzerland
Email: carlo.fiorina@epfl.ch

Abstract

The OpenFOAM Fuel BEhavior Analysis Tool (OFFBEAT) is a multidimensional fuel behavior solver under development at the Laboratory for Reactor Physics and Systems Behavior EPFL and at the Paul Scherrer Institut, in Switzerland. OFFBEAT relies upon the OpenFOAM C++ library and it aims to be a complement to traditional fuel performance codes for the study of 2D and 3D phenomena occurring in fuel rods. Although initially developed for light water reactors, the tool displays a wide flexibility and work is ongoing for its extension to Fast Reactor applications. Among various ongoing developments, this paper presents the integration of an accurate fission gas release model. The implementation, presented in this work, is based on the 0-D inert gas behavior code SCIANTIX, developed at Politecnico di Milano and designed to be coupled with fuel performance codes. The correct implementation of this fission gas release model in OFFBEAT is assessed with validation tests, using experimental data from the International Fuel Performance Experiments database, the Super-Ramp PWR program, and the Risø-3 experiment.

1. INTRODUCTION

Modelling the behavior of nuclear fuel rods under irradiation is essential to ensure the licensing and safe operation of nuclear reactors and to enable fuel design optimization. In that purpose, fuel performance codes have been developed to predict the multitude of complex multi-scale and multi-physics phenomena occurring in fuel rods [1]. Although the traditional approach to fuel analysis is based on 1.5-D models, several efforts have been recently directed towards the development of advanced 2-D and 3-D solvers that could help improve our understanding of the complex phenomena that characterize fuel behavior. Well-known examples of advanced codes are the BISON code developed at the Idaho National Laboratory (US) and the ALCYONE code developed at the CEA (France).

In this context, in 2017 the École Polytechnique Fédérale de Lausanne (EPFL) and the Paul Scherrer Institut (PSI) have started developing a new multi-dimensional code named OpenFOAM Fuel BEhavior Analysis Tool (OFFBEAT) [2]. It is based on the OpenFOAM C++ library [3], [4] and it allows for a full range of modelling possibilities, including 1.5-D, 2-D r-z, 2-D r-theta and full 3-D simulations. The choice of OpenFOAM as base library implies that the partial differential equations are discretized with finite volume techniques on unstructured meshes. The solver is fully parallelized through geometrical domain decomposition.

A main goal of OFFBEAT consists in enhancing the knowledge of poorly known 2-D and 3-D mechanisms relevant for reactor safety, such ridging and the PCMI in the presence of a missing pellet surface, as well as in-pile experiments featuring non-traditional geometries (see for instance [5]). Concurrently, the object-oriented programming and high-level API allows for quick tailoring of the solver to specific needs, testing of behavioral models, and extension to different fuel types.

OFFBEAT underwent a preliminary validation for the thermal behavior of Light Water Reactor (LWR) rods [6]. These first applications were limited to a linear-elastic framework, with the addition of fuel densification, swelling and relocation. A plasticity model was introduced in [7] and models for the thermal and irradiation creep of the Zircaloy cladding were implemented in [8] based on the work of Limbäck and Anderson. Models have then been introduced for fuel creep, based on the FCREEP routine from MATPRO, as well as for fuel isotropic cracking.

OFFBEAT can directly be coupled to Computational Fluid Dynamics (CFD), neutronics or chemical solvers developed by the OpenFOAM community while recent efforts have provided OFFBEAT with the ability to determine the fuel radial power profile either through a methodology similar to TRUBRNP or through a coupling with the Monte Carlo code Serpent2 [9]. In addition, a collaboration between the EPFL and the Joint Research Centre in Karlsruhe has been established, aiming at developing an optimal interaction strategy between OFFBEAT and the well-known fuel performance code TRANSURANUS [10].

The present paper focuses on the implementation in OFFBEAT of a mechanistic fission gas release model, based on the 0-D inert gas behavior code SCIANTIX [11]. This feature is preliminary validated against experimental data from the International Fuel Performance Experiments (IFPE) database, the Super-Ramp PWR program, and the Risø-3 experiment. The paper is structured as follows. Section 2 proposes a brief overview of the main characteristics of OFFBEAT. Section 3 presents the SCIANTIX fission gas release code. Section 4 introduces the experimental cases used for validation. Finally, Section 5 focuses on code testing and validation.

2. THE OFFBEAT FUEL BEHAVIOR ANALYSIS TOOL

OFFBEAT is an open-source, multi-dimensional fuel performance code. It solves for heat diffusion and deformations, and it features:

- Experimental correlations for the temperature- and burnup-dependent material properties.
- Semi-empirical models for fuel relocation, cracking, densification, and irradiation growth.
- Models for rate-independent plasticity and creep.
- A neutronics module derived from TUBRNP to calculate radial power profiles and isotopic evolution.
- A gap conductance model derived from the FRAPCON code but extended to a multi-dimensional framework.
- An explicit contact model based on the penalty method, as well as a novel implicit contact model to improve convergence, notably when modelling multiple separated pellets.
- Scripts and tools that simplifies the creation of geometries and post-processing of data.

Thanks to the use of OpenFOAM as base numerical library, OFFBEAT features:

- Routines for mesh generation and manipulation, with the additional possibility to readily import geometries and meshes from available tools such as Salome.
- Professional data processing and visualization with the ParaView open-source software.
- Finite volume discretization, with an intuitive formulation based on control volume balances.
- Unstructured meshes and arbitrary geometries, with the possibility of 1D, 2D or 3D analysis also for less conventional fuel configurations, such as experimental rods or plate-type fuel.
- State of the art linear algebra solvers.
- Massive parallelization.
- Streamlined multi-physics possibilities thanks to the straightforward coupling with the standard CFD solvers or any other code developed with the OpenFOAM library.

In terms of interactions with other codes, a coupling between OFFBEAT and the European fuel performance code TRANSURANUS has been developed. In addition, a coupling option has been developed for the Serpent2 Monte Carlo code for neutron transport.

3. IMPLEMENTATION OF SCIANTIX IN OFFBEAT

SCIANTIX is an open-source C++ code designed to be implemented in fuel performance codes to model fission gas release. The models implemented in SCIANTIX cover both the intra-granular and inter-granular inert gas behavior in UO2 under constant or transient conditions. The diffusion of gas atoms inside the grain can be treated either with the traditional FORMAS algorithm or with a novel methodology based on modal expansion [11]. The release from the grain boundaries takes into account the evolution of the inter-granular bubbles and it is based on the work of Pastore et al. [11]. Also, SCIANTIX includes models for grain growth, intra- and inter-granular gaseous swelling.

SCIANTIX is referred to as a 0-D code since it models the gas behavior at the scale of a fuel grain and all the variables are treated as average in space and evolving in time. The code being 0-D, it must be called at each mesh cell, for each iteration and for each time step of the fuel performance code it is coupled with. Thus, SCIANTIX is called a substantial number of times and has been designed to have a computational time in the order of milliseconds/call.

In the frame of this work, SCIANTIX has been wrapped in a C++ class and implemented in the solution scheme of OFFBEAT. This is composed of three loops: The time-iteration loop allows to advance in time; the outer-iteration loop to couple different physics; and the inner-iteration loop to solve each single physics. For each outer iteration, OFFBEAT feeds SCIANTIX with the values of temperature, fission rate and hydrostatic stress from the previous outer iteration. The physical state variables of SCIANTIX (i.e. grain radius, inert gas concentrations, gaseous swelling, etc.) are set and initialized in the class. SCIANTIX is then called for each cell of the fuel mesh, allowing to update the physical state variables. In addition to wrapping SCIANTIX into a class and integrating it into the solution algorithm of OFFBEAT, a model has been included for grain boundary sweeping.

SCIANTIX calculates the volume number density (atoms/m3) of helium, xenon and krypton, which is then converted into moles and transferred to the gap gas model. In particular, SCIANTIX provides for each cell the volume number density (atoms/m3) of gas released (nreleased) and gas produced (nproduced). These quantities are converted into atoms per cell and summed over the whole mesh, allowing to calculate the integral FGR (%) for each time step of OFFBEAT, as follows:

$$FGR[\%] = \frac{\sum_{cells} n_{released} Volume_{cell}}{\sum_{cells} n_{produced} Vol_{umecell}}$$

In the outer iteration, the gap model also uses the temperature and displacement values from the previous outer iteration to update the gap free volume and the gas pressure. The tasks described are performed iteratively until both the thermal and mechanical sub-solvers are converged.

The proper functioning of SCIANTIX in OFFBEAT was verified by ensuring that identical results are obtained with SCIANTIX as the stand-alone code and results obtained with SCIANTIX as fission gas release model in OFFBEAT.

4. EXPERIMENTAL DATA USED FOR VALIDATION

Three different fuel irradiation experiments from the OECD/NEA IFPE database have been considered for code validation, namely: the IFA-432 assembly, the Super-Ramp PWR program, and the Risø-3 experiment. The aim of the validation is mainly to reproduce the evolution of the fuel center temperature (FCT) in the rods and obtain an accurate amount of FGR at the end of irradiation.

4.1. IFA-432 assembly

The IFA-432 is composed of 6 rods that were irradiated in the Halden Boiling Water Reactor in Norway. The rods were designed to study the thermal and mechanical response of BWR fuel, up to a burnup of approximately 40 MWd/kgU, and were instrumented to monitor fuel centerline temperatures, cladding elongations, internal fuel rod pressures and local power during irradiation. In particular, two thermocouples (TCs) were inserted through holes in the bottom and top ends of the fuel stack. However, the precise position of the temperature measurement point was not indicated in the received database, leading to some uncertainties in the results.

No data related to Rod 4 is available, since this rod was discharged early during the experiment. Rod 2 and 6 presented instead specific features that make them unsuited to verify codes that are tailored to the analysis of standard fuel rods. In particular, rod 2 had a very large gap while rod 6 was loaded with a fuel with 92% theoretical density and unstable with respect to densification. For each of the 3 remaining rods (rods 1, 3 and 5.), a 2D axisymmetric model was built (including the two TCs holes).

4.2. Super-ramp program

The Studsvik PWR Super-Ramp project (1980 – 1983) aimed at investigating the failure propensity of LWR fuel rods subjected to power ramps. The 11 rods of interest belong to 3 rod groups: PK1, PK2 and PK6 and were first base irradiated in the Obrigheim power reactor in Germany, at time-averaged power ratings of approximately 14 – 26 kW/m, and to to peak burnups of approximately 33 – 45 MWd/kgU. The rods were then ramp tested in the research reactor R2 at Studsvik in Sweden. Rod puncturing allowed to measure integral FGR at the end of irradiation. Groups PK1 and PK2 are composed of standard fuel rods. Group PK6 is made of test fuel rods featuring large grain size, leading to a low FGR compared to groups PK1 and PK2.

4.3. Risø 3 experiment

The experimental fuel segments AN2 and AN3 from the Risø-3 fission gas project have also been considered. These 2 segments were first base irradiated in the Biblis A PWR in Germany from 1982 to 1986, reaching a final burnup of approximately 40 MWd/kgU, before being bump tested during 72 hours in the test reactor DR3 at Risø in Denmark, under PWR conditions. Prior to the bump test, after the base irradiation, the AN2 rod segment was neither punctured nor opened for refabrication. On the contrary, the AN3 rod segment was refabricated: in particular, the fuel segment was shortened, drilled at the top and refilled with helium at 14.7 bar. The segment was instrumented with a pressure transducer and a fuel centerline thermocouple, allowing to measure the temperature at a point situated 1.5 pellet lengths above the bottom of the thermocouple hole. The 72 hours ramp test reached a peak power around 40 kW/m and a final burnup around 41.8 MWd/kgU. The AN2 and AN3 segments were modelled in 1-D. For AN3, the refabricated geometry (with the presence of the hole) was assumed for both the base irradiation and the bump test. Moreover, the refabrication was taken into account by redefining specific parameters (i.e. helium filling pressure, coolant pressure, cladding outer surface temperature).

5. RESULTS AND DISCUSSION

5.1. FCT predictions

Figure 1 shows the comparison between FCTs predicted by OFFBEAT+SCIANTIX, and the experimental FCTs, for the mentioned 3 rods of the IFA-432 assembly. The difference between the measured and predicted FCTs appears to be low for Rods 1 and 3, considering the important source of uncertainties associated to the exact position of the thermo-couple and the fact that the description of the experiment only provides ranges for the value of the grain radius while it was arbitrarily decided to employ the average value in this range.

Discrepancies are instead more significant for rod 5. To better understand them, Fig 2 shows the results of rod 2 as a function of the irradiation time. For convenience, also the results obtained without fission gas release have been reported. One can observe how OFFBEAT+SCIANTIX can predict well FCTs at the beginning of the irradiation, while significantly overpredicting them for higher burnups. Although the exact reason for this behavior is not fully clear, one should notice that rod 5 is characterized by a 92% theoretical density of the fuel, which is not a typical value for which SCIANTIX was calibrated.

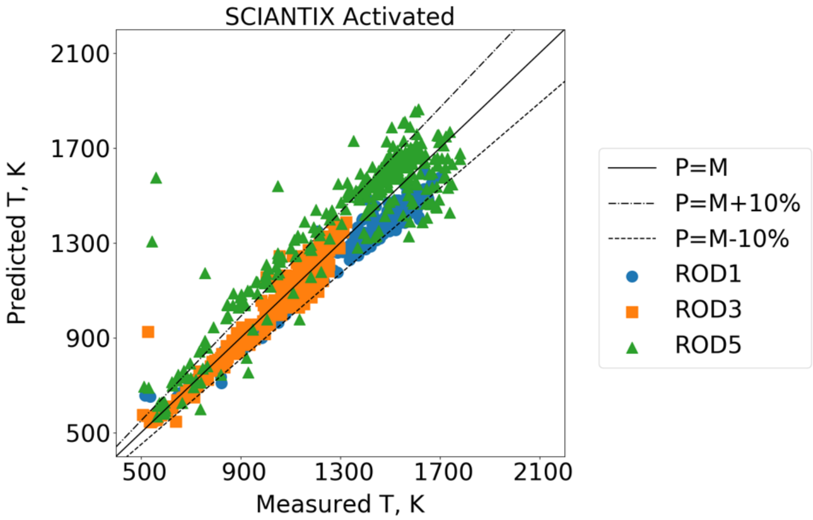

FIG. 1 – Comparison between measured and calculated FCTs for rods 1, 3 and 5 of the IFA-432 assembly

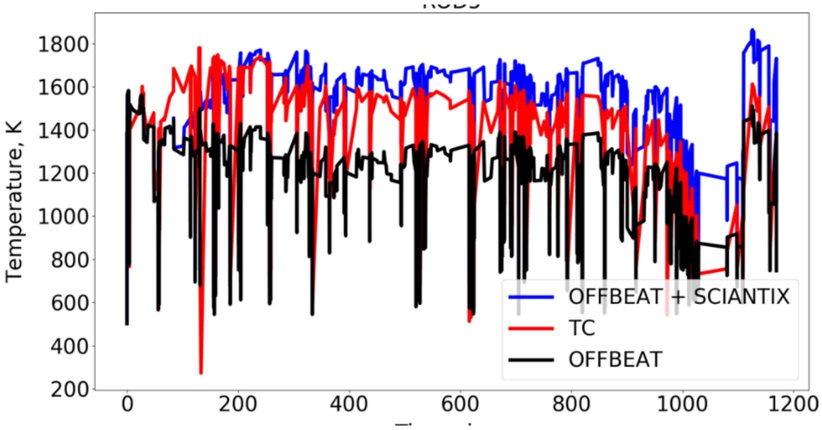

FIG. 2 – Comparison between measured and calculated FCTs (with and without SCIANTIX) for rod 5 of the IFA-432 assembly

Figure 3 illustrates the difference between the measured and calculated FCTs during the bump test of rod AN3. The 2 profiles are in very good agreement, though some discrepancies can be observed after the ramps, where the experimental temperature slightly decreases while the OFFBEAT temperature remains flat. However, this type of discrepancy is often observed in fuel performance codes and it is assumed to be due to fuel creep.

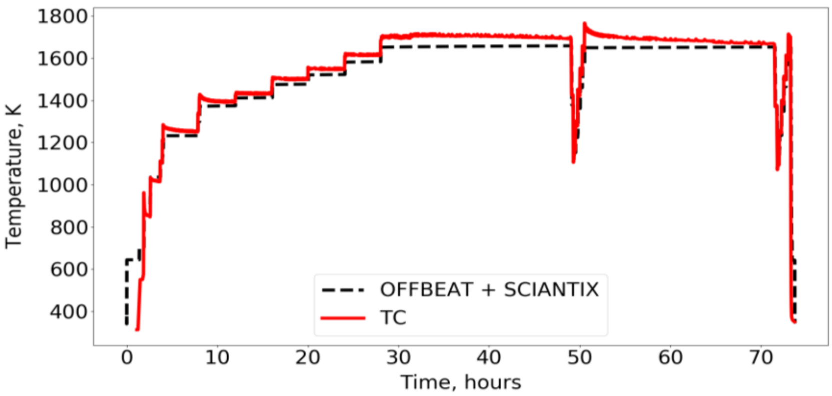

FIG. 3 – Comparison between measured and calculated FCTs for the AN3 rod

5.2. Fission gas release results

In this section, the integral FGR calculated at the end of irradiation is compared to the measured FGR, for the Super-Ramp and Risø-3 fuel rods. The integral FGR corresponds to the ratio of the fission gas released in the fuel rod free volume to the generated gas. The results are tabulated in Table 1 and plotted in Figure 4, with the two dashed lines representing a deviations of a factor of 2 from measured data. Due to the uncertainties embedded in FGR models coming for example from the correlations used for the gas diffusion coefficient, from the different modeling strategies adopted for the gaseous release from the grain boundaries etc., a factor of 2 is typically accepted in similar validation works [12]. One should also consider that the release of Kr and Xe atoms in the rod free volume affects only one portion of the total temperature jump from coolant to fuel centerline (namely, the gap temperature jump). In addition, large fractions of FGR are associated with high burnups, when the gap of a traditional LWR rod is closed and gap conductance is dominated by contact.

From Figure 4 it can be observed that OFFBEAT provides good prediction for most rods, notably considering the large deviations in predictions that are typically observed in the literature. It is worth noting that the FGR value for AN3 has been obtained based on an experimentally measured grain size of 6 um (2-D linear intercept). The result drastically improves (34% FGR) when using the 3 um that are indicated in the FUMEX international benchmark.

TABLE 1 – COMPARISON BETWEEN MEASURED AND CALCULATED FGRS

Fuel rod	Experiment	FGR measured (%)	FGR calculated (%)
PK1-1	Super-Ramp	8.5	13.9
PK1-2	Super-Ramp	13.6	15.7
PK1-3	Super-Ramp	22.1	18.5
PK1-4	Super-Ramp	13.0	15.5
PK2-1	Super-Ramp	28.0	18.9
PK2-2	Super-Ramp	32.1	23.9
PK2-3	Super-Ramp	44.9	26.8
PK2-4	Super-Ramp	9.5	11.4
PK6-2	Super-Ramp	3.5	3.3
PK6-3	Super-Ramp	6.7	3.6
PK6-S	Super-Ramp	6.1	3.2
AN2	Risø-3	29.7	24.9
AN3	Risø-3	35.5	25.6

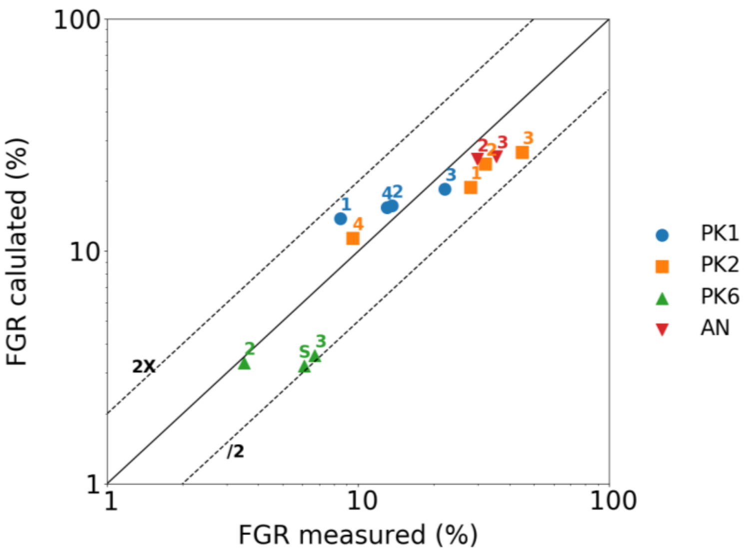

FIG. 4 – Comparison between measured and calculated FGRs

6. CONCLUSIONS

This work presented the implementation of the SCIANTIX inert gas behavior model into the OFFBEAT multi-dimensional fuel performance code, including its preliminary validation against experimental fuel rods from the IFA-432 assembly, Super-Ramp program and Risø-3 experiment. Obtained results can be considered as satisfactory and in-line with other results obtained by various authors.

7. AKNOWLEDGMENTS

This work is complementary to and partly motivated by the IAEA Open-source Nuclear Codes for Reactor Analysis (ONCORE) initiative, a collaborative framework for the development and application of open-source multiphysics software to support research, education, and training in analysis of advanced reactor designs.

REFERENCES

[1] P. van Uffelen, J. Hales, W. Li, G. Rossiter, and R. Williamson, “A review of fuel performance modelling,” *Journal of Nuclear Materials*, vol. 516. Elsevier B.V., pp. 373–412, Apr. 01, 2019. doi: 10.1016/j.jnucmat.2018.12.037.

[2] A. Scolaro, I. Clifford, C. Fiorina, and A. Pautz, “The OFFBEAT multi-dimensional fuel behavior solver,” *Nuclear Engineering and Design*, vol. 358, Mar. 2020, doi: 10.1016/j.nucengdes.2019.110416.

[3] “OpenFOAM,” 2021. www.openfoam.com

[4] C. Fiorina, I. Clifford, S. Kelm, and S. Lorenzi, “On the development of multi-physics tools for nuclear reactor analysis based on OpenFOAM®: state of the art, lessons learned and perspectives,” *Nuclear Engineering and Design*, p. 111604, Dec. 2021, doi: 10.1016/J.NUCENGDES.2021.111604.

[5] A. , Scolaro, P. , van Uffelen, C. , Fiorina, A. , Schubert, I. , Clifford, and A. ’ Pautz, “Investigation on the effect of eccentricity for fuel disc irradiation tests,” *Nuclear Engineering and Technology*, vol. 53, pp. 1602–1611, 2021.

[6] A. Scolaro, I. Clifford, C. Fiorina, and A. Pautz, “First steps towards the development of a 3D nuclear fuel behavior solver with openfoam,” in *International Conference on Nuclear Engineering, Proceedings, ICONE*, 2018, vol. 3. doi: 10.1115/ICONE26-82381.

[7] A. Scolaro, I. Clifford, C. Fiorina, and A. Pautz, “Cladding plasticity modeling with the multidimensional fuel performance code offbeat,” *TopFuel*, 2019.

[8] A. Scolaro, C. Fiorina, I. Clifford, and A. Pautz, "Multi-dimensional Creep Analysis Using the Novel OFFBEAT," *in Progress on Pellet–Cladding Interaction and Stress Corrosion Cracking. Experimentation, Modelling and Methodologies Applied to Support the Flexible Operation of Nuclear Power Plants. Report of a Technical Meeting*, 2019.

[9] J. Leppänen, M. Pusa, T. Viitanen, V. Valtavirta, and T. Kaltiaisenaho, "The Serpent Monte Carlo code: Status, development and applications in 2013," *Annals of Nuclear Energy*, vol. 82, pp. 142–150, Aug. 2015, doi: 10.1016/j.anucene.2014.08.024.

[10] A. Scolaro, C. Fiorina, P. van Uffelen, I. D. Clifford, and A. Pautz, "Coupling of the OFFBEAT 3-D fuel behaviour solver with TRANSURANUS," *Nuclear Engineering and Design*, vol. Submitted, 2022.

[11] D. Pizzocri, T. Barani, and L. Luzzi, "SCIANTIX: A new open source multi-scale code for fission gas behaviour modelling designed for nuclear fuel performance codes," *Journal of Nuclear Materials*, vol. 532, p. 152042, Apr. 2020, doi: 10.1016/j.jnucmat.2020.152042.

[12] G. Pastore *et al.*, "Uncertainty and sensitivity analysis of fission gas behavior in engineering-scale fuel modeling," *Journal of Nuclear Materials*, vol. 456, pp. 398–408, Jan. 2015, doi: 10.1016/j.jnucmat.2014.09.077.