Investigations Supporting MOX Fuel Licensing in ESNII Prototype Reactors

# D9.8 – Synthesis of the presentation of INSPYRE results to the User Group

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# SUMMARY


INSPYRE created a user group composed of key customers for the project's results, which included representatives of the designers of the ESNII reactor concepts (ASTRID, MYRRHA, ALFRED, ALLEGRO), as well as of fuel manufacturers and utilities (ORANO, EDF).

A first meeting had been organized in August 2018 to present the INSPYRE approach and activities to the users and discuss their needs in the area covered by INSPYRE activities. The synthesis of the meeting is reported in INSPYRE Deliverable D9.4.

Three meetings with the user group were then organised throughout the project to present the approach and results of the project to the Users, get their feedback on these results and discuss follow-up activities.

- The Second User Group meeting took place on January 17th, 2020 and was dedicated to the developments made in the fuel performance codes considered in the project and their assessment against the selected fast reactor irradiation experiments
- The third User Group meeting was held on May 31st, 2021 and was dedicated to the simulation of the fuel elements in normal operating conditions of the ASTRID reactor concept
- The final User Group meeting was organised jointly with the second Scientific Advisory Committee meeting on May 24th, 2022 and concerned the overall scientific outcomes of INSPYRE.

The present deliverable reports the presentations made during the meetings and the synthesis of the exchanges that followed.

# CONTENT

# GLOSSARY

| | |
|---|---|
| ADS | Accelerator Driven System |
| ALFRED | Advanced Lead Fast Reactor European Demonstrator |
| ALLEGRO | Gen-IV helium-cooled fast reactor |
| ASTRID | Advanced Sodium Technological Reactor for Industrial Demonstration |
| BOI | Beginning Of Irradiation |
| BPJ | Beam Power Jump |
| ESNII | European Sustainable Nuclear Industrial Initiative |
| EOI | End Of Irradiation |
| ESFR-SMART | European Sodium Fast Reactor - Safety Measures Assessment and Research Tools |
| FGR | Fission Gas Release |
| FPC | Fuel Performance Code |
| FR | Fast Reactor |
| Gen-IV | Generation IV International Forum |
| GFR | Gas-cooled Fast Reactor |
| H2020 | Horizon 2020 |
| INSPYRE | Investigations Supporting MOX Fuel Licensing for ESNII Prototype Reactors |
| JOG | Joint Oxyde-Gaine |
| JPNM | Joint Programme Nuclear Materials |
| LBE | Lithium-Beryllium Eutectic |
| LFR | Lead Fast Reactor |
| MOX | Mixed Oxide |
| MYRRHA | Multi-purpose hYbrid Research Reactor for High-tech Applications |
| PIE | Post-Irradiation Examination |
| ppn | peak power node |
| SA | Sensitivity Analysis |
| SFR | Sodium Fast Reactor |
| TAF-ID | Thermodynamics of Advanced Fuels – International Database |
| TF | Task Force |
| UA | Uncertainty Analysis |
| UG | User Group |
| WP | Work Package |

# 1 INTRODUCTION

INSPYRE created a user group composed of key customers for the project's results, which included representatives of the designers of the ESNII reactor concepts (ASTRID, MYRRHA, ALFRED, ALLEGRO), as well as of fuel manufacturers and utilities (ORANO, EDF).

A first meeting had been organized in August 2018 to present the INSPYRE approach and activities to the users and discuss their specific and common needs in the area covered by INSPYRE. The synthesis of the meeting is reported in INSPYRE Deliverable D9.4 [1].

Three meetings with the user group were then organised throughout the project to present the approach and results of the project to the Users, get their feedback on these results and discuss follow-up activities.

- The Second User Group meeting took place on January 17th, 2020 and was dedicated to the developments made in the fuel performance codes considered in the project and their assessment against the selected fast reactor irradiation experiments
- The third User Group meeting was held on May 31st, 2021 and was dedicated to the simulation of the fuel elements in normal operating conditions of the ASTRID reactor concept
- The final User Group meeting was organised jointly with the second Scientific Advisory Committee meeting on May 24th, 2022 and concerned the overall scientific outcomes of INSPYRE.

The Sections 2, 3 and 4 of the present deliverable report the presentations made during the meetings and the synthesis of the exchanges that followed. Conclusions and perspectives are given in Section 5.

# 2 SECOND USER GROUP MEETING (AT MONTH 28)

The second meeting with the User Group was held online on January 17th, 2020. The goals of the meeting were to present the status of INSPYRE activities at Month 28, in particular

- the models developed for the improvement of fuel performance codes in Work Package 6 and their implementation ion the three FPC considered in the project (GERMINAL, TRANSURANUS, MACROS) done in WP7
- the results of the assessment of the pre-INSPYRE versions of the GERMINAL, MACROS and TRANSURANUS fuel performance codes against the SUPERFACT-1 experiment
- the case studies selected for the application of the codes improved in INSPYRE.

## 2.1 Participants

Users

- A. Alemberti (Ansaldo Nucleare, Italy), Nuclear Science Development Manager
- B. Fontaine (CEA/DEs, France), Manager of CEA/DEs project on fuel development for Gen IV nuclear reactors
- V. Garat (ORANO, France), in charge of R&D on safety of nuclear fuels

- G. Grasso (ENEA, Italy), in charge of the core design of ALFRED
- G. Kennedy (SCK.CEN), Head of Nuclear Technology Engineering Unit
- F. Laugier (EDF-DPNT, France), Expert on back-end of nuclear fuel cycle
- Z. Hózer (EK CER, Hungary), Head of Fuel and Reactor Materials Department

Representatives of INSPYRE

- M. Bertolus (CEA/DEs), INSPYRE Coordinator
- L. Luzzi (POLIMI), INSPYRE Work Package 7 Leader
- T. Barani (POLIMI), Participant in WP6 and 7
- A. Magni (POLIMI), Participant in WP6 and 7
- D. Pizzocri (POLIMI), Participant in WP6 and 7
- F. Errecart (LGI), INSPYRE Project management office.

## 2.2 Achievements of the project at Month 28

M. Bertolus recalled the objective and organisation of the project and presented the activities and achievements of the project during the first two years. The first half of INSPYRE enabled the consortium to lay solid foundations for the activities planned in the Project by analysing in detail the available data and models and identifying gaps, by assessing the pre-INSPYRE versions of fuel performance codes on previous irradiation experiments and by developing new experimental set-ups enabling the precise characterization of Pu and Am bearing oxides in hot labs of several partners. It also brought the first results as follows:

- First detailed characterizations were performed on fresh uranium-plutonium oxide samples and on fission products compounds for the understanding of JOG.
- Significant progress was made in the preparation of the experiments planned for the measurement of creep under irradiation in the CNRS cyclotron in Orléans and in the High Flux Reactor in Petten.
- First-of-a-kind calculations at the atomic scale were performed of thermodynamic properties, defect behaviour and fission gas incorporation in $(U,Pu)O_2$, as well as on the impact of primary damage on mechanical properties.
- An improved thermodynamic model for (U-Pu-Am-O) was built.
- At the microscale, physics-based models describing the inert gas behaviour in irradiated fuels, as well as the thermal and mechanical evolution as a function of the parameters of interest were developed

Two reviews were conducted at mid-project, by the scientific advisory committee of the project and by experts chosen by the EC. These emphasized the quality of the work performed and of the results obtained.

M. Bertolus also presented briefly the communication, dissemination and education and training activities. She then described the main results obtained in WP6, which focuses on the derivation of parameters and development of models for FPCs. These results are presented in the deliverables D6.1 (Review of available models and progress on the sub-models dealing with the intra- and intergranular inert gas behaviour) [2] and D.6.2 (Report on improved models of melting temperature and thermal conductivity for MOX fuels and JOG) [3] of the Project.

## 2.3 Description of the irradiation experiments selected for the assessment of Fuel Performance Codes

L. Luzzi presented in detail the three irradiation experiments selected for the assessment of the European fuel performance codes considered in INSPYRE: SUPERFACT-1, RAPSODIE-I, NESTOR-3. The detailed characteristics of the as-fabricated fuel pins (fuel, cladding and geometry), the irradiation histories (linear heat rate and fast neutron flux as a function of time), final fuel burn-ups and cladding damage were described in an internal INSPYRE report (R7.1), which is accessible to the User Group. The open information is available in the public deliverable D7.1 (Report describing the Irradiation Experiments selected for the assessment of fuel performance codes) [4].

The assessment strategy defined in INSPYRE an presented in D7.1 consists in the simulation of selected pins from these three irradiation experiments, representative for sodium fast reactor conditions, employing first the state-of-the-art version of the codes [4]. The assessment, which involves the code validation against experimental measurements, code-to-code benchmark and possible uncertainty and sensitivity analyses, will be repeated with the improved versions of the FPCs, which will include the models that developed in INSPYRE WP6 based on the data and information on MOX fuel achieved by WPs 1 – 5 [5].

Z. Hózer underlined the importance of comparing the results of the simulations with experimental data (fission gas release, FGR, margin to melting) and asked about the availability of PIE data from the selected irradiation experiments. L. Luzzi answered that the database of the measured quantities of the selected irradiation experiments is limited (cladding outer diameter axial profile at end-of-irradiation, central hole and columnar-grains region size at specific heights in the fuel column, radial profiles of actinide and fission product concentrations at specific heights in the fuel column, fission gas release at end-of-irradiation). A code-to-code benchmark was therefore performed on quantities of interest that had not been measured during the experiments (e.g., the fuel centreline temperature). This is the object the internal report R.7.3 and public deliverable D7.3 (Results of the benchmark between pre- and post-INSPYRE code versions on selected experimental cases) [6], which was published later in the project.

G. Grasso noticed that the final peak burnup attained by RAPSODIE-I pins is high (~ 10% FIMA) but the corresponding peak cladding damage is rather low (~ 35 $dpa_{NRT}$), especially if compared to SUPERFACT-1 and NESTOR-3. L. Luzzi answered that RAPSODIE-I values correspond to those provided by SCK.CEN, who has access to the experimental database. Further investigations by SCK.CEN are necessary to check and understand this result.

B. Fontaine asked whether the FGR was very high (i.e., ~ 90%) in all these three irradiation experiments. D. Pizzocri confirmed that this is the case. No discrimination is directly possible based on the FGR, but the three irradiation experiments differ from each other on other parameters and figures of merit, e.g., the cladding outer diameter profile at end of irradiation and the extension of the restructured zones within the fuel.

## 2.4 Assessment of fuel performance codes against SUPERFACT-1 experiment

A. Magni presented the assessment of the pre-INSPYRE version of FPCs performed in WP7 using the codes considered (GERMINAL, MACROS, TRANSURANUS) against the SUPERFACT-1 SFR irradiation experiment [7]. The results of the codes on integral FGR and pin elongation, axial cladding profilometry, fuel central void radius and columnar grain extension, radial concentrations of plutonium, americium, neptunium, xenon and caesium were compared to the available experimental data. Then, the results of the various codes on the fuel central temperature, fuel-cladding gap size, fuel inner radius and FGR at peak power node (ppn) were compared. A preliminary sensitivity analysis on the fuel-cladding gap conductance modelling was also performed using TRANSURANUS. Topics needing improvements and further developments were identified from the results obtained on the simulation of SUPERFACT-1.

A. Alemberti asked to what extent the three selected irradiation experiments were representative of fast reactor conditions and whether the community could be confident about the assessment results. D. Pizzocri answered that the selected experiments are representative of GEN IV core designs in terms of fast spectrum and composition of the fuel and cladding. In addition, given that the case studies selected correspond to very different fuel design and irradiation conditions, they represent a good test for the improved physics-based models that will be implemented in the FPCs. The simulation of other irradiation experiments would probably show that other specific developments are needed, each partner is responsible to extend the validation matrix internally depending on the complementary data available to them.

V. Garat proposed to investigate in detail the differences in the fuel central temperatures yielded by the various codes (which can be as large as 500°C), since fuel temperature strongly impacts the fuel performance and induces large differences in practically all the engineering figures of merit. She also asked about a sensitivity analysis on the various inputs or models, e.g., fuel thermal conductivity or redistribution and relocation models, which should have a strong impact on the results. The fuel temperature regimes predicted by the codes will be re-evaluated using the improved models and parameters obtained in INSPYRE and it is hoped that the new models will improve the description of the integral quantities [8]. A detailed sensitivity analysis is planned in this final assessment step.

## 2.5 Selection of case studies representative of ESNII cores: ASTRID and MYRRHA

D. Pizzocri first described the design and irradiation scenario considered for the simulation of the Gen-IV SFR concept ASTRID, i.e., the base irradiation of the hot channel fuel pin [9], [10], together with the preliminary simulation results obtained using the TRANSURANUS FPC. Key safety criteria to be assessed are the power-to-melt margin at beginning of irradiation (BOI) and the cladding maximal hoop stress at the end of irradiation. This case study will be simulated by POLIMI and CEA using both the pre-INSPYRE and improved versions of TRANSURANUS and GERMINAL FPCs, respectively. The preliminary simulations performed using TRANSURANUS predict an FGR around 50-60%, a value expected also for other Gen-IV concepts, e.g., MYRRHA, ALFRED, much lower than the 90% observed in FR irradiation experiments. For this reason, the assumption usually made for FR conditions of 100% FGR is not valid, confirming the need for a more mechanistic modelling of fission gas behaviour in the fuel.

D. Pizzocri then presented the design and irradiation scenario considered for the Gen-IV LBE-ADS concept MYRRHA, i.e., base irradiation and Beam Power Jump of the hot, average and cold channel fuel pins [11], [12]. The preliminary simulation results yielded by the TRANSURANUS FPC regarding both the normal operating conditions and the BPJ over-power transient scenario were also presented. The key safety criteria to be assessed are the margin to melting and the maximum cladding plastic strain enabling one to avoid pin failure due to fuel melting or to severe pellet-cladding mechanical interaction. This case study will be simulated by all the INSPYRE partners involved in WP7 (JRC, ENEA, POLIMI – TRANSURANUS; CEA – GERMINAL; SCK.CEN – MACROS) using both the state-of-the-art and improved versions of the FPCs.

G. Kennedy asked if uncertainty and sensitivity analyses (UA, SA) on the MYRRHA case study would also be performed. D. Pizzocri answered that UA and SA are optional for the case studies according to the INSPYRE Work Plan. It would be a great added value if several partners performed them using various codes. The preliminary TRANSURANUS simulations performed show that different models for the cladding swelling and creep yield very different behaviour of the MYRRHA fuel pin with/without fuel-cladding gap closure.

## 2.6 General discussion and wrap-up

L. Luzzi indicated that the INSPYRE partners are completely open to feedback and suggestions from the Users regarding the selected case studies, the transient scenarios, the kind of UA and SA to be performed, the figures of merit in which the Users are interested the most.

B. Fontaine expressed some doubts about the completeness of the conclusions from only three irradiation experiments and two case studies. For example, MYRRHA reactor power is much lower (half) than the power in the selected irradiation experiments. L. Luzzi answered that the strategy of testing the improved models in different fuel performance codes to evaluate if their impact on the results is comparable in all codes is key to conclude on the applicability of the improved model itself. For instance, improving the modelling of burst release from micro-cracked fuel pellets should improve the overall FGR prediction, independently of the fuel performance code and of the application considered.

G. Kennedy asked if, among the INSPYRE objectives, there is the compilation of a database to be delivered to nuclear companies or fuel vendors. M. Bertolus specified that this is one of the objectives of the ESFR-SMART Project, while the INSPYRE Project is complementary and focuses on the investigation of MOX fuel behaviour and underlying mechanisms and their modelling starting from the atomic scale.

# 3 THIRD USER GROUP MEETING (AT MONTH 44)

This meeting, held online on May 31st, 2021, aimed at presenting to the Users:

- the status of INSPYRE activities at Month 44, focusing in particular on the achievements of WP6 and WP7
- the results obtained on the ASTRID case study, representative of the SFR Gen-IV technology, selected for the application of both "pre-INSPYRE" and "post-INSPYRE" (extended with the models developed during the Project) fuel performance codes.

## 3.1 Participants

Users

- V. Garat (ORANO, France), in charge of R&D on safety of nuclear fuels
- G. Grasso (ENEA, Italy), in charge of the core design of ALFRED
- Z. Hózer (EK CER, Hungary), Head of Fuel and Reactor Materials Department
- J. Lamontagne (CEA, France), Head of the CEA project on Gen IV fuel development was excused and represented by M. Bertolus (CEA).

INSPYRE participants

- M. Bertolus (CEA/DEs), INSPYRE Coordinator
- A. Del Nevo (ENEA), INSPYRE Work Package 6 Leader
- L. Luzzi (POLIMI), INSPYRE Work Package 7 Leader
- B. Michel (CEA, DEs), Participant in WP7
- M. Lainet (CEA, DEs), Participant in WP7
- A. Magni (POLIMI), Participant in WP7

- D. Pizzocri (POLIMI), Participant in WP7
- A. Schubert (JRC), Participant in WP7
- P. Van Uffelen (JRC), Participant in WP7.

## 3.2 Overview of the project achievements at Month 44

M. Bertolus recalled the objective and organisation of the project and presented the activities of the project after 3 years and a half, which brought significant advances in the understanding and simulation of nuclear fuels. In particular,

- Detailed characterizations of structural, thermal, mechanical properties of fresh and irradiated uranium-plutonium oxide samples were performed.
- Fission product compounds were synthesised and characterized to get further insight into the formation and properties of JOG.
- Measurements of swelling under irradiation in the CNRS cyclotron in Orléans and the High Flux Reactor in Petten have started in 2020.
- Atomic scale calculations of thermodynamic properties, defect behaviour and fission gas incorporation in $(U,Pu)O_2$ and impact of primary damage on mechanical properties were completed.
- An improved thermodynamic model for (U-Pu-Am-O) and a thermo-kinetic model of MOX were built.
- At the microscale, physics-based models describing inert gas behaviour, thermal and mechanical evolution were developed.
- The data obtained and models developed were implemented in the three fuel performance codes considered in INSPYRE.
- The validation of new versions was performed and these versions were applied to the simulation of irradiation experiments.

M. Bertolus also presented briefly the communication, dissemination and education and training activities of the project.

## 3.3 Overview of activities concerning modelling and simulation using fuel performance codes

L. Luzzi presented an overview of the achievements of Work Packages 6 and 7. These two WPs represent the end of the INSPYRE Project chain, transferring the results yielded by the basic research investigations in WPs 1 – 5 to the codes and using these codes for the simulation of GENIV reactor cores.

Concerning WP6, some examples of the results obtained on the grain boundary venting of fission gases (Task 6.1, [13]), on the modelling of thermal expansion of MOX fuels (Task 6.2, [14]) and on the validation of the novel correlation for the thermal conductivity of MOX fuels proposed in INSPYRE (Task 6.3, [3], [15]) were presented. Additional WP6 deliverables cover the modelling of thermal properties extended to minor actinide-bearing MOX fuels (D6.5, [16]), the modelling of micro-mechanical rupture of nuclear fuels (D6.6, [17]) and the development of a polycrystalline mechanical model for the visco-plastic behaviour of $UO_2$ and $(U,Pu)O_2$ fuels (D6.7, [18]).

For WP7, the activities completed include on the one hand the extension of FPCs with the models developed in WP6, e.g., the coupling of the SCIANTIX inert gas behaviour module with the GERMINAL FPC [5] performed in Task 7.1, and on the other hand the assessment of pre and post-INSPYRE code versions against three irradiation experiments (SUPERFACT-1, RAPSODIE-I, NESTOR-3). This activity involved both the integral validation of codes against available experimental data and the benchmark of codes on quantities of engineering interest (e.g., the fuel temperature regime). It is reported in Deliverable D7.3 [6]. The application of FPCs to the ASTRID and MYRRHA case studies is in progress.

Z. Hózer asked if the validation of the novel INSPYRE correlation for the MOX melting temperature leads to results as good as the ones for the MOX thermal conductivity (shown as an example in the presentation). L. Luzzi answered that the validation of the novel melting temperature correlation against the available experimental data is also satisfactory and is shown in Deliverable D6.2 [3] and in a journal publication [15]. The effect of a high Pu content (up to 50 – 60%) in the MOX fuel on these thermal properties will be further investigated in the PuMMA H2020 Project [19].

P. Van Uffelen remarked that, besides the models fitted mainly on experimental data, CEA derived a novel correlation for the heat capacity of MOX fuels based on data obtained at the atomic scale in the WP1 of the project [20], [21].

## 3.4 Application of GERMINAL and TRANSURANUS to the ASTRID case study

B. Michel and D. Pizzocri presented the main results obtained by CEA and POLIMI applying the GERMINAL and TRANSURANUS FPCs, respectively, to the ASTRID case study [9], [10]. The simulation of the ASTRID case study presented during the meeting (benchmark GERMINAL – TRANSURANUS between CEA and POLIMI) is reported in Deliverable D7.4 [9] and in a journal publication focusing on fission gas-related aspects via the coupling of FPCs with the SCIANTIX module [10]. This case study is representative of sodium-cooled Gen-IV irradiation conditions and focuses on two key criteria under nominal irradiation, namely: the margin to fuel melting at the beginning of irradiation and the cladding maximum hoop stress at the end of irradiation. The main objective of this benchmark activity is to assess the behaviour of the hot channel fuel pin under nominal irradiation conditions and to discuss the impact of the modelling improvements brought about by the INSPYRE Project.

Attention was drawn on the heterogeneous axial structure of the ASTRID fuel pin, featuring alternate fertile and fissile fuel segments, which leads to a specific pin axial power profile. The main results of the two codes (using both pre and post-INSPYRE versions) were presented and discussed in detail, in particular the evolutions in time of fuel central temperature, the fuel-cladding gap size, the cladding outer radius, the fission gas release; the axial profiles of cladding swelling, the hoop stress, fuel-cladding contact pressure at the end of irradiation. The differences in the results yielded by the two codes were highlighted, and ascribed to the differences in the modelling of phenomena in the codes (e.g., the different treatment of fuel relocation and fuel-cladding contact pressure). The results of additional sensitivity analyses performed using TRANSURANUS concerning the fuel grain growth and the conservative modelling of cladding swelling, which impact the fission gas release dynamics and the cladding stress levels, were also presented.

Z. Hózer asked about the level of validation of the various modelling improvements implemented in the codes. B. Michel and D. Pizzocri answered that all the models developed in WP6 and implemented in FPCs (or in the SCIANTIX module coupled to FPCs) were assessed against available data, both from literature, coming from past European Projects or obtained by INSPYRE WPs 1 – 5. More data would be needed to validate these models further.

## 3.5 General discussion and wrap-up

Z. Hózer added that the European gas cooled fast reactor community (GFR), which works on the ALLEGRO Gen-IV reactor concept, is currently focusing again on the application of highly enriched $UO_2$ fuel, after having considered the MOX fuel option.

M. Bertolus remarked that the fuel performance code results on the MYRRHA case study, out of the scope of this UG meeting, are collected and will be reported in Deliverable D7.5 (Fuel performance simulations of ESNII prototypes: Results on the MYRRHA case study) [11]. Moreover, the User Group is invited to participate to the final workshop of the INSPYRE Project (November 2021).

# 4 FINAL USER GROUP MEETING (AFTER THE END OF THE PROJECT)

The final User Group meeting was held online on May 24th, 2022 in combination with the final meeting with the Scientific Advisory Committee. The objectives of the meeting were to:

- present a synthesis of the Project activities and results to the UG and SAC and exchange on them
- discuss further research activities that could be included in future European collaborative projects on fuels or in the possible European partnership on nuclear materials.

## 4.1 Participants

Users

- G. Kennedy (SCK.CEN, Belgium), Head of Nuclear Technology Engineering Unit
- Z. Hózer (EK CER, Hungary), Head of Fuel and Reactor Materials Department.
- F. Laugier (EDF-DPNT, France), Expert on back-end of nuclear fuel cycle
- L. Diaz (EDF, France)
- J. Lamontagne (CEA/ DEs, France), Head of the CEA project on Gen IV fuel development
- G. Kauric (ORANO, France)
- G. Grasso (ENEA, Italy) was excused.

Members of the Scientific Advisory Committee

- D. Haas (NC2 SPRL, Belgium), Independent consultant
- C. Stanek (LANL, USA), National Technical Director of the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program
- T. Ivanova (OECD/NEA), Head of the Division of Nuclear Science
- R. Grimes (Imperial College, UK) was excused.

INSPYRE WP leaders and participants

- M. Bertolus (CEA/DEs), INSPYRE Coordinator
- D. Staicu (JRC), Work Package 1 Leader
- M. Krack (PSI), Work Package 2 Leader
- M.-F. Barthe (CNRS/CEMHTI), Work Package 3 Leader
- C. Guéneau (CEA), Work Package 4 Leader
- T. Wiss (JRC), Work Package 5 Leader
- A. Del Nevo (ENEA), INSPYRE Work Package 6 Leader
- L. Luzzi (POLIMI), INSPYRE Work Package 7 Leader
- A. Smith (TU Delft), INSPYRE Work Package 8 Leader

- S. Maurice (LGI), Work Package 9 Leader.

## 4.2 Overview of the objectives of the INSPYRE activities

M. Bertolus introduced the meeting by recalling the context, structure and strategic objectives of the INSPYRE Project. The focus was particularly on the approach adopted in INSPYRE, which brought significant advances in the understanding and simulation of the behaviour of oxide nuclear fuels under irradiation towards an improved description of FR MOX behaviour in fuel performance codes. This approach involved use of data from irradiation tests and separate effect studies, modelling at various time and length scales and characterizations of fresh and irradiated $UO_2$ and MOX fuels.

The main advances reached in the understanding and simulation of nuclear fuels on the thermochemical behaviour of MOX, thermomechanical properties of $UO_2$ and MOX, atomic transport properties and fission gas behaviour, were summarized to introduce the next presentations. These consisted of:

- A large number of new experimental set-ups developed in hot labs enabling the characterization of Pu- and Am- bearing oxides
- Characterization of the structural and thermal properties of fresh and irradiated uranium-plutonium oxide samples
- Characterization of the mechanical properties of fresh $UO_2$ and uranium-plutonium oxide samples, as well as the measurement of swelling of $UO_2$ samples under ion irradiation and of swelling of MOX samples under neutron irradiation
- Synthesis and characterization of fission product compounds for the understanding of the Joint Oxyde-Gaine (JOG) in fast reactor fuel pins
- Atomic scale calculations of thermodynamic and transport properties and development of improved thermodynamic model for (U-Pu-Am-O) and of a thermo-kinetic model for (U-PU-O)
- Development of physics-based models describing the inert gas behaviour in nuclear fuels and the evolution of thermal and mechanical properties
- Assessment of the pre and post-INSPYRE versions of the three fuel performance codes on previous irradiation experiments.

The difficulties encountered during INSPYRE were also indicated: changes in regulations which induced delays in the fabrication and transportation of fuel samples and in the commissioning of set-ups in hot labs, capsule leaks during the fuel creep measurements in the HFR. An important unforeseen difficulty was the COVID-19 crisis: the experimental activities of almost all partners stopped completely for between 4 and 9 months, laboratories reopening progressively in 2021.

M. Bertolus also highlighted the connections between INSPYRE and other projects that have started or been proposed during INSPYRE and involve a large number of the INSPYRE participants, i.e., PUMMA, PATRICIA, RODEO and OperaHPC [19], [22]–[24].

## 4.3 Dissemination & Communication activities

Communication and dissemination activities were an important aspect of the activities of the INSPYRE project.

First, the INSPYRE website [25] has been online since the Project Kick off Meeting (September 2017) and has been regularly updated with INSPYRE deliverables and publications, as well as the latest news and events of interest for the INSPYRE community.

Then, about 45 articles have been published in peer-reviewed journals and several more have been submitted or under preparation. Moreover, INSPYRE partners presented approximately 90 communications at workshops and conferences, held in 12 European countries (including the UK), 4 non-European countries (Argentina, Japan, Mexico and the USA), plus 8 online conferences. Four INSPYRE newsletters describing the achievements of INSPYRE were also distributed to members of the nuclear research community in December 2018, February 2020, March 2021 and June 2022.

Finally, concerning communication for the general public, a poster exhibition describing in layman terms the simulation to guarantee the safety of nuclear fuels in reactor was prepared in October 2019 and presented at 60$^{th}$ birthday of the CEA Cadarache centre. These posters are available in English and French. Moreover, the INSPYRE partners prepared and released a video explaining the objectives and results of the Project. The video is available on the INSPYRE website [26].

## 4.4 Education & Training activities

A. Smith presented the three pillars of the INSPYRE Education & Training activities.

- The organization of two schools to train the next generation of researchers in the nuclear field: the first INSPYRE School "Generation IV reactors fuel cycle" (May 2019, Delft, The Netherlands) and the European School on Nuclear Materials Science 2020 (November 2020, online), in collaboration with other H2020 European Projects under the EERA-JPNM (GEMMA, M4F, Il Trovatore).
- The (co-)organization of three workshops to disseminate the results of the project to the nuclear materials research community and users: the first INSPYRE Workshop NuFuel-MMSNF 2019 (November 2019, PSI Villigen, Switzerland), the NuFuel Conference 2021 (September 2021, Bangor University, UK / online) and the final INSPYRE Workshop (November 2021, Marseille, France / online). The participation of students and young researchers was promoted and supported.
- The training through research performed in INSPYRE. 20 PhD students and Post-Docs were involved in the technical activities of the Project and 15 PhD theses were successfully defended during the project. In addition, a mobility scheme supported the travel and accommodation costs of young researchers to foster their mobility between partner institutions, giving them access to specific facilities or expertise. Despite the COVID-19 pandemic, a total of 33 months of mobility concerning 8 people took place.

## 4.5 Technical activities

The Work Package Leaders presented the results obtained during the project and the issues faced on the operational issues considered.

### 4.5.1 Margin to fuel melting

D. Staicu first described the new thermodynamic modelling of the (U-Pu-Am-O) fuel system developed on the basis of the materials properties both calculated at the atomic scale and measured on new samples synthesised and characterized during the project. He presented the review of the mechanisms governing MOX thermal conductivity evolution with burn-up, which led to recommendations for modelling activities. He finally reported the determination of MOX heat capacity using atomic scale calculations, covering the whole range of Pu contents and in a form suitable for implementation and use in fuel performance codes.

Future activities should focus on the experimental determination and atomic scale modelling of the melting point on well-characterised MOX samples with higher Am contents to determine the effects of

Am content and deviation from stoichiometry. Moreover, the thermal diffusivity of irradiated fuels at varying burnup should be investigated, enabling one to quantify the effects of O, Pu and fission products redistribution. These aspects will be investigated in the H2020 PATRICIA project [22] and in the EERA-JPNM Pilot Project RODEO [24].

### 4.5.2 Irradiated fuel thermochemistry and chemical interaction with the cladding

C. Guéneau presented the results of INSPYRE activities on the thermochemistry of irradiated MOX fuel.

The main focus of these activities was on the phases composing the “Joint Oxyde-Gaine” (JOG) layer. Thermodynamic properties and phase diagrams of these systems were determined and introduced in the TAF-ID database [27], [28]. The new data enables to get further insight into the various phases that can form and into the thermodynamic properties. The impact on the thermal conductivity of the JOG layers, which is one of the key elements governing the temperature in the fuel pellet at high burn-up, still needs to be determined. This will be investigated inter alia in the RODEO pilot project of the EERA-JPNM [24].

INSPYRE also investigated the phase diagrams of uranium, plutonium, iron and oxygen at high temperature. The first measurements of thermodynamic data at high temperatures in the U-Fe-O and $PuO_2$-$Fe_3O_4$ systems allow for better predictions of the chemical interaction between MOX/steel in case of severe accidents.

### 4.5.3 Atom transport properties and fission product behaviour

M. Krack presented the results obtained on the modelling of atom transport and inert gas (helium, fission gases) behaviour in $UO_2$ and $(U,Pu)O_2$ using experimental and modelling methods from the atomic to the microstructure scale. New experimental devices dedicated to MOX were developed. The combination of different techniques and methods provided input parameters for higher scale methods and simulation tools. Additionally, the microstructure and the release of inert gases of irradiated fuel samples (NESTOR-3, TRABANT-1) were investigated in the CEA and JRC laboratories.

Some experiments could not be performed because of the COVID-19 crisis and the modelling of transport properties in MOX fuels has only started. Activities will continue in particular in the EERA-JPNM Pilot Project RODEO [24].

### 4.5.4 Mechanical properties of fuels

M.-F. Barthe presented the INSPYRE activities on the investigation of the mechanical properties of $UO_2$ and MOX out of and under irradiation. The goal was to understand the underlying mechanisms governing the evolution of properties and phenomena (creep, swelling, fracture) as a function of Pu content, oxygen partial pressure, temperature and irradiation conditions, fill the literature gaps on MOX and justify or overcome the approximation of using $UO_2$ data for MOX. Dedicated experimental set-ups were developed to enable measurements on fresh fuels at high temperature, as well as under ion irradiation and neutron irradiation. Complementarily, correlations for MOX mechanical properties (elastic moduli, thermal expansion) and advanced micro-mechanical modelling approaches targeting the fuel visco-plastic and rupture behaviour were developed. The experimental irradiation activities encountered some difficulties, above all the closure of the laboratories during the COVID-19 pandemic, but also the leaks in the capsules enabling the in situ measurement of creep in HFR. Activities will continue on $UO_2$ based fuels in the OperaHPC Horizon Europe project [23].

### 4.5.5 Knowledge transfer to fuel performance codes and to users

L. Luzzi presented the activities aiming at improving and applying the GERMINAL, MACROS, and TRANSURANUS fuel performance codes, which represent the final link of the INSPYRE Project chain.

The first objective was to transfer the experimental and modelling knowledge acquired in the Project into FPCs [5]. The focus was on multi-scale and physics-based modelling approaches acting as a bridge from the lower-length (atomic) scale to the engineering scale of the fuel pin.

The involved codes, both in their reference PRE-INSPYRE and their post-INSPYRE versions, were then assessed against three fast reactor irradiation experiments (SUPERFACT-1, RAPSODIE-I, NESTOR-3) [6]–[8].

Finally, the post-INSPYRE versions of GERMINAL, TRANSURANUS and MACROS were used to simulate normal operation conditions in the ASTRID sodium fast reactor prototype and normal and transient conditions in the lead-bismuth cooled reactor of the MYRRHA accelerator driven system. The results of these simulations, which are the first openly available, enabled the evaluation of the safety margins of the fuel designs, e.g., the margin to fuel melting or the cladding plasticity for these two systems in representative operational conditions.

The FPC activities are continuing in the PATRICIA [22] and PUMMA [19] H2020 Projects, which focus on modelling developments for Am-bearing fuels and high-Pu MOX fuels, respectively, analysing additional scenarios relevant for MYRRHA and the SFR technology, as well as in the Horizon Europe OperaHPC [23], which concerns fuels with enhanced accident tolerance for current reactors.

## 4.6 General discussion and wrap-up

During the final discussion, the approach combining basic and applied research an the important results obtained it brought on uranium-plutonium mixed oxides in the INSPYRE Project were acknowledged. INSPYRE also gathered the various communities needed to make progress on the understanding and simulation of nuclear fuel, improving the understanding between the researchers and reinforcing the links between the research communities.

The results of INSPYRE are described in detail in the INSPYRE deliverables and publications and synthetized in Deliverable D7.6 [29] and in the presentations of the Final International Workshop (November 2021, Marseille, France).

# 5 CONCLUSIONS AND PERSPECTIVES

The conclusions of the User Group members regarding the approach and results of INSPYRE are as follows:

- The inclusion in fuel performance codes of improved MOX properties obtained is important for the Users. More generally the availability of updated and accurate MOX properties and behaviour models, even if not yet implemented in codes, will be useful since they constitute a significant basis for future improvements of fuel performance codes.
- The benchmark of fuel performance codes on relevant fast reactor irradiation cases ensures improved confidence in fuel performance simulations, supporting the design and licensing of Gen IV fast reactors.
- The detailed assessment of fuel performance codes for their application to fast reactor conditions was an important goal of the INSPYRE Project. Extending this validation using further data is key for their effective use.

Medium to long-term needs, to be addressed by follow-up European Projects and international initiatives, were also identified:

- The analysis of the interaction between the fuel and the cladding and the investigation of the JOG formation in fast reactor pins should continue, with the aim of improving its description in fuel performance codes.
- The modelling and simulations activities must be extended to demonstrate the improved predictive capabilities of fuel behaviour in accidental transient conditions.
- The investigations must also be extended to fuels with higher Pu and minor actinide contents.
- Fuel fabrication processes, which were not targeted in the INSPYRE Project, should be investigated using the approach developed and implemented in INSPYRE.

The regular exchanges of INSPYRE participants with the Project's user group were very fruitful. It enabled on the one hand the presentation of the approach and results of INSPYRE to the designers of fuel elements for the next generation of reactors. On the other hand, it enabled the INSPYRE researchers to get first-hand information on the needs of designers. This two-way exchanges will be a key element to accelerate the qualification of future fuels.

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