

ANALYSIS OF THE BEHAVIOR UNDER IRRADIATION OF HIGH BURNUP NUCLEAR FUELS WITH THE COMPUTER PROGRAMS FRAPCON AND FRAPTRAN

Regis Reis and Antonio Teixeira e Silva

Instituto de Pesquisas Energéticas e Nucleares (IPEN/CNEN-SP)
Av. Professor Lineu Prestes 2242
05508-000 São Paulo, SP
teixeira@ipen.br

ABSTRACT

The objective of this paper is to verify the validity and accuracy of the results provided by computer programs FRAPCON-3.4a and FRAPTRAN-1.4, used in the simulation process of the irradiation behavior of Pressurized Water Reactors (PWR) fuel rods, in steady-state and transient operational conditions at high burnup. To achieve this goal, the results provided by these computer simulations are compared with experimental data available in the database FUMEX III. Through the results, it was found that the computer programs used have a good ability to predict the operational behavior of PWR fuel rods in high burnup steady-state conditions and under the influence of Reactivity Initiated Accident (RIA).

1. INTRODUCTION

Reliable prediction of nuclear fuel performance under operational conditions is a basic requirement for a safe and reliable design of a nuclear reactor. However, predicting the behavior of constituent components of a fuel element under operational conditions is an extremely complex task, since it involves the interaction of a large number of variables, which encompass the physicochemical properties of the materials involved, metallurgy, structural mechanics, mass transfer and heat transfer mechanisms and irradiation effects. Thus, a great effort has been made to study the behavior of nuclear fuel elements under operational conditions and, through these studies, to develop models that represent this behavior, so that they can be used in computer programs that simulate fuel performance under normal or transient operating conditions.

Since computer programs use dozens of these models interactively, the results generated by the programs may have a relatively high degree of uncertainty. Therefore, it is essential that studies are conducted comparing the results provided by these computer programs with experimental data related to the behavior of fuel rods of nuclear reactors.

The main interest of this article is to verify the validity and precision of the results provided by the software FRAPCON-3.4a and FRAPTRAN-1.4 [1], [2], used in the simulation process of the behavior of fuel rods used in light water reactors (LWR), in different power situations, under permanent and transient operating conditions, and under high burnup conditions. In order to reach this objective, the data provided by these computer programs are compared with the experimental results made available in the FUMEX III database [3], [4], [5].

In this article, special emphasis is given to the fuel elements used in pressurized light water reactors (PWR), composed of fuel rods consisting of UO₂ fuel pellets and Zircaloy-4 cladding.

2. EFFECTS OF NUCLEAR FUEL IRRADIATION

During operation in the nuclear reactor core, the fuel rod is in a very severe environment, involving high levels of radiation and the application of high thermal and mechanical loads. This causes numerous and complex phenomena to occur in the various components of a fuel element, phenomena that cause a series of chemical, physical, metallurgical and structural changes.

As for the behavior of the UO₂ fuel pellets, because it is a ceramic material, besides the intense radiation, the pellets are subjected to severe thermal conditions. Due to the low thermal conductivity of this material, the heat generated due to the nuclear fissions occurring inside the fuel pellet finds great resistance to its propagation, which causes enormous temperature differences between the central region and the peripheral region of the fuel pellet. A typical UO₂ pellet operates at temperatures near the melting point in its central region and at temperatures slightly above those of the refrigerant in its peripheral region, implying a radial temperature gradient of the order of 2000-2200 °C/cm [6]. Such a thermal gradient results in a rapid cracking of the fuel pellet due to the appearance of thermal stresses. In addition, the irradiation process provides conditions for manifold transport mechanisms in the fuel, which lead to significant changes in the microstructure, composition and size of the fuel. According to ROY and SAH [7], the main effects of irradiation and high thermal gradients on UO₂ fuel pellets can be divided into five main categories: (1) densification; (2) restructuring; (3) redistribution of fuel and fission products; (4) effects related to fission gases: swelling and gas release; and (5) irradiation creep.

With regard to the behavior of the fuel rod cladding during the operation, one of the major concerns is to avoid perforations in the cladding wall. The appearance of these perforations can lead to damage that renders the entire fuel element inoperative and contaminates the refrigerant with radioactive material. Such perforations, in general, are due to corrosion and mechanical ruptures, or a combination of these two effects.

Currently, the most widely used material for the cladding of fuel rods for pressurized water reactors (PWR) is Zircaloy-4, but this has been gradually replaced by newer alloys such as ZIRLO and M5 [8]. Some characteristics that make this material suitable for such application are its low thermal neutron absorption section and its good mechanical characteristics and resistance to corrosion when subjected to normal operating conditions in a nuclear reactor, i.e. under irradiation conditions, corrosion, and with thermal and mechanical loads [9].

3. HIGH BURNUP EFFECTS IN THE NUCLEAR FUEL

With respect to the fuel pellet, three phenomena are significantly influenced by the high burnup conditions and, consequently, considered as life-limiting factors of the fuel rod: (1) fuel restructuring; (2) release of fission gases and; (3) degradation of the thermal conductivity [10], [11].

In relation to the cladding tube, high burnup conditions result in higher levels of corrosion, greater absorption of hydrogen and a greater degradation of its mechanical properties [12], [13]. Additionally, a very critical effect, which is more likely to manifest under high burnup conditions, is the mechanical interaction between pellet and cladding (Pellet-Clad Mechanical Interaction -PCMI).

4. ANALYSIS OF RESULTS

As previously emphasized, the main purpose of this study is to evaluate the accuracy of the FRAPCON-3.4a and FRAPTRAN-1.4 computer programs for determining the behavior of fuel rods under operational conditions. To achieve this goal, the FUMEX III database was used. Through the use of the information provided by this database, analyses were performed that allowed the results provided by the FRAPCON-3.4a and FRAPTRAN-1.4 programs to be compared with experimental data and also with results provided by other computer programs. From the experiments provided by the FUMEX III database, the following cases were selected for the analyses carried out in this article:

- For steady-state conditions, the following experiments were selected:
 - 1) IFPE/US-PWR-16x16 LTA (NEA-1738/01);
 - 2) IFPE/RISOEIII-GE7 (NEA-1493/17) with PCMI.
- For transient regime conditions, considering the occurrence of a RIA transient type, the following experiment was selected:
 - 1) IFPE/NSRR-FK1 (NEA-1724/01).

4.1. Case of US-PWR-16

The US-PWR-16x16-LTA experiment was conducted during the 1980s in the United States, in a commercial PWR reactor, to demonstrate the behavior of fuel rods in high burnup regimes. In this experiment, two test fuel elements, called D039 and D040, were used. Each of these elements consisted of a set of 236 fuel rods mounted on a 16x16 assembly, with five guide tubes for control rods and twelve spacer grids. The lower spacer grid was constructed with Inconel 625. All other spacer grids and all guide tubes were constructed with Zircaloy-4. In all assemblies, Zircaloy-4 was used as cladding tube material and fuel rod buffers.

The test fuel element D039 was subjected to three irradiation cycles with a total exposure of 885 effective days of maximum power, while the D040 element was subjected to five irradiation cycles with a total exposure of 1,641 days of maximum power. The burnup achieved for each of the assemblies is identical over the first three irradiation cycles, due to their placement in symmetrical central positions, and involves average values of the order of 39 MWd/kgU. For element D040, an average burnup of approximately 58 MWd/kgU was achieved as it was subjected to two additional cycles of irradiation.

The data documented by the FUMEX III final report for the IFPE/US-PWR-16x16-LTA experiment, fuel element D040, fuel-rod TSQ002, make it possible to perform the following analyses:

- Release of fission gases;
- Free volume of the fuel rod at the end of life;
- Fuel rod internal pressure;

- cladding creep.

Although the FUMEX III program does not provide data for the fuel temperature and fuel rod internal pressure for this experiment, the final report of the FUMEX III program presents an analysis of these quantities using data provided by the computer codes used by program participants. These analyses were also performed in this study.

4.1.1 Fuel Pellet Central Temperature

The final FUMEX III report (IAEA-FUMEX-III, 2013) provides, for the experiment in question, a graph with the temperature in the central region of the fuel pellet as a function of the average burnup obtained through computer simulation performed by the computer programs that participated in the project. This graph is presented in Figure 1. The results presented in this figure are of interest for this article as they allow a comparison of the result provided by the FRAPCON-3.4a code with the results provided by the other codes.

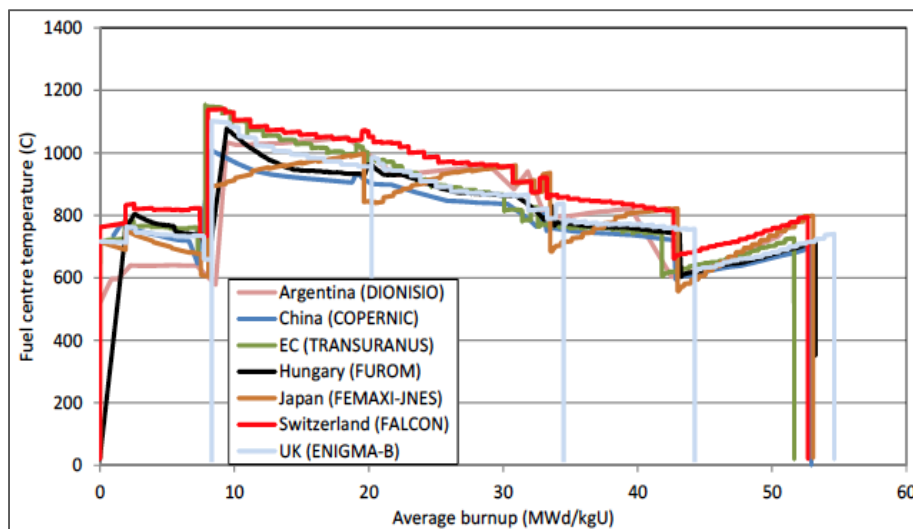


Figure 1 - Temperature variation of the central region of the fuel rod in function of the average burnup (Source: FUMEX III Final Report).

Figure 2 presents the result obtained for the temperature in the central region of the fuel pellet as a function of the burning through the execution of the code FRAPCON-3.4a for this experiment. Comparing Figures 1 and 2 it can be observed that there is a good convergence of the data provided by the FRAPCON-3.4a code with the data provided by the other codes, with a variation in relation to the mean of the values around 100 °C, considered acceptable by the FUMEX III Final Report.

4.1.2 Fission Gas Release

As for the percentage of fission gases released, the experiment obtained a value of 1.18% of the total gas produced at the end of the life of the fuel rod (approximately 58 MWd/kgU). This value is plotted in the graph provided in Figure 3, which also provides the values obtained for the release of fission gases through the use of computer codes used by the FUMEX-III program participants.

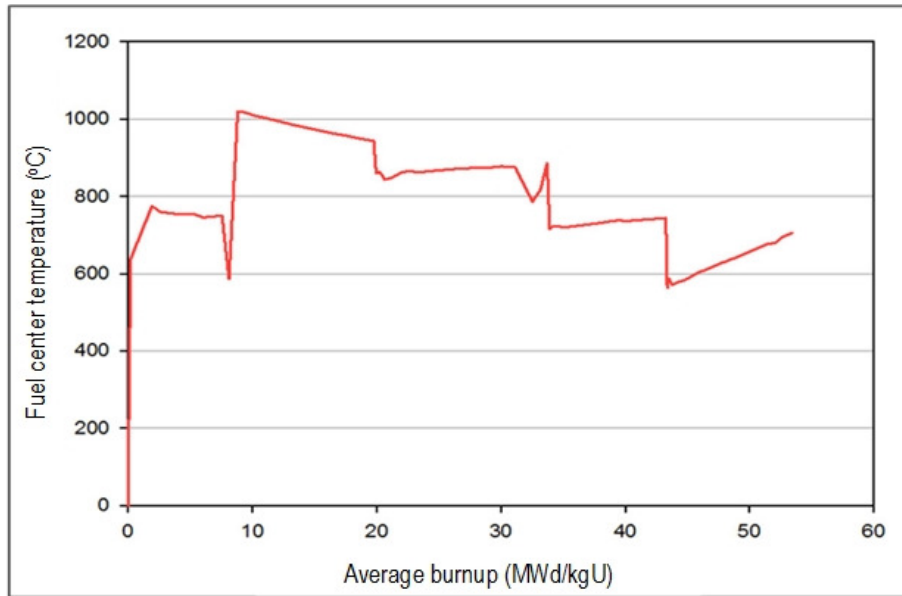


Figure 2 - Temperature variation of the central region of the fuel rod as a function of the average burnup provided by FRAPCON-3.4a (Source: Authors).

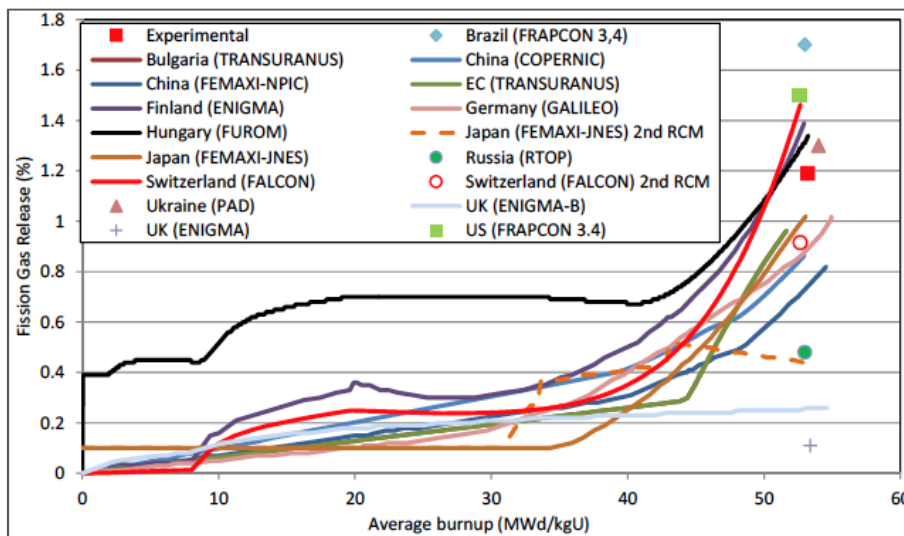


Figure 3 - Experimental value and predictions of computer codes for fission gas release (Source: FUMEX III Final Report).

Figure 4 shows the comparison between the result obtained through the experiment with the result obtained using the FRAPCON-3.4a code. In this figure there is a relatively sharp discrepancy of the result provided by the code when compared to the result obtained experimentally, and the result provided by the code has a value approximately 66% greater than the result obtained experimentally.

The most plausible explanation for this discrepancy is due to the complexity of the phenomena involved in the fission gas release process. This complexity makes it difficult to design models that allow simulating the behavior of the release of fission gases in the fuel pellet. Another factor that supports this hypothesis is the great dispersion of the results

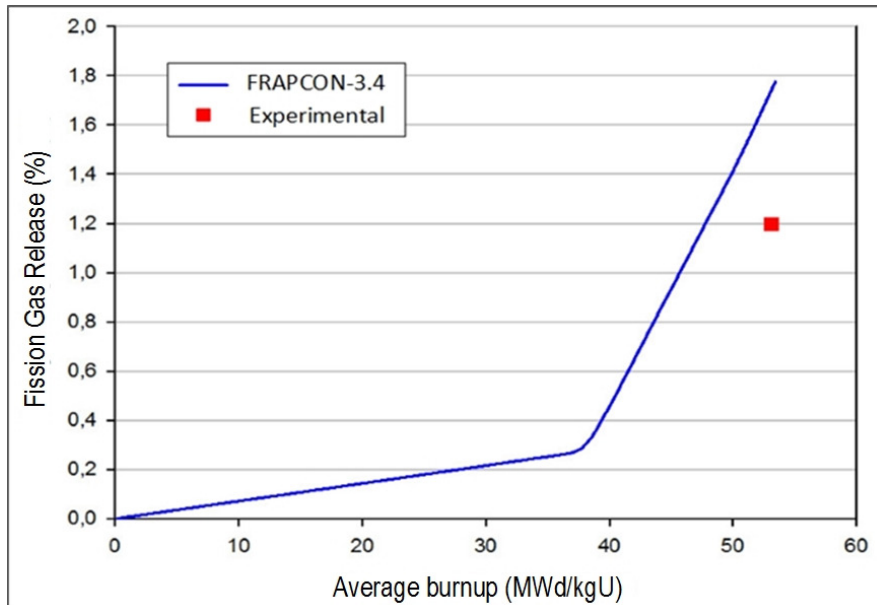


Figure 4 - Experimental value and prediction of the FRAPCON-3.4a code for the release of fission gas (Source: Authors).

provided by the various codes employed. As can be seen in Figure 3, there is a large divergence between the results provided by the models employed by the codes to represent the amount of gas released by the fuel. Despite the discrepancy observed in the result, a fact in favor of the result provided by code FRAPCON-3.4a for the release of fission gas is that the result provided by the code is conservative when compared to the experimental value, which is desirable for the validation of the design conditions of a fuel rod.

4.1.3 Fuel rod free volume

The determination of the free volume inside the fuel rod is of fundamental importance for the calculation of its internal pressure. The experimental value obtained at the end of the life for the test fuel rod TSQ002 was 17.8 ml. This value is plotted in the graph provided in Figure 5, compared to values obtained using the computer programs used by the FUMEX-III program participants. Figure 6 shows the comparison of the value obtained experimentally with the result provided by the FRAPCON-3.4a code for the determination of the free volume of the fuel rod, considering the conditions used in the experiment. In this figure, it can be observed that there is a good convergence between the experimental result and the value provided by the code.

4.1.4 Fuel rod internal pressure

Although the experiment IFPE/US-PWR-16x16-LTA did not provide results regarding the internal pressure at the end of the life of the fuel rod, a comparative analysis of the results obtained by the computational codes used by the various project participants was presented in the FUMEX final report III. The data obtained in this analysis are given in Figure 7.

Figure 8 shows the result obtained for the internal pressure variation in the fuel rod TSQ002 by using the code FRAPCON-3.4a for the conditions employed in the experiment. The comparison of Figures 7 and 8 shows that the result provided by the program FRAPCON-

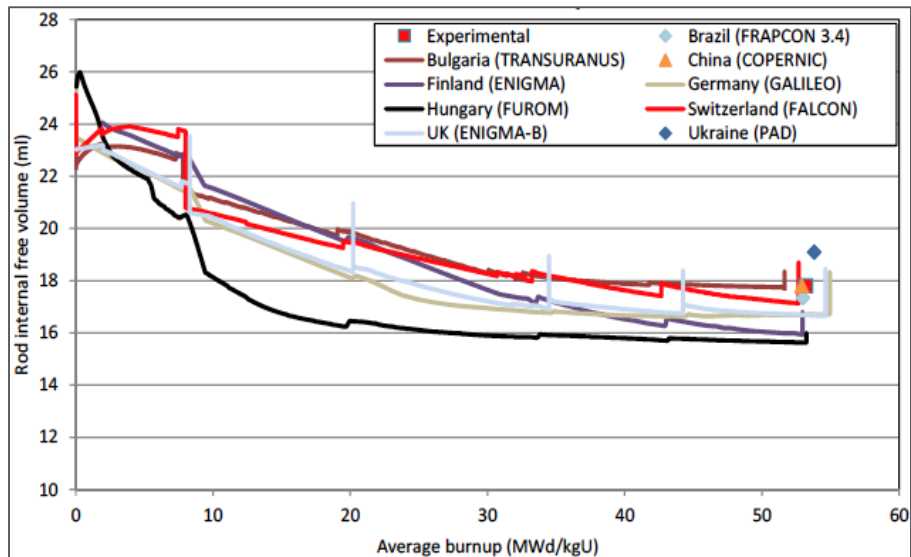


Figure 5 - Experimental value and predictions of the computer programs for the free volume inside the fuel rod (Source: FUMEX III Final Report).

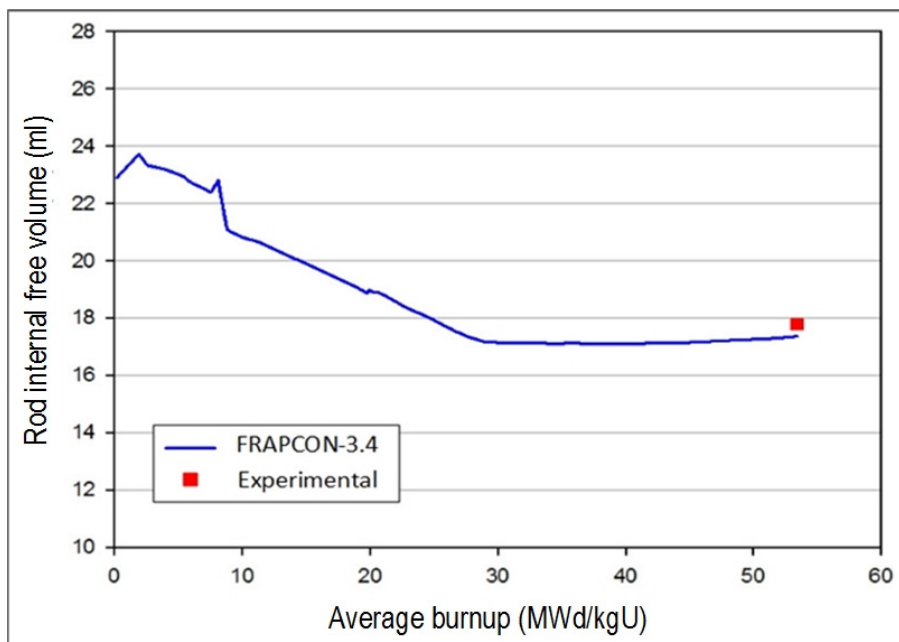


Figure 6 - Experimental value and prediction of the FRAPCON-3.4a code for the determination of the fuel rod free volume (Source: Authors).

3.4a is presented within the expected when compared with the results provided by the other codes used in this analysis. The variations between the results provided by the various codes are mainly due to the variation of the amount of fission gas released, which varies significantly from code to code, as discussed above.

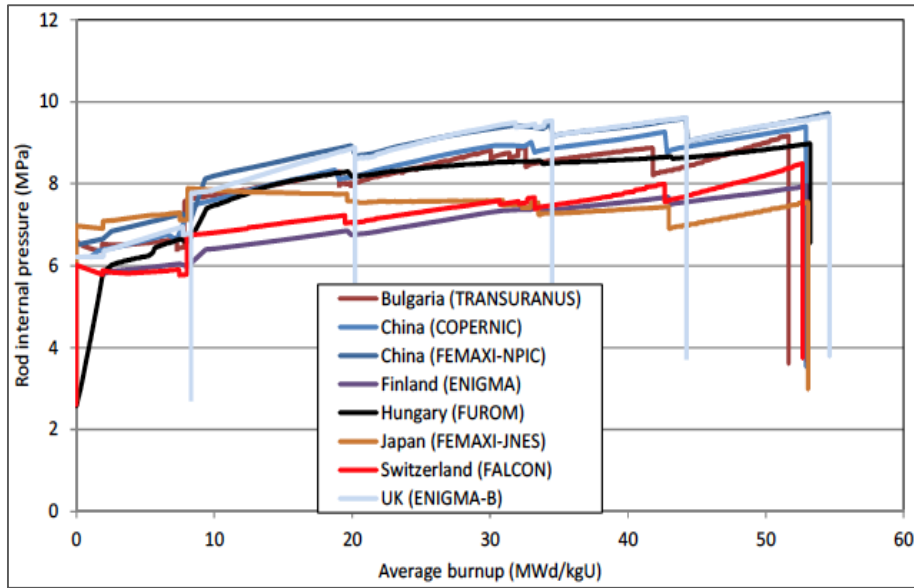


Figure 7 - Predictions of computer programs for fuel rod internal pressure (Source: FUMEX III Final Report).

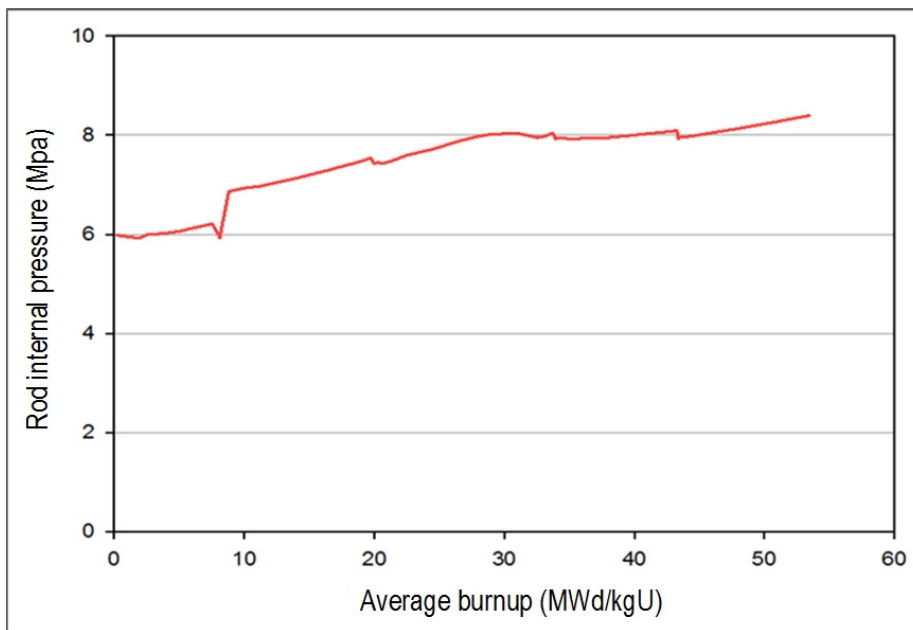


Figure 8 - Variation of the fuel rod internal pressure as a function of the average burnup provided by code FRAPCON-3.4a (Source: Authors).

4.2 Case RISOE-III-GE7

The experiment IFPE/RISOEIII-GE7 (NEA-1493/17) is part of a project consisting of three programs of irradiation of slow-power ramp fuel rods, called bump tests, with the objective of evaluating the release of fission gas and microstructural changes in fuel. The third and last project, whose data will be used in the present work, involved the irradiation of fuel rods used

in PWR and BWR reactors and was carried out from 1986 to 1990. The data documented by the FUMEX III final report for the IFPE/RISOEIII experiment (NEA-1493/17), ZX115, make it possible to perform the following analyses:

- Fission gas release;
- Temperature of the central region of the fuel pellet;
- Temperature of the central region of the fuel pellet emphasizing the power ramp applied at the end of the life of the fuel rod.

4.2.1 Fuel pellet central temperature

The database provided by the FUMEX III program does not present, for this case, experimental data related to the temperature distribution in the fuel pellet. However, the final FUMEX III report (IAEA-FUMEX-III, 2013) provides two graphs on the temperatures in the fuel pellet: the first, given in Figure 9, shows the temperature in the central region of the pellet as a function of the average burnup and the second, presented in Figure 10, shows the temperature behavior in the central region of the fuel pellet taking into account the power ramp applied at the end of the life of the fuel rod. These two curves were obtained through the computational codes used by the teams that participated in the project.

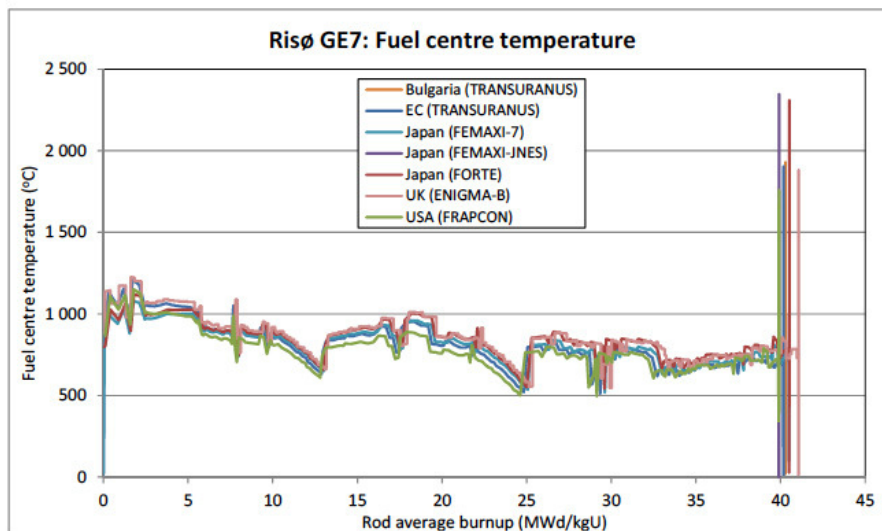


Figure 9 - Temperature variation of the central region of the fuel rod (Source: FUMEX III Final Report).

By using the FRAPCON-3.4a code, the graphs shown in Figures 11 and 12 were obtained. The graph provided in Figure 11 shows the temperature variation in the central region of the fuel pellet as a function of the average burnup and the graph provided in Figure 12 shows the temperature variation of the central region of the fuel rod during the power ramp applied at the end of the life of the fuel rod.

A first analysis of the curves presented in the graphs of Figures 9 and 11 shows a good convergence between the data provided by the FRAPCON-3.4a code when compared to the results provided by the other codes. However, when comparing the curves provided in Figures 10 and 12, which show the temperature behavior in the central region of the fuel pellet when the rod is subjected to a power ramp, a relatively large discrepancy is observed

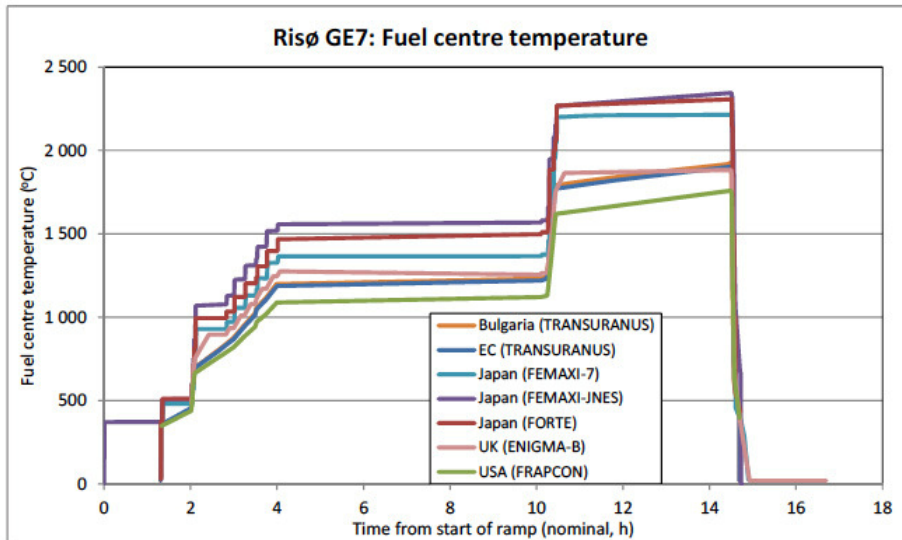


Figure 10 - Temperature variation of the central region of the fuel rod during the power ramp applied at the end life of the fuel rod (Source: FUMEX III Final Report).

between the results provided by the computer programs, reaching, in some points, differences of the order of 500 °C. This discrepancy is probably due to the fact that the power ramp was applied at the end of the life of the fuel rod with an approximate burnup of 40-42 MWd/kgU, a condition in which a series of phenomena in the fuel influence the thermal behavior of the pellet, phenomena that are not yet adequately modeled by the codes.

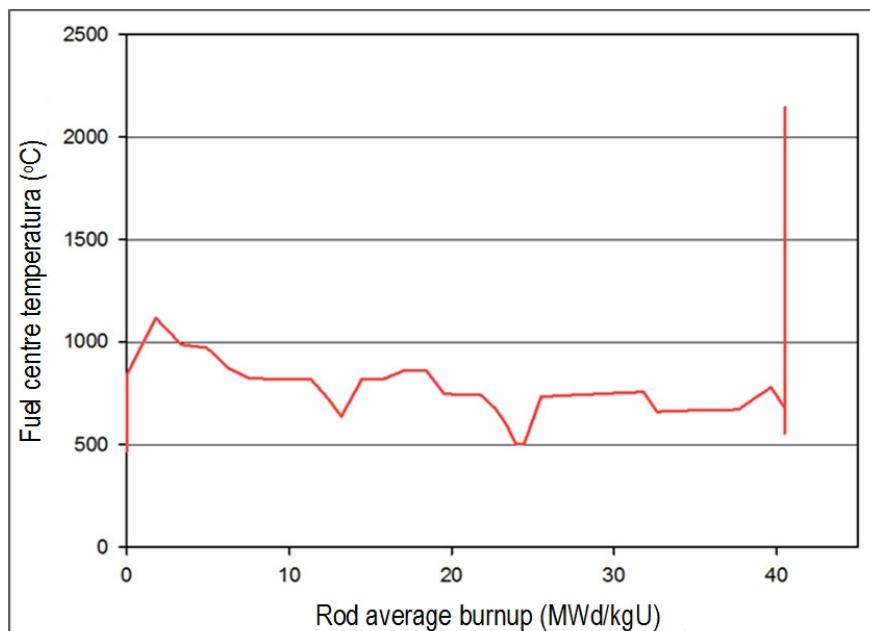


Figure 11 - Temperature variation of the central region of the fuel rod as a function of the average burnup obtained by FRAPCON-3.4a (Source: Authors)..

4.2.2 Fission gas release

The main objective of the IFPE/RISOEIII-GE7 experiment (NEA-1493/17) was to study the effect that a power ramp applied at the end of the life of a fuel rod causes to the fission gas release process. It is well known that power ramps result in a rapid increase in temperature in the fuel pellet, a fact that can be observed in Figure 12. This fact, added to the conditions present in the fuel pellet with high burnup, tend to accelerate the process of fission gas release. This fact was also observed in the experiment carried out, and can be observed in the graph provided in Figure 13, which presents a comparison between the result obtained experimentally for the release of fission gases with the results obtained through the computer simulation. In this graph it can be seen that, as soon as the power ramp (approx. 40 MWd/kgU) is applied, there is a marked increase in the amount of gas released, reaching an experimental value of 14.4% of the total of gas produced.

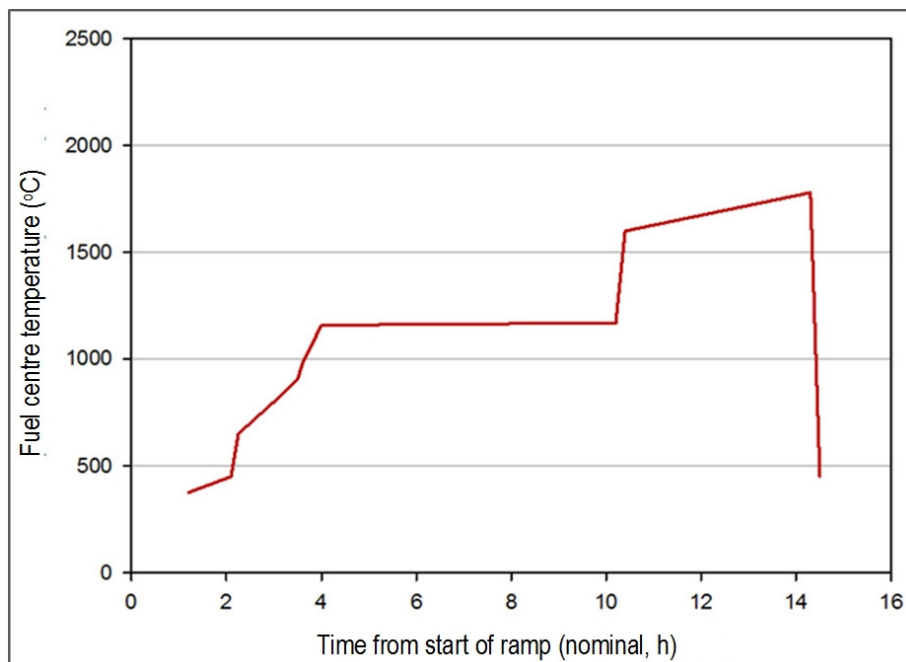


Figure 12 - Temperature variation of the central region of the fuel rod during ramp applied at the end of the life of the fuel rod obtained by Code FRAPCON-3.4a (Source: Authors).

Figure 14 shows the graph with the results obtained for the release of fission gas through computer simulation performed with code FRAPCON-3.4a. The result obtained by this simulation was 12.8% of the total gas produced, which is about 11% lower than the result obtained experimentally (14.4%). This discrepancy is probably due to the complexity of the phenomena involved and the difficulty of the models used by the code to represent these phenomena.

4.3 Case NSRR-FK1

The experiment IFPE/NSRR NEA-1724/01 was carried out from 1984 to 1997 and was aimed at investigating the behavior of the fuel when subjected to a reactivity-initiated accident (RIA). In its final phase, this experiment analyzed the behavior of three fuel rods used in BWR reactors, called FK-1, FK-2 and FK-3. For this work the data obtained through

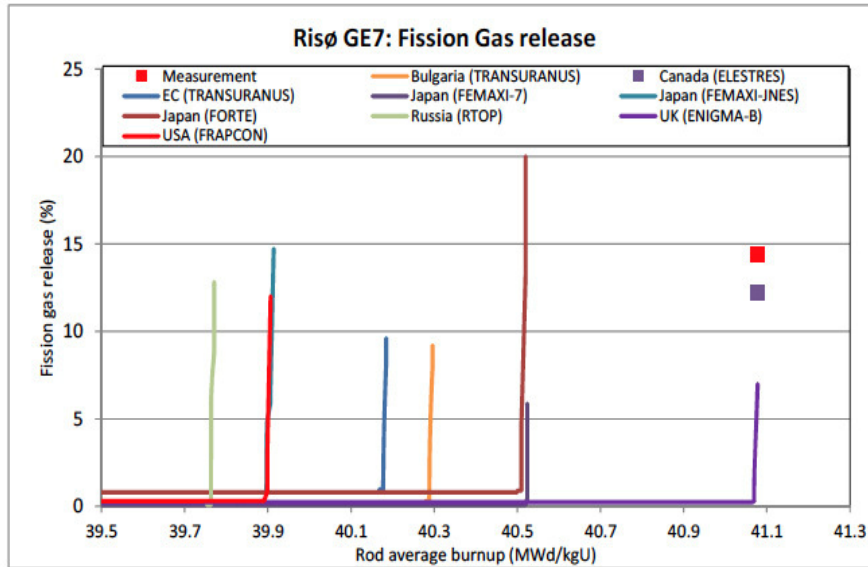


Figure 13 - Experimental value and predictions of computer programs for fission gas release (Source: FUMEX III Final Report).

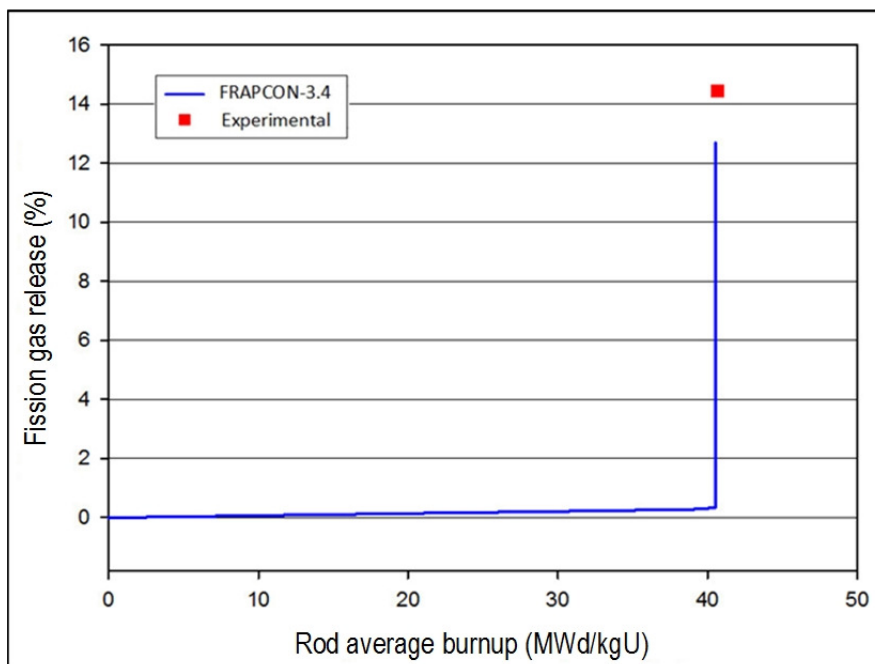


Figure 14 - Experimental value and prediction of the FRAPCON-3.4a code for fission gas release (Source: Author).

the experiment with the fuel rod FK-1 were used. The IFPE / NSRR-FK1 NEA-1724/01 experiment was carried out in two stages: in the first step, 8x8 BJ-STEP I fuel elements from Unit 3 of the Fukushima Daiichi Nuclear Power Plant were used, which were irradiated under steady-state conditions up to a burnup of 41-45 MWd/kgU. In the second step, the FK-1 rod was remanufactured from the rods used in the spent fuel element in the Fukushima reactor and transferred to the Nuclear Safety Research Reactor (NSRR), being subjected to enthalpy

pulses of the order of 293-607 J/g, for periods of 4.4 ms, in order to simulate initialized reactivity accidents (RIA). In order to perform the simulation of the behavior of the fuel rod used in the IFPE/NSRR-FK1 experiment NEA-1724/01, the computer programs FRAPCON-3.4a and FRAPTRAN-1.4 were used together. The FRAPCON-3.4a program was used in order to obtain behavior of the fuel rod during the initial irradiation carried out on a steady state condition, and also to generate the input data file for the FRAPTRAN-1.4 code, which was used for the analysis of the behavior of the rod under the action of a transient, simulating a reactivity-initiated accident (RIA).

4.3.1 Fuel pellet central temperature

As in the previous cases, the data base provided by the FUMEX III program does not present, for this experiment, data related to the temperature distribution in the fuel pellet. However, the final FUMEX III report (IAEA-FUMEX-III, 2013) provides, for the experiment in question, a graph with the temperature in the central region of the fuel pellet as a function of time during the pulse period for RIA simulation. These temperatures were obtained through computer simulation performed by the various codes that participated in the project and are provided in Figure 15. In this figure it can be observed that there is a good agreement between the temperatures provided by the FRAPTRAN and TRANSURANUS codes and a significant discrepancy between the temperatures provided by these codes when compared to the results provided by the FAIR code.

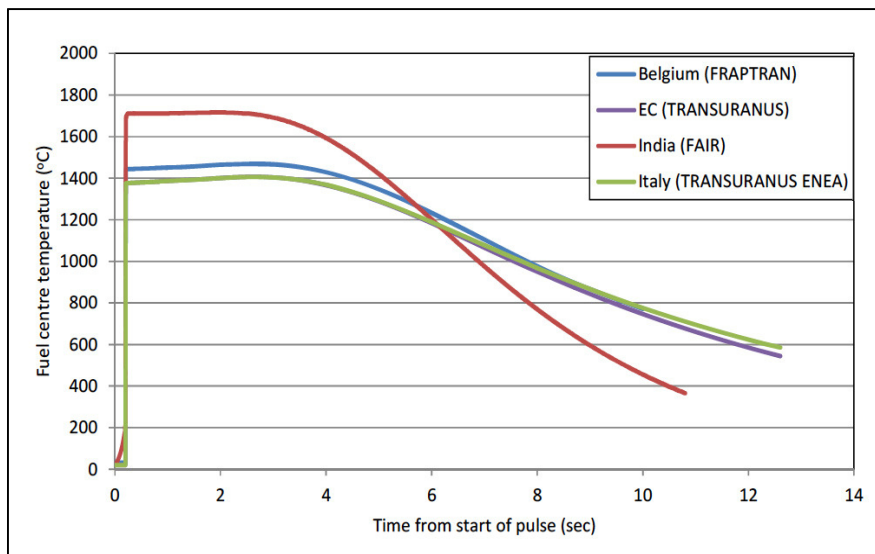


Figure 15 - Temperature in the central region of the fuel pellet during application Of the pulse for RIA simulation (Source: FUMEX III Final Report).

Figure 16 shows the result obtained for the temperature in the central region of the fuel pellet as a function of the time from the beginning of the pulse to the RIA simulation using the FRAPTRAN-1.4 code. Comparing Figures 15 and 16 it can be observed that there is a good convergence of the data provided by the FUMEX-III final report with the data obtained through the computational simulation performed in this work.

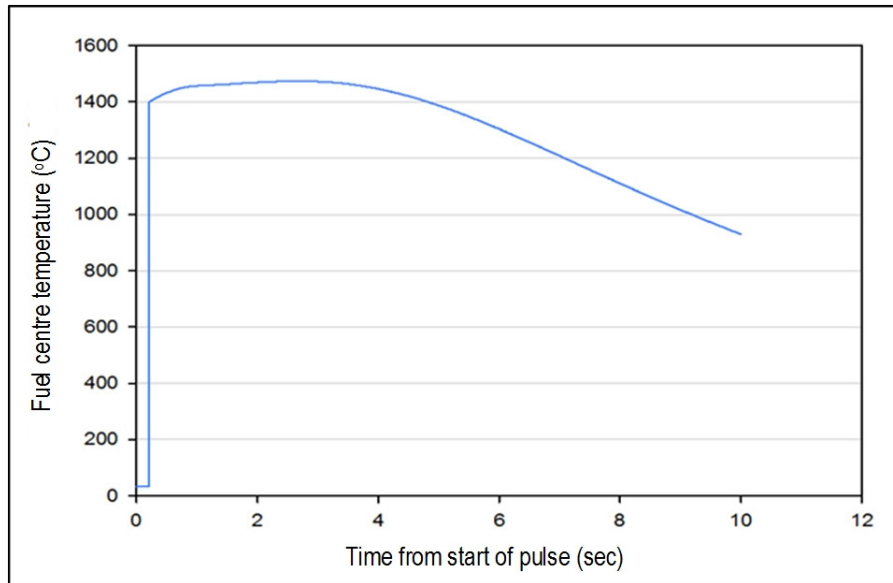


Figure 16 - Temperature variation of the central region of the fuel rod as a function of time elapsed from the pulse provided by FRATRAN-1.4 (Source: Authors).

4.3.2 Internal pressure of fuel rod

Figure 17 shows the result obtained for the internal pressure in the fuel rod FK-1 during the time of application of the pulse for simulation of RIA, through the codes used by the teams that participated in the FUMEX-III program and performed the analysis of this experiment.

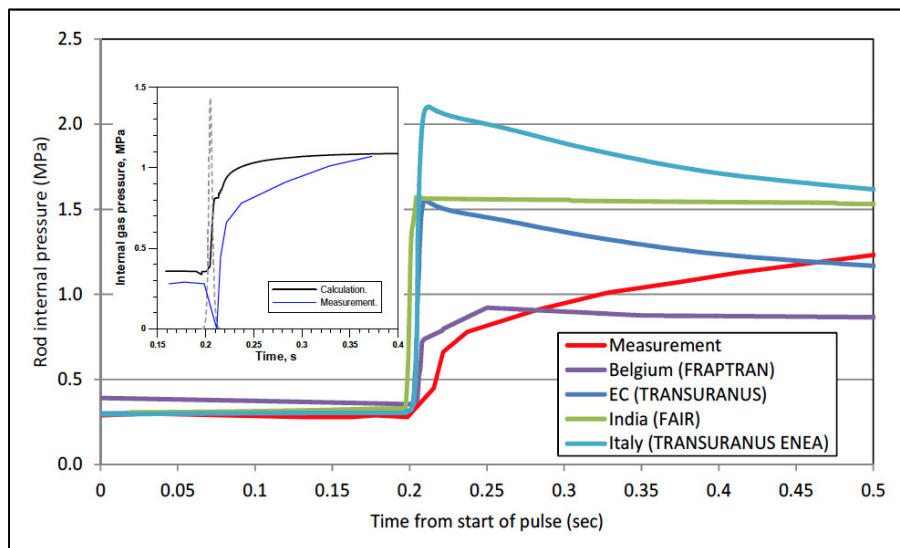


Figure 17 - Predictions of the computer programs for the internal pressure of the fuel rod FK-1 as a function of the time elapsed from the application of the pulse to the simulation of RIA (Source: FUMEX III Final Report).

In this figure we can observe the existence of an appreciable divergence between the pressures provided by the various computer programs when compared to the results obtained experimentally. These divergences probably occur due to the variation in the amount of fission gas released calculated by the models used by the codes, which varies significantly

from computer program to computer program. Figure 18 shows the result obtained through the simulation performed by the FRAPCON-3.4a and FRAPTRAN-1.4 codes for the experiment in question. The comparison of Figures 17 and 18 shows that the result obtained by the simulation performed in this work has a marked discrepancy in relation to the results obtained by the Belgian team that also used the FRAPTRAN code. After several revisions of the data used to simulate the experiment in question, no inconsistency was found in the input data. As the FUMEX-III report does not provide the input data used by the Belgian team for such a simulation, nor the version of the FRAPCON and FRAPTRAN codes that were used, it was not possible to conduct a more in-depth analysis of such discrepancy.

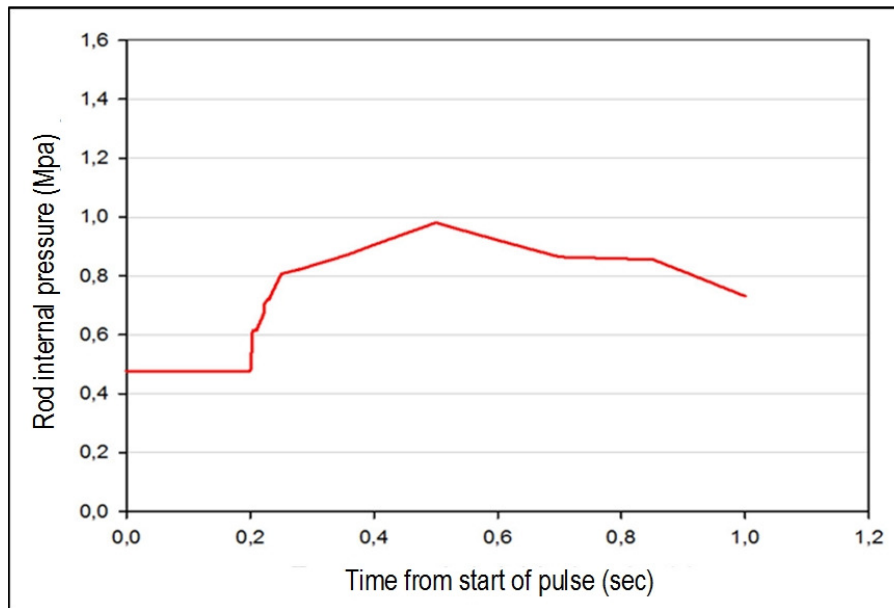


Figure 18 - Variation of the internal pressure of the fuel rod FK-1 as a function of the elapsed time of the pulse for the simulation of RIA provided by the FRAPTRAN-1.4 code (Source: Authors).

4.3.3 Elongation of pellet column

Figure 19 shows the result obtained for the elongation of the fuel pellets column of the FK-1 fuel rod during the pulse application time period for RIA simulation, through the codes used by the teams that participated in the FUMEX-III program and performed the analysis of this experiment. In this figure it can be observed that there is an acceptable agreement between the results provided by the codes TRANSURANUS, RANN-Sliding and FRAPTRAN when compared to the data obtained experimentally. However, the RANNS-Bonding and TRANSURANUS ENEA codes have a significant discrepancy when compared to the experimental data. Figure 20 illustrates the result obtained for the elongation of the fuel pellet stack through the computational simulation performed in this work through the use of the FRAPTRAN-1.4 computational code. Comparing the results obtained in this simulation with the results shown in Figure 19, we can observe that it is in agreement with the result obtained by the Belgian team that also uses the FRAPTRAN code.

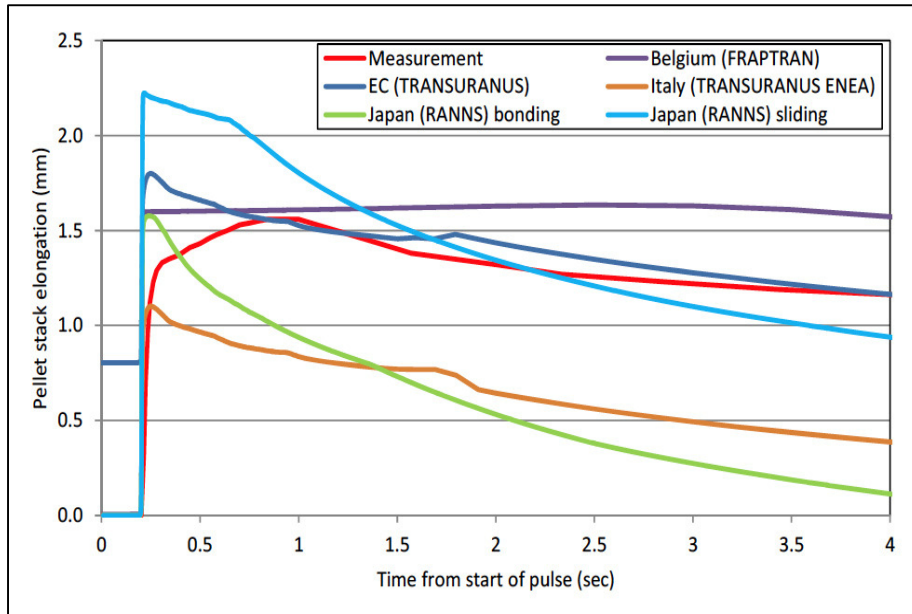


Figure 19 - Predictions of computer programs for elongation of fuel pellet stack of FK-1 rod as a function of time elapsed from pulse application to RIA simulation (Source: FUMEX III Final Report).

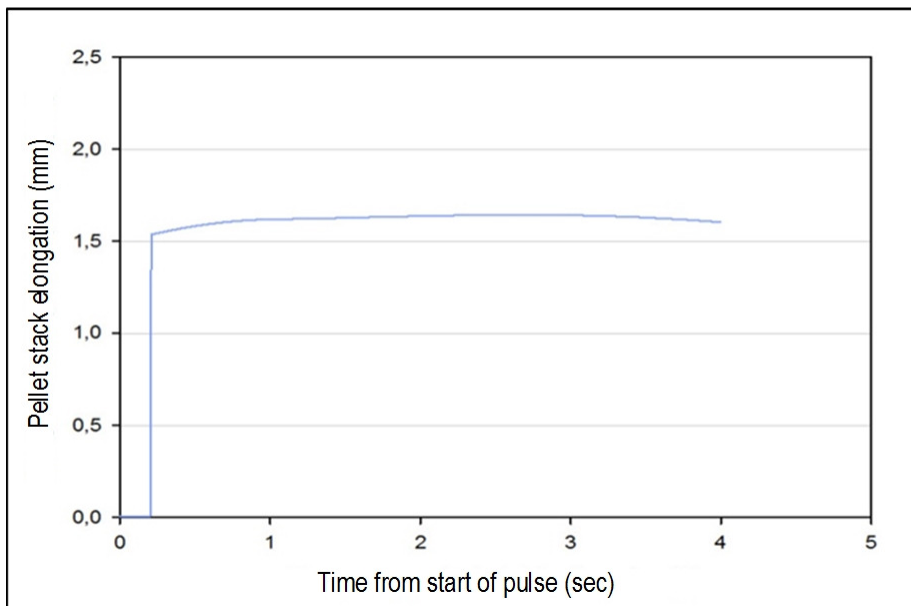


Figure 20 - Fuel pellet stack elongation of fuel rod FK-1 as a function of elapsed pulse time for RIA simulation provided by FRAPTRAN-1.4 code (Source: Authors).

4.3.4 Fuel rod cladding elongation

Figure 21 shows the results obtained for the elongation of the fuel rod cladding of the FK-1 during the pulse application time for RIA simulation, through the programs used by the teams that participated in the FUMEX-III program and performed the analysis of this experiment. In this figure it can be observed that there is an acceptable agreement between the result provided by the TRANSURANUS, RANNS-Bonding and FRAPTRAN codes when

compared to the data obtained experimentally. However, the RANNS-Sliding and TRANSURANUS ENEA codes have a significant discrepancy when compared to the experimental data.

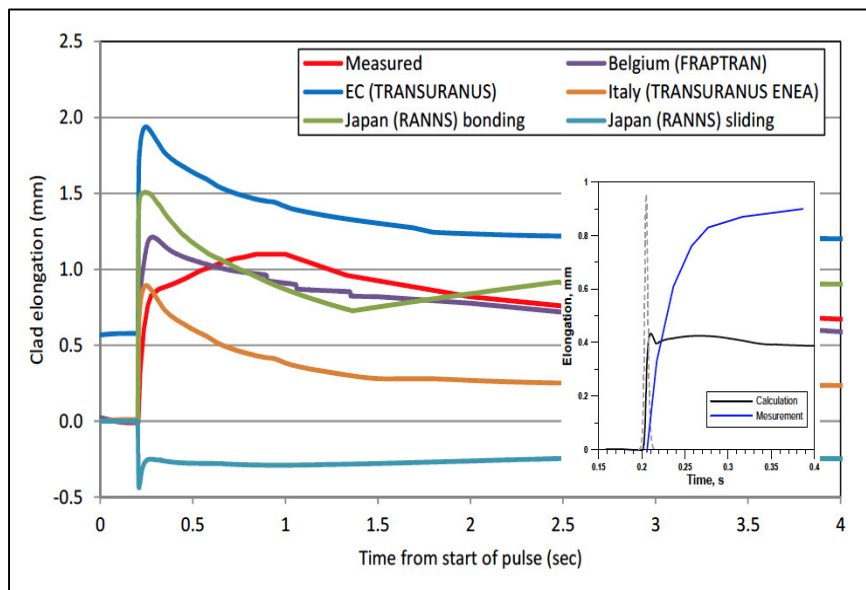


Figure 21 - Predictions of computer programs for cladding elongation of the FK-1 rod as a function of the elapsed time of the RIA pulse (Source: FUMEX III Final Report).

Figure 22 shows the result obtained for cladding elongation through the computer simulation performed in this work using the FRAPTRAN-1.4 computer program. Comparing the results obtained in this simulation with the results shown in Figure 21, we can observe that it is in agreement with the result obtained by the Belgian team that also uses the FRAPTRAN code.

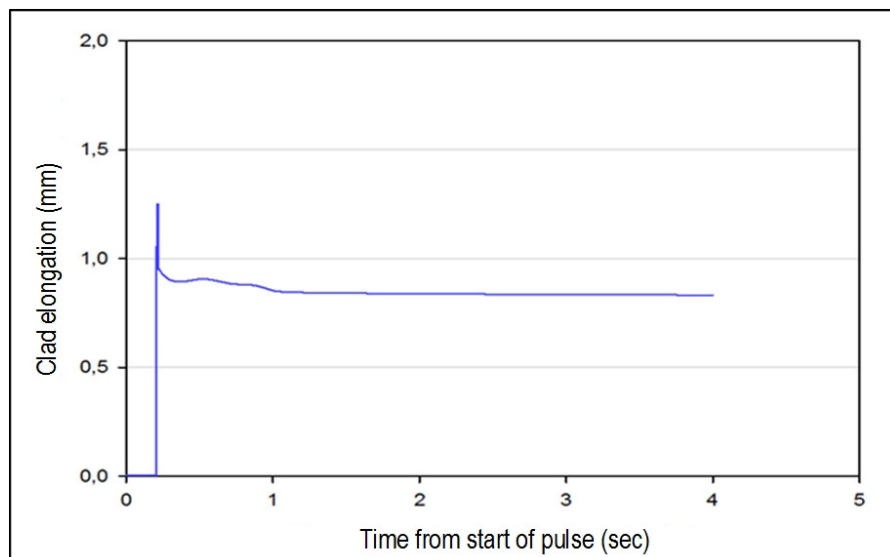


Figure 22 - Elongation of the fuel rod cladding of the fuel rod FK-1 as a function of the elapsed time of the RIA pulse provided by the FRAPTRAN-1.4 code (Source: Author).

5. CONCLUSIONS

Through the results provided by the computer programs FRAPCON-3.4a and FRAPTRAN-1.4 for the cases analyzed in this work, it can be seen that they are within the expected when compared to the data provided by the FUMEX-III final report. An important point to be emphasized in the analyzes carried out using the FRAPCON and FRAPTRAN software programs is that, in general, the results provided by these codes are either close to or slightly higher than the experimental data, which shows that the models employed by the codes are conservative. This fact is of great importance for the validation of fuel rod design. A more detailed analysis of the models simulating the behavior of the uranium dioxide (UO₂) fuel rods at high burnup in the pressurized light water reactors is recommended for future work. These models include the formation of the microstructure of UO₂ at high burnup, the restructuring of the fuel, the porosity in the restructured material, the release of athermal fission gases into the restructured material, the release of thermally activated fission gases, including models of gas release, grain growth, release of gases that occur due to grain growth, thermal conductivity of UO₂ at high burnups and models for the behavior of the cladding tube with zirconium alloys, including the corrosion of the various cladding types used, the hydrogen embrittlement and the mechanical properties at high burnup. From this analysis, it will be possible to evaluate with greater consistency the results obtained from the simulation of the fuel rod in conditions of high burnup with the experimental data obtained and disclosed for this rod in the FUMEX-III program.

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