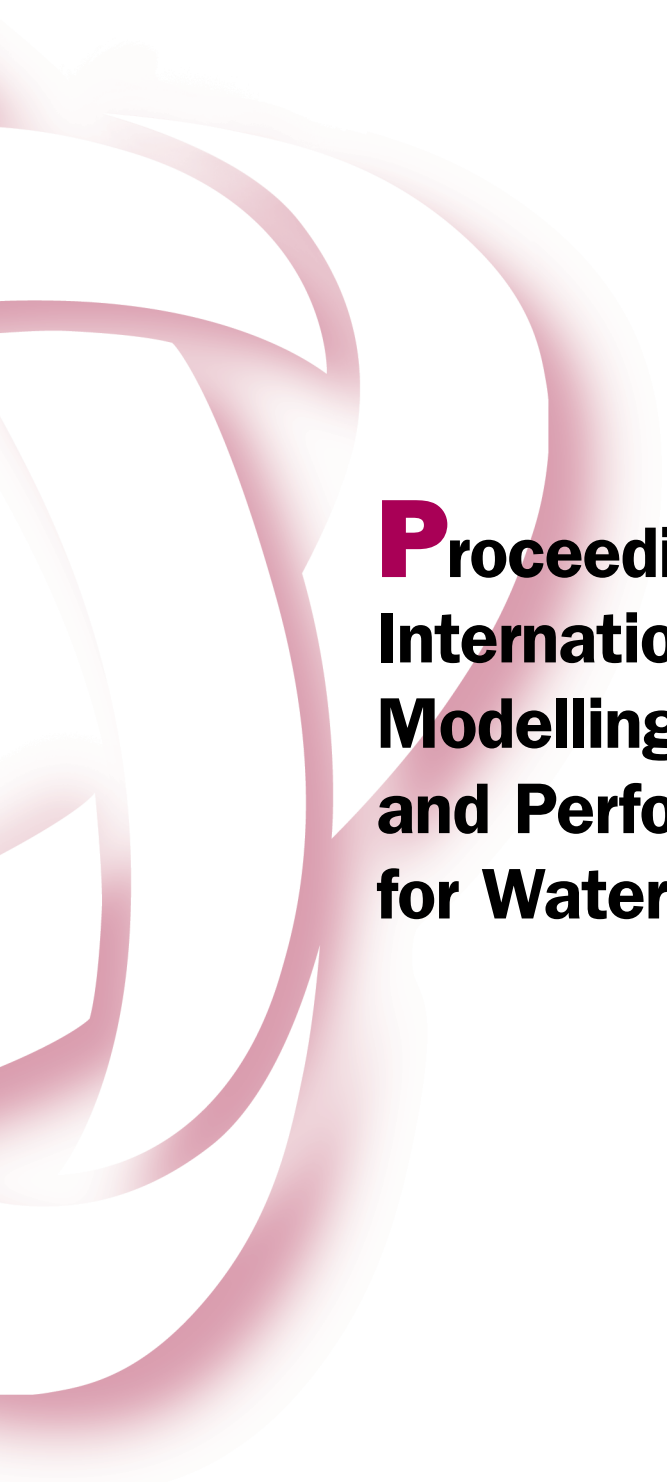




Proceedings of the 2017 International Workshop on Fuel Modelling to Support Safety and Performance Enhancement for Water-cooled Reactors

**NUCLEAR ENERGY AGENCY
COMMITTEE ON THE SAFETY OF NUCLEAR INSTALLATIONS**

**Proceedings of the 2017 International Workshop on Fuel Modelling to Support
Safety and Performance Enhancement for Water-cooled Reactors**

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List of abbreviations and acronyms

ACTOF	Analysis of Options and Experimental Examination of Fuels with Increased Accident Tolerance
AESJ	Atomic Energy Society of Japan
ANS	American Nuclear Society
AOO	Anticipated operational occurrences
ATF	Accident-tolerant fuel
BEPU	Best-estimate calculation plus uncertainty
BWR	Boiling water reactor
CEA	Commissariat à l'énergie atomique et aux énergies alternatives (Alternative Energies and Atomic Energy Commission, France)
CHF	Critical heat flux
CHROMOX	Cr doped mixed oxide fuel
CIM	Conductivity integral to melt
CIPS	Crud induced power shift
CPU	Central processing unit
CRP	Co-ordinated research project
CSNI	Committee on the Safety of Nuclear Installations (NEA)
DBA	Design-basis accident
DEC	Design extended condition
DEM	Discrete element method
DFT	Density functional theory
DiD	Defence in depth
DNBR	Departure from nucleate boiling ratio
DSA	Deterministic safety analysis
EATF	Enhanced Accident-tolerant Fuel
ECCS	Emergency core cooling system
EDF	Électricité de France
EGMPEBV	Expert Group on Multi-Physics Experimental Data, Benchmarking and Validation (NEA)
ENSI	Swiss Nuclear Safety Inspectorate
EPMA	Electron probe micro-analysis
EPRI	Electric Power Research Institute (United States)

FEM	Finite-element method
FFRD	Fuel fragmentation, relocation and dispersal
FGR	Fission gas release
FP	Fuel performance
FR	Fast reactor
FRM	Fuel Rod Module
FUMAC	Fuel Modelling in Accident Conditions
GB	Grain boundary
GTRF	Grid-to-rod-fretting
HBS	High burnup structure
HBWR	Halden boiling water reactor
HEDL	Hanford Engineering Development Laboratory
HPG	Halden Programme Group
HTR	High-temperature reactor
IAEA	International Atomic Energy Agency
IBRAE	Nuclear Safety Institute of the Russian Academy of Sciences
IEA	International Energy Agency
IFPE	International Fuel Performance Experimental Database
INL	Idaho National Laboratory
IRSN	Institut de Radioprotection et de Sûreté Nucléaire (Institute of Radiological Protection and Nuclear Safety, France)
JAEA	Japan Atomic Energy Agency
JHR	Jules Horowitz Reactor
JRC	Joint Research Centre
KAERI	Korea Atomic Energy Research Institute
KEPCO	Korea Electric Power Corporation
KINS	Korean Institute of Nuclear Safety
KIT	Karlsruhe Institute of Technology
KNF	KEPCO Nuclear Fuel
LANL	Los Alamos National Laboratory
LHR	Linear heat rate
LOCA	Loss-of-coolant accident
LWR	Light water reactor
M&S	Modelling and simulation
MD	Molecular dynamics
MEAM	Modified embedded-atom method

MNF	Mitsubishi Nuclear Fuel
MOOSE	Multiphysics Object-Oriented Simulation Environment
MOX	Mixed oxide fuel
NDC	Nuclear Development Committee (NEA)
NEA	Nuclear Energy Agency
NPI	Nuclear Promise Initiative
NPIC	Nuclear Power Institute of China
NRA	Nuclear Regulation Authority (Japan)
NRC	Nuclear Regulatory Commission (United States)
NSC	Nuclear Science Committee (NEA)
OMD	Order of magnitude deviation
ORNL	Oak Ridge National Laboratory
PCI	Pellet-clad interaction
PCMI	Pellet-cladding mechanical interaction
PIE	Post-irradiation examination
POLIMI	Politecnico di Milano
PPN	Peak Power Node
PSA	Probabilistic safety assessment
PSI	Paul Scherrer Institute (Switzerland)
PWR	Pressurised water reactor
Q&A	Questions and answers
R&D	Research and development
RCM	Research Coordination Meeting
REV	Representative elementary volume
SA	Severe accident
SAFDL	Specified acceptable fuel design limits
SCC	Stress corrosion cracking
SiC	Silicon carbide
SIMS	Secondary ion mass spectrometry
SMIRT	International Conference on Structural Mechanics in Reactor Technology
SRSS	Square root of the sum of the squares
SSM	Swedish Radiation Safety Authority
TCD	Thermal conductivity degradation
TEM	Transmission electron microscope
TEPCO	Tokyo Electric Power Company

TH	Thermal-hydraulic
TMOL	Thermo-mechanical operational limit
TRL	Technology-readiness levels
TSO	Technical support organisations
UKAEA	United Kingdom Atomic Energy Authority
US DOE	United States Department of Energy
V&V	Verification and validation
VVER	Water-water energetic reactor
WGFS	Working Group of Fuel Safety (NEA)
WPMM	Working Party on Multiscale Modelling (NEA)

Executive summary

Advanced techniques for fuel modelling have progressed considerably in the last decade, in part aided by progress in high-performance computational capability. At the engineering scale, this has resulted in improved mechanistic descriptions within fuel performance codes. There has been a trend to progressively replace empirical models and correlations with physical models that allow, in principle, an extension of the predictive capability of the codes beyond the domain for which experimental results are available. As an example, mesoscale codes (at the fuel-grain scale and typically microns) provide predictions of microstructure evolution and determine their impact on fuel properties. The codes describe phenomena such as grain boundary sweeping, grain growth, bubble nucleation, growth and coalescence, precipitation of solid fission products and their speciation and phase separation. The inclusion of these models within engineering-oriented fuel performance codes offers improved predictions of thermal conductivity, elastic constants, swelling, pellet-clad interactions and fission-gas release under conditions beyond their usual range of validity and creates an exploratory capability.

At the Nuclear Energy Agency (NEA), the importance of fuel modelling and its improvement through development of phenomenological representations has been recognised and multiple technical groups related to materials modelling and the support of advanced fuels and safety codes are considering these issues. One example is the Working Party on Multiscale Modelling (WPMM) of Fuels and Structural Materials for Nuclear Energy Systems, and in particular the Expert Group on Multiscale Modelling of Fuels, which published in October 2015 a state-of-the-art report on Multi-scale Modelling of Nuclear Fuels. Another example is the Reactivity Initiated Accident (RIA) Fuel Codes Benchmark that was organised by the Working Group of Fuel Safety (WGFS), who released first results in November 2013 – “RIA Fuel Codes Benchmark - Volume 1”¹ – and results of a second phase in April 2016 – “Reactivity Initiated Accident (RIA) Fuel Codes Benchmark Phase-II”².

The International Workshop on Nuclear Fuel Modelling to Support Safety and Performance Enhancement for Water-Cooled Reactors was held on 7-9 March 2017 in Paris to further improve the co-ordination of these activities, both within the NEA and in the broader technical world, and to identify future needs. The workshop was an excellent opportunity to bridge the gap between the WGFS and WPMM activities and identify future perspectives of nuclear fuel modelling.

The main objectives of the workshop were to:

- identify areas where advanced rod scale, mesoscale or microscale plus multiscale integration modelling of nuclear fuels is contributing or may contribute to significant progress or insights on fuel safety and/or fuel performance for water-cooled reactors; the focus was on the design and operation of nuclear fuel, with a consideration of normal and off-normal operating conditions, including design-basis accidents;

¹ NEA (2013), “RIA Fuel Codes Benchmark - Volume 1”, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_19332.

² NEA (2016), “Reactivity Initiated Accident (RIA) Fuel Codes Benchmark Phase-II: Volume 1: Simplified Cases Results Summary and Analysis”, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_19710.

- identify the impacts these advanced modelling approaches might have on current nuclear fuel design safety limits (evolution or new types of safety limits);
- identify gaps and possible experimental needs;
- identify areas for enhanced international collaboration and the NEA contribution.

The workshop included keynote speeches, technical talks and panel discussions involving experts from a broad spectrum of stakeholders from NEA member countries, which included research and development (R&D) organisations, academia, industry and regulatory bodies along with representatives of other international bodies. The workshop covered major topics related to performance and safety improvements during normal operation and under off-normal conditions for water-cooled reactor nuclear fuel. These include:

- the release of fission gas;
- the formation of high burn-up structures (rim and MOX clusters);
- fuel swelling (diametral and axial) and pellet-clad interactions;
- the impact of dopants such as gadolinia;
- an analytical investigation of margins associated with fuel safety criteria including uncertainties;
- other issues such as clad oxidation, crud deposition, fretting and fuel rod bowing;
- factors affecting burn-up and cycle length, power uprates and more flexible operating modes;
- the reduction of uncertainties in the fuel design process and consequences for licensing margins;
- fuel behaviour such as relocation under LOCA conditions.

Technical discussions also addressed – but were not limited to – the development of accident-tolerant fuels, which included: improved uranium oxide fuels; various types of high-density fuels and ceramic microencapsulated fuels; advanced cladding materials including coated/improved zirconium-based alloys, ceramic composites, advanced steels and refractory metals.

The workshop promoted discussion among the different communities of fuel experts, i.e. experts in advanced modelling, safety and fuel performance. The key aim was to identify fuel issues in normal and off-normal/design-basis accident conditions that would strongly benefit from the application of advanced modelling techniques made available within a reasonable time frame (of 5-10 years). Such efforts made within that time period are expected to generate better insights into fuel behaviour and the use of integrated advanced modelling should, as an example, lead to progress in the improvement of fuel efficiency and provide alternative methodologies for the assessment of fuel safety.

For this purpose, the workshop was organised into 3 main sessions:

- Session 1 on “recent developments and future challenges for nuclear fuel”;
- Session 2 on “nuclear-fuel modelling in support of performance and safety improvements under off-normal conditions”;
- Session 3 on “nuclear-fuel modelling in support of performance and safety improvements during normal operating conditions”.

The major outcomes and observations to emerge from the workshop were discussed during the last “workshop wrap-up” session (session 4) and can be summarised as follow:

- Modelling and simulation (M&S) are driving experiments (rather than experiments driving M&S) and tackle problems and provide insights that would not have been possible five or more years ago.
- An assessment was made of whether an enhanced use of advanced M&S in the design and licensing of new products is having an impact, which led to the observation that there is progress in this direction but that the impact is not yet major. There is some limited evidence that the fuel and/or experimental designers are using advanced M&S tools for the development of fuel and experimental procedures, while the key focus of regulators is dealing with convincing safety cases based on reliable (experimental) validation and not with M&S tools per se. On the other hand, advanced M&S tools may be used by the regulators to challenge the historical safety case analysis provided by the designers.
- It was observed that most of the current “historical” design/safety limits are not adapted to approaches based on multi-physics or multi-scales tools.
- Some needs were identified: further progress on instrumentation to accompany the progress on M&S tools; smaller-scale experiments (as opposed to integral and/or power reactor) for the validation of individual models and the quantification of uncertainties; and the development of a methodology for assessing uncertainties in fuel performance codes (licensing).
- Collaboration driving the resolution of some of these issues is occurring effectively and well, if not too formally and not on a very large scale. One key element that needs to progress is gathering modellers and experimentalists.
- Some areas for future collaboration were identified, as follows: fuel densification and fission-gas swelling; ballooning and fuel relocation in accident conditions; fuel restructuring during normal operation; microstructure/properties in the high burn-up region; interaction between the fission-product and fuel microstructure; an investigation of which mechanism drives fuel fragmentation; and cladding failure and the modelling for design of accident-tolerant fuels.
- The presentations by international organisations (the NEA and the International Atomic Energy Agency [IAEA]) underlined the importance of international benchmark exercises for the validation of fuel behaviour codes using common databases. It was concluded that the development of accident-tolerant fuel concepts could also profit from advanced modelling carried out in international co-operation.
- The possibility of assessing priorities and needs as a group was raised. Therefore, it is recommended that a table of needs and priorities be built.

Overall, advanced modelling was thought to be contributing to fuel design. However, its direct application in the licensing process is not currently established (although regulators may use advanced M&S tools to challenge historical safety cases' analysis). The NEA Working Group on Fuel Safety (WGFS) will continue discussions on this issue to identify further areas where advanced techniques for fuel modelling could be utilised from the fuel safety viewpoint.

1. Introduction

The International Workshop on Nuclear Fuel Modelling to Support Safety and Performance Enhancement for Water-Cooled Reactors was held on 7-9 March 2017 with the objectives of clarifying the status of modelling capabilities and bringing together people from diverse communities with an active interest in advanced nuclear fuel modelling.

The workshop aimed to focus on advanced nuclear fuel modelling and simulation (M&S) in order to:

- provide insights into the phenomenology governing the evolution of current fuels in normal conditions (fission-gas release, high burnup structures, swelling, pellet-clad interactions and impact of dopants, etc.);
- provide insights into the phenomenology governing the evolution of current fuels in off-normal conditions;
- assess the potential to investigate the criteria of fuel safety margins including uncertainties;
- identify which topics/developments are considered to be key areas for progress by the international community in the medium term ($\geq$ five years);
- identify major challenges for the experimental validation of advanced M&S methods (data availability, availability and cost of experimental capabilities);
- clarify the implementation by industry of new fuels requiring licensing, e.g. the possible optimisation of the qualification process;
- seek a common understanding of the role of the NEA in tackling these challenges through international co-operation.

The workshop featured technical sessions about developments from the perspectives of modellers, utilities, fuel vendors and safety bodies, as well as about modelling in support of improvements during normal and off-normal operating conditions. The event brought together 80 participants from 18 member countries who represented a broad spectrum of stakeholders including academic and R&D institutions, industry, technical support organisations (TSOs), regulatory bodies and international organisations.

2. Overview of Session 1: Recent Developments and Future Challenges for Nuclear Fuel

Co-chairs: Kemel Pasamehmetoglu (the Idaho National Laboratory [INL], United States), Marc Petit (Institute for Radiological Protection and Nuclear Safety [IRSN], France) and Theodore Besmann (the University of South Carolina [USC], United States)

This session comprised nine presentations that provided an overview of the status of advanced modelling and simulations of nuclear fuel, needs and expected progress in the next decade from the perspective of nuclear utilities and fuel vendors, the regulators' perspective, and related activities within the NEA and International Atomic Energy Agency [IAEA]:

- Chris Stanek (the Los Alamos National Laboratory [LANL], United States) and Michel Freyss (Commissariat à l'énergie atomique et aux énergies alternatives [CEA], France), "Recent developments in advanced modelling applied to nuclear fuel";
- Nicolas Waeckel (Électricité de France S.A. [EDF], France), Jinzhao Zhang (Tractebel-Engie, Belgium) and Ken Yueh (the Electric Power Research Institute [EPRI], United States), "Utility perspective on needs related to nuclear-fuel operation".
- Fuel vendor perspectives on current trends and future needs for improvements:
 - Nozomu Murakami (Mitsubishi Heavy Industries [MNF], Japan), "Expectations from progress in fuel modelling in order to optimise fuel design and safety analysis";
 - Pierre Mailhé (AREVA NP, France), "Current and upcoming issues for fuel modelling";
 - Simon Middleburgh (Westinghouse, Sweden), "Modelling accident -tolerant fuel concepts: gaining a mechanistic understanding to aid licensing";
 - Jongsung Yoo (KEPCO Nuclear Fuel [NF], Korea), "Current issues and future needs for fuel modelling in LWRs".
- Marc Petit (IRSN, France) and Toyoski Fuketa (Nuclear Regulation Authority [NRA], Japan), "Safety and regulatory aspects related to nuclear fuel and activities within CSNI Working Group on Fuel Safety";
- Marc Deffrennes (NEA), "Link with NEA Innovation 2050 initiative";
- Mikhail Veshchunov (IAEA), "IAEA activities on fuel performance".

2.1. Summary

Session 1, on the recent developments and future challenges for nuclear fuel, was designed to set the stage for discussions about the needs, contributions and developments in modelling in support of safety and performance enhancement for water-cooled reactors. Presentations were therefore given by representatives of the technical support organisation of the French nuclear safety authority (IRSN), the regulatory body of Japan (NRA), as well as the IAEA, with an NRC representative in attendance but not presenting. Modelling needs from the vendor perspective, the current status and future developments were highlighted

by representatives of Westinghouse Electric Co., LLC, KEPCO, AREVA NP, and Mitsubishi Nuclear Fuel Co., Ltd. The power producers' views were well presented by EDF, Tractebel-Engie and EPRI. While modelling developments are underway largely among all these organisations, the fundamental underpinnings are being provided by universities and national/government laboratories, with the US Department of Energy (US DOE) and CEA programmes described in the programme. Finally, IAEA activities on fuel performance and the NEA efforts on modelling and simulation were presented.

2.1.1. Chris Stanek (Los Alamos National Laboratory, United States)

Empirical models can accurately interpolate between regions of known data but cannot confidently extrapolate outside of test bounds. A goal is thus to develop improved, mechanistic and predictive models for fuel performance using hierarchical and multiscale modelling applied to existing, advanced (including accident-tolerant) and used (spent) fuel. Work has started on extending the BISON code to accident-tolerant fuel, for example, U-Si fuel issues such as U_3Si_2 non-stoichiometry, fission gas release, potential derivation, radiation tolerance, etc. Validation cases are being added to the current suite that corresponds to specific capability development with near-term validation experiments being planned for the Halden reactor. On a more specific issue, the successful effort to understand and model anomalous heat capacity behaviour in UO_2 was described and is being incorporated into fuel performance codes.

2.1.2. Michel Freyss (CEA)

Efforts made at CEA with fuel performance codes aim to predict the mechanical integrity of fuel, microstructure evolution, swelling, fission gas release and pellet-cladding interaction. These efforts include recent developments in fuel performance modelling such as a micromechanical approach that includes the influence of the microstructure on fuel properties; and the integration of thermochemistry into fuel performance codes in order to better represent the thermochemical interactions involved in pellet-clad interactions (PCIs) and stress corrosion cracking (SCC). In addition, the role of defects and stoichiometry on fission-product migration is being taken into account in fuel performance code fission gas release models. These are through the Macro-scale Mean Grain Fission-Gas behaviour (MARGARET) approach with the use of representative elementary volume (REV) methodology. The 3D continuum damage approach for the simulation of crack initiation and growth due to fission gas bubbles, as well as fuel fragmentation at the microscopic scale simulated by a full 3D finite-element method (FEM) approach, are both being pursued. Beyond conventional light water reactor (LWR) fuel, there is an effort on MOX to incorporate composition heterogeneity into the fuel performance code ALCYONE (PLEIADES); 3D simulation of microstructure (heterogeneity) of MOX based on experimental characterisation; derivation of a micromechanical constitutive law (homogenisation); and effect of MOX heterogeneities on fuel behaviour (swelling, fission gas release). Finally, the recent coupling of fuel performance codes and thermochemistry calculations to investigate the impact of thermochemistry on fuel behaviour was described. This aims to understand the key role of thermochemistry on irradiated fuel behaviour. Challenges for the future were identified, which included obtaining the optimal use of modelling/simulation and analytical experiments for defining critical irradiation tests and contributing to their interpretation; and the further development of uncertainty and sensitivity analysis in nuclear fuel behaviour modelling.

2.1.3. Jinzhao Zhang (Tractebel-Engie), Ken Yueh (EPRI) and Nicolas Waeckel (EDF)

The utility representatives asked the general question: How could advanced modelling help reduce costs? The reality is that if all physical mechanisms/phenomena are well-identified and characterised, experimental validation using advanced calculation tools (verification and validation [V&V] Uncertainty Quantification [UQ]) is inevitable. Multi-scale and multi-physics tools may even require new ways of demonstrating validation. These might include dedicated, advanced research and development (R&D) tests, new methods for analysing test results or commercial in-reactor measurements. Specific big data algorithms will perhaps need to be developed. Advanced modelling may help increase design/operation margins. However, the use of advanced modelling (i.e. multi-scale and multi-physics approaches) is not always adapted to fuel core design where the behaviour of thousands of fuel rods must be considered. Current standards are based on former decoupled 1D static methods, which has now been surpassed by advanced modelling. Some areas of interest include PCI-SCC, where the pellet behaviour includes thermochemistry and thermomechanical modelling and the SCC mechanisms of the cladding include crack initiation and propagation, determining susceptibility and developing a SCC damage model.

In another area, the utility representatives are looking for help regarding the management of design and safety margins. Although margins are included in the safety assessments, definitions of them are somehow unclear and confusing. The margins might be different for each organisation/country (e.g. the IAEA, NEA, NRC and industry) and can be divergent according to the specialty/discipline (such as mechanics; neutronics; thermal-hydraulics; deterministic and probabilistic safety assessments). Margins can also evolve alongside advances in safety standards and technology. However, the utilities' representatives promote a simple and practical approach that is based on the NEA definitions and Tractebel/EDF margin models.

Lower scale and complex models need more validation efforts. Simple models could be helpful by providing insights and improving experimental designs.

Finally, the utility representatives note that modelling needs include improved codes' coupling features, the identification of the various mechanisms/phenomena leading to grid-to-rod-fretting (GTRF), impacting loss-of-coolant accidents (LOCAs), reactivity-initiated accidents (RIAs), PCIs and crud induced power shift (CIPS) events.

In general, utilities worldwide are facing cost-related difficulties and see advanced modelling as a way, among others, of reducing expensive fuel research and restoring design margins. Such an approach of course must remain fully compatible with the standard fuel and core design/safety requirements.

2.1.4. Nozomu Murakami (Mitsubishi Nuclear Fuel Co., Ltd.)

The fuel vendor identified a need to improve evaluation methods for cladding failure under transient conditions to quantify/clarify safety margins. Long-term coolability after a LOCA event has been focused upon since 2011 and more discussions on how to treat this topic are necessary. It was noted that the fuel designer should collaborate with safety analysis groups. Concerning high burnup fuel, issues revolve around the onset of fuel pulverisation, fragmentation, relocation and/or dispersion outside of the cladding following the ballooning/burst point during a LOCA event, i.e. in high-temperature transient conditions. A threshold burnup of 60-70 GWd/t was preliminarily investigated in current Halden and Studsvik studies. The phenomena are likely to limit burnup from a coolability point of view. Models of the mass of fragmented, relocated and dispersed pellets material and

models for evaluating coolability with such dispersed/relocated pellets are therefore important. V&V test programmes and code benchmarking are also important. There is an expectation that future efforts made in these areas will involve international collaboration.

2.1.5. Pierre Mailhé, Christophe Garnier and Jérôme Roland (AREVA NP)

Current trends and future needs for fuel modelling include improving predictive capabilities to justify increased fuel performance for improved fuel management, fuel manoeuvrability (e.g. load following) and safety margins. These trends are necessarily accompanied by some evolution in the design methods such as the development of statistical methodologies for a realistic assessment of fuel performance. In addition, support is needed for the development and licensing of new fuel products (e.g. doped fuels and enhanced accident-tolerant fuel) and for compliance with safety authorities' new rules and requirements. Issues encompass improvement in fuel model predictive capabilities and improved transient and accident modelling. New fuel products will be strong drivers for fuel modelling in the next years, covering subjects such as fission gas release, gaseous swelling, fuel fragmentation, PCI, high burnup structure (HBS), clad oxidation and silicon carbide (SiC) irradiation behaviour. Codes need improved predictive capabilities, validation and robustness.

2.1.6. Simon Middleburgh, Ed Lahoda, Peng Xu, Magnus Limbäck and Yun Long (Westinghouse Electric Co., LLC)

Westinghouse discussed accident-tolerant fuels (ATFs) UN, U_3Si_2 , UN- U_3Si_2 , advanced doped UO_2 and SiC-SiC composite and coated cladding. Current fuel modelling activities within Westinghouse are reliable for UO_2 -Zr systems, but likely to be inefficient for new materials' licensing without first undergoing serious architectural alterations. Extensive data collection efforts will be required for some new systems. Mechanistic modelling is also seen as an aid to licensing. Mechanistic modelling reduces the need for experimental work, but it does not replace experimental validation. However, mechanistic modelling enables a degree of extrapolation and understanding of experimental data and provides a mechanistic multi-input model that functions over more of the experience space.

2.1.7. Jongsung Yoo and Jaemyung Choi (KEPCO Nuclear Fuel)

This group focused on issues in fuel modelling like fuel thermal conductivity and its uncertainty, as well as crud deposition and thermal conductivity. There is also a need to improve PCI/ pellet-cladding mechanical interaction (PCMI) analysis and accidents' analysis. Concerning the enhancement of safety and performance margins, fuel modelling in particular needs to address the refinement of fuel representations and properties in order to allow for more accurate predictions of fuel rod behaviour during normal operation and transients such as in PCI, LOCA and RIA.

2.1.8. Marc Petit (IRSN, France) and Toyoski Fuketa (NRA, Japan): CSNI Working Group on Fuel Safety

Discussions focused on the work of the NEA Committee on the Safety of Nuclear Installations (CSNI) Working Group on Fuel Safety (WGFS). The reports about RIA fuel behaviour, RIA code benchmarking, behaviour under LOCA – including spent fuel pool – fuel fragmentation, relocation and dispersal were highlighted. Recent activity on leaking fuel and impacts, SCC and PCI, oxygen and hydrogen in cladding, fuel performance (FP) behaviour during transients, behaviour in spent fuel pools and the fuel assembly bow were described. It was noted that a number of topics related to fuel safety offer opportunities to advance modelling, particularly in areas such as uncertainty evaluation that is becoming

more important due to modelling sophistication. New fuel concepts such as ATFs were also mentioned as areas that may similarly benefit from advanced modelling.

2.1.9. Marc Deffrennes (NEA)

Nuclear Innovation 2050, a NEA incubator intended to accelerate R&D and the market deployment of innovative nuclear fission technologies in order to contribute to a sustainable energy future, was described. Relevant identified elements that deserve further development include the following: the enhanced collection of basic data (databases in nuclear data, mechanical properties, chemistry and experimental databases); development of novel experimental techniques to address the need for more fundamental and precise data; organisation of basic experimental campaigns to obtain such data; use of this data to develop and validate new models that will enable deeper understanding; benchmarking of resulting codes and comparisons of coupling techniques; development of validation methodologies, including extrapolation; organisation of large-scale validation experimental campaigns; joint exercises in code validation; and, finally, the resolution of major challenges and problems in order to demonstrate the value of the new products.

2.1.10. Mikhail Veshchunov (IAEA)

The Nuclear Fuel Cycle and Materials Technologies Subprogram comes under the IAEA Nuclear Power and Fuel Cycle major programme and runs three related projects: the Nuclear Power Reactor Fuel; Nuclear Power Reactor Fuel Engineering; and the Action Plan to Support Nuclear Power Reactor Fuel. These projects are designed to enable member states to organise adequate R&D programmes to support the effective design and manufacturing of technologies and to optimise the in-pile performance of current and advanced fuels and materials for reliability and efficiency. There are currently co-ordinated research projects on Fuel Modelling in Accident Conditions (FUMAC); Analysis of Options and Experimental Examination of Fuels with Increased Accident Tolerance (ACTOF); and a new effort on Fuel Materials for Fast Reactors. The IAEA believes that the development and modelling of advanced fuel types that can better withstand the extreme conditions found in severe accidents will improve safety margins. The projects listed above strive to achieve the goal within the IAEA Nuclear Safety Action Plan of enhancing the safety of nuclear reactor operations.

2.2. Overall summary of Session 1

The lecturers identified the following objectives and development directions for advanced modelling and the simulation of nuclear fuel in session 1:

- the development of improved, mechanistic and predictive models for fuel performance using hierarchical and multiscale modelling;
- applications to existing, advanced and used (spent) fuel;
- the introduction of material properties, correlations and models for new materials used in accident-tolerant fuel designs (e.g. UN, U_3Si_2 , doped UO_2 pellets, and SiC-SiC composite and coated Zr claddings);
- predictions of the mechanical integrity of fuel, microstructure evolution, swelling, fission gas release and pellet-cladding interaction;
- the micromechanical approach that aims to include the influence of the microstructure on fuel properties;

- the integration of thermochemistry in fuel performance codes in order to better represent thermochemical interactions;
- the development of statistical methodologies for a realistic assessment of fuel performance during normal operating, anticipated operational occurrence and pre-accidental conditions;
- the development of big data algorithms;
- the application of multi-scale and multi-physics approaches;
- models for fuel pulverisation, fragmentation, relocation and/or dispersion outside of the cladding after the cladding burst;
- the justification of increased fuel performance for improved fuel management, fuel manoeuvrability (e.g. load following) and safety margins;
- enhancing knowledge on crud deposition and thermal conductivity issues.

The presentations by international organisations (NEA and the IAEA) underlined the importance of international benchmark exercises for the validation of fuel behaviour codes using common databases. It was concluded that the development of accident-tolerant fuel concepts could also benefit from advanced modelling carried out through international co-operation.

3. Overview of Session 2: Nuclear-Fuel Modelling in Support of Performance and Safety Improvements under Off-Normal Conditions

Co-Chairs: Anna Alvestav (Strålsäkerhetsmyndigheten [SSM], Sweden) and Brian Wirth (Oak Ridge National Laboratory [ORNL]/ University of Tennessee [UT], United States)

This session comprised five presentations followed by a panel discussion.

- Gaétan Guillard (Institute for Radiological Protection and Nuclear Safety [IRSN], France), “Computational analysis of multi-rod ballooning and fuel relocation during loss-of-coolant accident (LOCA) using the multi-physics DRACCAR code”;
- Masaki Amaya (the Japan Atomic Energy Agency [JAEA], Japan), “Key issues in fuel safety studies on the modelling of fission-gas behaviour inside fuel pellet under normal and off-normal conditions”;
- Hyo-Chan Kim (the Korea Atomic Energy Research Institute [KAERI], Korea), “Development status of the fuel module for simulation of LOCA and reactivity-initiated accident (RIA) in KAERI”;
- Vladimir Ozrin (the Nuclear Safety Institute [IBRAE], Russia), “Modelling of irradiated oxide-fuel behaviour and fission-product releases under transient and severe-accident conditions by the fuel performance and safety code SFPR”;
- Kevin Govers (SCK CEN, Belgium), “Granular simulation of fuel relocation and dispersal in LOCA conditions”.

3.1. Summary

The second session was devoted to consideration of the phenomena that occur in off-normal conditions and how they can be modelled. The discussions were mainly centred on the current fuel and reactor systems (UO_2 in Zircaloy in the light water reactor [LWR]) due to the maturity of these systems and the level of knowledge that has been built around their types of events. Among the major events relevant for LWR are loss-of-coolant accidents (LOCAs), reactivity-initiated accidents (RIAs) and power transients resulting in pellet-clad interactions (PCIs).

3.1.1. Gaétan Guillard (IRSN, France)

In the framework of its research activities related to loss-of-coolant accidents (LOCAs) the IRSN is developing a multi-rod computational tool named DRACCAR. Modelling has to take into account many coupled phenomena in order to realistically describe the behaviour of the reactor core during a LOCA. This implies complex computations involving multidimensional aspects. The presentation included a description of models in DRACCAR and an example of an application: the simulation of multi-rod ballooning and fuel relocation during a LOCA. IRSN presented plans for the further development of the DRACCAR tool and tools to be used in combination with it about the validation of mechanics with azimuthal temperature gradients and also about contact aspects and the validation of reflooding models on deformed geometries.

3.1.2. Masaki Amaya (JAEA, Japan)

Fuel failure phenomena under accident conditions have been extensively studied at JAEA. Experimental analyses are being performed using the fuel performance code, RANNS, and the steam explosion simulation code, JASMINE. The results show that some fission gas behaviours are likely to dominate both fuel deformation and the intensity of destructive force at fuel failure. Specifically, the timing of gas release to the free volume in the fuel rod, gas communication in the axial direction of fuel rod and the mixing of the fission gas released by fuel failure with coolant water have been identified as elementary processes that should be clarified to properly reflect the knowledge obtained from experiments in safety criteria. The contribution of meso- and/or micro-scale studies seems important for the establishment of a more physics-based modelling. These studies will be able to provide key information about, for example, the mobility of single gas atoms and gas bubbles and influential factors on the effective rate of coalescence between single gas atoms and gas bubbles.

3.1.3. Hyo-Chan Kim (KAERI, Korea)

KAERI has been developing a new methodology of safety analysis code system that incorporates the best-estimated fuel module for rule revision. For LOCA, the development is ongoing with a fully coupled safety analysis code system with a fuel module. As the first step, the modified FRAPTRAN (so-called SFRAPTRAN) will be embedded into a safety analysis code system (MARS-KS). As the next step, KAERI's fuel module, which is based on finite-element method (FEM), will be developed. In the case of RIA, the development of a fuel module is not yet very advanced because fuel behaviours during RIA are not fully understood and in-pile experiments for RIA should first be more accumulated. One of the failure mechanisms of fuel during RIA that needs further understanding and code development is pellet-cladding mechanical interaction (PCMI). The following items have been recognised to support development at KAERI:

- the development of a FEM-based fuel behaviour module for a LOCA;
 - models of single rod behaviour during a LOCA;
 - a thermo-mechanical model for fuel;
 - a performance basis fuel model and new models;
 - a FEM solver and core module;
 - a flow blockage prediction model;
 - a multi-rod analysis methodology;
 - a rod-to-rod contact model;
- the development of an integrated TH code system;
 - the coupling of a TH code (CUPID) system-KAERI's fuel module;
 - embedding fuel models into a TH code system;
 - the evaluation of an integrated TH code using international fuel experiment database;
- the development of an out-of-pile fuel behaviour experiment;
 - the development of multi-dimension measurement at high temperature;
 - the experiment of cladding deformation (Balloon&Burst);
 - an experiment of rod-to-rod contact for a flow blockage prediction model.

3.1.4. Vladimir Ozrin (IBRAE, Russia)

The SFPR code for mechanistic and multi-scale modelling of single fuel rod behaviour under various regimes of light water reactor operations (normal and off-normal, including severe accidents) has been developed at IBRAE during the last decade. The code was designed by coupling together the two stand-alone codes MFPR (for mesoscale modelling of irradiated UO₂ fuel behaviour) and SVECHA/QUENCH (for macro-scale modelling of Zr cladding thermo-mechanical and physico-chemical behaviour). The phenomena discussed in the presentation were microscopic mechanisms of enhanced fission gas release and microstructure evolution as well as the transport of chemically-active elements. The further development of the SFPR code would consist of, for example, its implementation in best-estimate codes, further validation and extension to fast reactor (FR) fuel.

3.1.5. Kevin Govers (SCK CEN, Belgium)

At SCK CEN, discrete element method (DEM) simulations have been performed with the LAMMPS code in order to generate better understanding about the mechanisms leading to fuel relocation and dispersal during LOCA accidents. The fall of fuel fragments in a rapidly expanding cladding (balloon zone) was modelled and used to evaluate the packing density in the ballooned area. The adopted methodology has also shown the capabilities of addressing fuel dispersal through the burst and therefore opens the way for linking the amount of dispersed fuel to the balloon and burst geometrical characteristics. Further analyses are necessary to derive a relation between the amount of dispersed fuel and the geometrical parameters of the balloon and burst. A development of the method includes, for example, physical and geometrical descriptions and non-spherical particles.

3.2. Panel discussion moderated by session co-chairs

A panel summarised the session and reflected upon the state of knowledge. The participants were Thierry Forgeron (Commissariat à l'énergie atomique et aux énergies alternatives [CEA], France), Timothy Valentine (ORNL, United States), Nicolas Waeckel (Électricité de France S.A. [EDF], France) and Ken Yueh (the Electric Power Research Institute [EPRI], United States). The panel discussed the efforts that have been and are being made for PCI and off-normal situations (RIA and LOCA). The topics discussed included: thermomechanical and thermochemical models, the coupling of codes, failure and burst mechanisms and criteria. Large benefits were acknowledged in the recognition and understanding of which phenomena are important and where current methods could be improved.

3.2.1. Thierry Forgeron (CEA, France)

The speaker first introduced the CEA fuel simulation platform PLEIADES, which includes models and data applicable to different reactor technologies (pressurised water reactors [PWRs], boiling water reactors [BWRs], materials testing reactors [MTRs], high-temperature reactors [HTRs] and fast neutron reactors [FBRs]). The speaker focused on ongoing developments for off-normal conditions, in particular RIA and LOCA. He then briefly summarised the major conclusions of a workshop on PCI that was held in 2016 in Lucca (Italy).

3.2.2. Timothy Valentine (ORNL, United States)

The speaker opened his presentation on multi-physics calculations from the perspective of fuel modelling (a major theme of the workshop), which is the primary focus of the NEA Expert Group on Multi-Physics Experimental Data, Benchmarking and Validation

(EGMPEBV, www.oecd-neo.org/science/egmpebv/). EGMPEBV will in 2017-18 carry out a first exercise of application to a specific PCI problem of the methodology of a multi-physics calculation that is under development within this group.

During the questions and answers (Q&A) the discussion focused on:

- how to scale up uncertainty related to fuel phenomena in multiscale modelling and simulations (M&S);
- the need for M&S and experimental work to proceed jointly in order to advance phenomenological knowledge of key issues (i.e. PCI and fuel cracking), which is needed to allow M&S to evolve into a predictive and validated tool that could be effectively adopted into the design process.

3.2.3. *Nicolas Waeckel (EDF, France)*

The speaker developed the perspectives offered by advanced multiscale multi-physics modelling tools in terms of the consequences for the safety demonstration and its potential impact on safety as a whole. The presentation offered several items for further discussion, including:

- the need to confirm that current safety design limits are still adapted to multiscale/multi-physics calculations;
- the need to develop relevant experiments/ways to validate multiscale/multi-physics tools (an essential condition for using them in a safety analysis);
- the fact that multiscale M&S is well suited to defining mechanistic scenarios and helping to analyse complex in-pile tests;
- opportunities for valuable synergies between “big data” analysis, multiscale/multi-physics M&S and experiments (including start-up tests in nuclear power plants).

3.2.4. *Ken Yueh (EPRI, United States)*

The speaker focused on various issues including:

- fuel fragmentation and fission gas release: grain boundary fission gas is certainly a driver for fuel fragmentation, but not the only one;
- unit mechanisms contributing to ballooning and burst;
- RIA evaluation (experimental values versus M&S).

3.2.5. *Daniel Wachs (INL, United States)*

The speaker briefly introduced the planned restart of the Transient Reactor Test Facility (TREAT) that is scheduled for 2018 and provided elements on the Fuel Safety Research/Transient Testing Program, which is being elaborated in conjunction with stakeholders and industrial partners.

3.3. Summary of panel discussion

The panel discussion revealed that there is no expectation that advanced modelling in the current design of LWRs will bring about any significant benefits; the methods used for safety analyses are quite mature and the materials well-known. There are even some indications that most actors are happy with the situation with respect to models, methods, safety analysis and regulations. Larger benefits are anticipated to arise from the

development of accident-tolerant fuel (ATF). It is expected that advanced modelling will allow their behaviour and phenomena in off-normal conditions to be simulated. Simulations with advanced models can be used to design ATF and plan tests of them in a more efficient way than in previous testing of promising prototypes.

Margins in safety analysis is always a topic of interest. Multiscale models have enabled an even better understanding of what the safety margin consists of and what they should consist of. A more detailed understanding of phenomena means that they can be incorporated in computational methods instead of being treated as general margins. However, this approach might make it necessary to redefine some safety margins because current safety margins could be too penalising when examining very local effects. Yet at the same time margins should not be too reduced in situations where they also are necessary for other unknown phenomena.

PCI is a phenomenon that would be suitable for multiscale modelling, which could be used both in the development stages of new pellets and also for the verification of operation. Multiscale models are perceived as capable of incorporating all complex phenomena that contribute to damage due to PCI: pellet cracking pattern, fission gas impact, stress and strain.

3.4. Overall summary of Session 2

Session 2 met the objective of having interested parties meet and share their experiences. More specifically, the key items and possibilities for further international collaboration that were discussed were as follows.

Key items:

- Fission gas pressure/plenum volume and axial gas behaviours (gas mixing, axial gas communication within the fuel rod, coalescence within the fuel pellets, etc.) at the onset of the transient and during the transient.
- Onset of ballooning/cladding rupture and loss of coolable geometry (along with high-temperature, neutron irradiated cladding mechanical properties and fuel pellets and cladding behaviours).
- Multi-rod analysis methodology used to estimate the risks and consequences of multi-rod ballooning.
- Multiscale models for describing the behaviour of doped pellets, specifically with regards to mechanistic models that can predict fission-product retention and cracking behaviour in steady states and transient conditions.
- Multiscale models for cladding-to-coolant heat transfer that might help improve the experimental determination of critical heat flux (CHF) correlations and generate better estimations of the onset of critical heat flux in the safety cases analysis.
- The role of hydrogen regarding the cladding embrittlement, including a hydriding model for spent fuel and hydrogen absorption and resolution (using an out-of-pile test).
- Chemical effects, including the fission products' effect on cladding stress corrosion cracking (SCC), for example the enhancement of SCC by Te and I; radiochemistry approaches that can be beneficial to include in codes; specific tests are under development and a first step to develop analysis methods.

International collaboration:

- Validation and benchmark activities for multi-scale (and) coupled codes on topics such as PCI or sensitivity analysis.
- Uncertainty qualification, including an improved understanding of uncertainties from tests and statistical treatments leading to the quantification of margins.
- Testing in an international consortium. For example, Halden and Studsvik, among others, have ongoing NEA projects. The TREAT test reactor (United States), the BR2 test reactor (Belgium) and the future JHR facility (France) are open for establishing similar international projects.

4. Overview of Session 3: Nuclear-Fuel Modelling in Support of Performance and Safety Improvements during Normal Conditions

Co-chairs: Marie Moatti (Électricité de France S.A. [EDF], France) and Glyn Rossiter (the National Nuclear Laboratory [NNL], United Kingdom)

This session comprised eight presentations followed by a panel discussion:

- Christophe Durand (EDF, France), “Fuel assembly bowing during normal operation”;
- Grigori Khvostov (the Paul Scherrer Institute [PSI], Switzerland), “On effects of high-temperature fuel restructuring during the steady-state irradiation in the context of the selected fuel design criteria”;
- Brian D. Wirth (Oak Ridge National Laboratory [ORNL]/ University of Tennessee [UT], United States), “Multiscale modelling of fission-gas bubble evolution in UO₂ under nominal operating conditions”;
- Larry Aagesen (the Idaho National Laboratory [INL], United States), “Modelling Fission-Gas Bubble Swelling in Silicide Fuel using Marmot”;
- Paul Van Uffelen (European Commission [EC]- the Joint Research Centre [JRC]), “Current meso-scale modelling developments for TRANSURANUS”;
- Giovanni Pastore (INL, United States), “Recent Developments in Modelling Fission Gas Behaviour for BISON”;
- Jerome Julien (Commissariat à l’énergie atomique et aux énergies alternatives [CEA], France), “ALCYONE calculations of GONCOR experiment for the kinetics of gaseous swelling during a power transient”;
- P. Demianov (JSC Bochvar Institute, Russia), “A model of irradiation-induced densification of oxide nuclear fuel”.

4.1. Summary

The third session was devoted to the phenomena that occur at normal conditions and anticipated operation occurrences. The following aspects were mentioned in the introduction:

- different modelling and experimental disciplines, while emphasising the importance of communication and openness to new techniques;
- an assessment of quantified benefits, both in anticipated operation occurrences, with enhanced fuel performance at stake (reduction of fuel failures and assembly bow), and in accidental transients with an improved modelling of the fuel initial states, with increased safety margins at stake that lead to increased operational margin and associated benefits;
- accounting for the limitations on length, time scales and computer time;
- implications of the consequences of those limitations (for example, on detailed pellet-clad interaction [PCI] assessments...);
- the need to understand the physics before undertaking the modelling;
- linking with experiments.

All the presentations – except for the CEA and the EDF presentations – focused on UO_2 fuel pellet microstructure in a light water reactor (LWR) and sometimes extended their scope to U_3Si_2 fuel. The CEA presentation focused on cladding deformation due to gaseous swelling. The EDF presentation relied on data analysis to explain the mechanisms of fuel assembly bowing in EDF four-loop pressurised water reactors (PWRs). Most presentations focused on the level of accuracy of the proposed modelling, except for the EDF presentation, which relied on data analysis only.

4.1.1. Christophe Durand (EDF, France)

The DAMAC tool operated by EDF provides easy and complete measurements of the bowing of all fuel assemblies during the core unloading. The measurement data clearly illustrate the main impact of hydraulic flows in the core, which lead to symmetric deformation core phenomena. However, an asymmetric deformation can be observed in the top of the core in the direction not impacted by the hot legs suction, which occurs due to contact forces between neighbouring assemblies. This situation can induce significantly increased rod drop times and difficulties with handling assemblies. The ability of the structure to resist creeping under irradiation can lead to lower residual deformations. The deployment of reloads of suitable fuel assembly design shows encouraging results.

4.1.2. Grigori Khvostov (PSI, Switzerland)

Licensing calculations for the justification of fuel reliability usually deal with hypothesised challenging power histories, which is referred to as Thermo-Mechanical Operational Limit (TMOL) and for which the high-temperature fuel restructuring and its consequences are expected. A FALCON-based methodology enables a relevant modelling of fuel restructuring applied to a BWR MOX fuel irradiated under high-power conditions, with a peak local linear heat rate (LHR) up to 56 kW/m. The model properly predicts the resulting increase in local fuel density and formation of a significant central void. Compared to calculations based on fuel without central-hole formation, the central void predicted by the model leads to a reduced calculated peak temperature, fission gas release, rod pressure, cladding stress and strain during a power ramp. Including these effects in licensing analysis would suggest a reduction of its conservatism; moreover, it may eventually result in alternative approaches to the optimisation of parameters of rod design and fuel cycles.

4.1.3. Brian D. Wirth (ORNL/UT, United States)

There is a critical need to identify and characterise the diffusive behaviour of Xe on the atomic scale and then use this as the foundation of higher-level models in order to predict the gas bubble formation and evolution. A multiscale modelling approach to simulate the behaviour of fission gas and intragranular fission gas bubble populations is presented. That modelling is based on an information-passing paradigm, which relies on both a “bottom-up” atomistic-based approach and a “top-down” continuum perspective that focuses on kinetic models of intragranular gas bubble evolution. Specific mechanisms of Xe and Xe cluster diffusion, as well as Xe re-solution from fission gas bubbles, have been investigated for UO_2 fuel. Molecular dynamics (MD) simulations have also been used to investigate the mechanisms of Xe re-solution from fission gas bubbles; they confirm theoretical estimates of the magnitude of re-solution by homogeneous re-solution. The heterogeneous re-solution mechanism produces a much larger re-solution by at least 103 times for UO_2 fuel. MD simulations generally match literature data for heterogeneous re-solution and show that there is a critical electronic stopping energy of a little above two eV/atom. These results will ultimately provide a comprehensive model for heterogeneous re-solution that will be used to predict intragranular bubble populations in the Xolotl-fission code.

4.1.4. Larry Aagesen (INL, United States)

The modelling of fuel performance is historically connected to temperature and burnup parameters; that approach is relevant as long as the same types of fuel and operating conditions as those associated with historical data are considered. However, historical data are unsuitable for considering different materials and different plants. More relevant models have been developed that are based on microstructure rather than burnup. Structure/property relationships connect the fuel and cladding microstructure variables to the property values. Atomistic and mesoscale simulations (implemented in the MARMOT application based on the MOOSE framework) inform the development of analytical materials models. One example is BISON, which predicts fuel performance at an engineering scale. MARMOT predicts the co-evolution of microstructure and physical properties in reactor fuel and cladding for UO_2 and U_3Si_2 fuel using a phase-field model. That type of approach can be used to present the example of swelling due to fission gases in U_3Si_2 fuel, leading to a simulation-based analytical expression of swelling as an input to BISON.

4.1.5. Paul Van Uffelen (EC-JRC)

There has been a general trend of developing more mechanistic models in the fuel rod performance codes like TRANSURANUS:

- High burnup structure (HBS) formation and evolution:
 - Correlation for the fuel Young's modulus by accounting for the decrease due to burnup accumulation: the new correlation correlates with the experimental results, extending its range of experimental validation from non-irradiated to irradiated UO_2 .
 - Exponential reduction of the average grain size with local effective burnup, paired with a simultaneous depletion of intragranular fission gas driven by diffusion.
- Fission gas behaviour: extension of conventional diffusion-based models to introduce the burst release effect, with quantitative improvements of the integral fission gas release (FGR) predictions in two structurally different fuel performance codes, TRANSURANUS (JRC) and BISON (INL).
- Helium modelling: introduction of a new modal algorithm that can efficiently solve the helium diffusion problem.

There are other planned and ongoing fields of model development. These are: hydrogen uptake, fission coupling of the MFPR code (IRSN) and TRANSURANUS for a multiscale approach for fuel rod behaviour under normal, off-normal or accident conditions in a reactor or storage facility; revision of the model for plenum temperature and pressure on the basis of multidimensional and multi-physics calculations with the COMSOL software package in the frame of the collaboration between JRC-Karlsruhe and Nuclear Power Institute of China (NPIC); and extension of the modelling in the frame of the INSPYRE project with a focus on MOX fuel.

4.1.6. Giovanni Pastore (INL, United States)

Developments have been made on the BISON fuel performance code that rely on the improved modelling of intragranular fission gas bubble evolution for UO_2 and a new multiscale model of fission gas behaviour in U_3Si_2 . The evolution of intragranular fission gas bubbles in nuclear fuel is controlled by bubble nucleation, gas atom trapping at the

bubbles and irradiation-induced gas atom re-solution occurring from bubbles back into the lattice. Heterogeneous mechanisms of nucleation and re-solution are dominant for UO_2 based on the available knowledge, whereas the homogeneous mechanisms are assumed to dominate in U_3Si_2 . The PolyPole-1 algorithm provides a more accurate solution than other algorithms for UO_2 for intragranular fission gas release at normal conditions. The PolyPole-2 algorithm shows good results for intragranular fission gas release for fast transients such as a reactivity-initiated accident (RIA). A cluster dynamics approach has been used to track bubble evolution. A simplified model is used for the calculation of the bubble mean size and concentration and the associated fuel gas swelling. Either lower length scale modelling or experimental work were adopted for UO_2 parameters. The model was informed with density functional theory calculations for U_3Si_2 for the gas atom diffusivity, as well as for the trapping rate and molecular dynamics calculations for the re-solution rate. The results for UO_2 demonstrated a clear improvement compared to the experimental data of bubble number density and size of previous attempts to model bubble evolution with a mean and single size approach. The application to U_3Si_2 was integrated with a description of grain boundary processes, leading to an initial engineering model for fission gas swelling and release in this type of fuel at power reactor temperatures.

4.1.7. Jerome Julien (CEA, France)

The CEA, in collaboration with EDF and AREVA, has developed the multidimensional fuel performance code ALCYONE in the simulation platform PLEIADES in order to study PWR fuel behaviour during incidental conditions. 1D and 3D modelling are available. ALCYONE has good correlation between the calculations and measurements for power ramps used to establish the pellet-cladding interaction (PCI) technological limit. 1D modelling aims to estimate integral parameters (such as fission gas release) or mean local parameters (such as external cladding diameter); 3D modelling focuses on local parameters. A close correlation is found between 1D and 3D modelling for the external cladding diameter at the mid-pellet plane both after base irradiation and after a power ramp. The modelling of the kinetics' evolution of external cladding diameters impacted by the gaseous swelling throughout a ramp test was investigated, which relied on the GONCOR experiment carried out in 1993 at the SILOE MTR with a maximum power level that was maintained over six days. The decrease of the diameter was well predicted during the period of time at maximum power, which demonstrates an accurate modelling of the evolution of the fuel rod deformation due to fission gas release for either the 1D or 3D calculation. The shape of the diameter evolution at the beginning of the step at maximum power has been well reproduced by the 3D modelling. Future analysis will focus on the cladding diameter increase at the mid-pellet and inter-pellet plans and the evolution of the heights of primary and secondary ridges in order to produce a better adjustment of the models used in ALCYONE.

4.1.8. P. Demianov (JSC Bochvar Institute, Russia)

A model of irradiation-induced densification of nuclear fuel was presented. A densification has been observed that starts at the beginning of irradiation due to the closing of submicron fuel pores. After a maximum densification at intermediate burnup levels, the swelling process of uranium dioxide starts to overcome the densification process. Xe gas yielded by ^{235}U fission excites electrons, with a resulting lattice heating exceeding the UO_2 melting temperature. Compressive stresses, which are due to the variance of specific volumes of melted and solid phases on the tracks created by the fission fragments, lead to pore decreases in size in the plastic medium zones around the melted track. The size of the submicron pores is equal to the radius of the yield zone and therefore the process of pores closing for that size occurs exponentially quickly. Experimental data show more significant

and faster irradiation-induced densification for a VVER fuel than for a PWR fuel; that data is consistent with the pores' size distributions in each type of reactor, with an important portion of pores being in the submicron size for the VVER fuel. That result illustrates that the densification of UO_2 is a consequence of the closing of pores resulting from the plastic flow and influenced by the stresses appearing in the fission fragment tracks in UO_2 .

4.2. Panel discussion moderated by session co-chairs

4.2.1. *Fumihisa Nagase (JAEA, Japan)*

The speaker focused on the developments required to adapt the fuel performance code FEMAXI to ATF modelling and, in particular, SiC cladding. Phenomenological differences between SiC and Zircaloy on specific phenomena (i.e. stress relaxation and stress generation induced by swelling) were mentioned, including specific characteristics of SiC cladding (wall-thinning due to corrosion and multi-layer cladding) requiring ad-hoc developments, which is also required to improve the modelling of swelling and fracture behaviour.

4.2.2. *Chris Stanek (LANL, United States)*

The speaker expanded on the role of advanced fuel performance modelling and simulation (M&S) tools that, far from being in competition with existing M&S tools currently used by industry (vendors and utilities) and regulators, instead provide complementary insights on specific issues (such as load following, transient analysis, CRUD and manufacturing flaws). These tools also help identify areas of relevance for fundamental research.

4.2.3. *Mikhail Veshchunov (IAEA)*

With reference to an ongoing review of experimental needs for the validation of fuel performance codes (carried out by the NEA Expert Group on Reactor Fuel Performance, www.oecd-nea.org/science/wprs/egrfp), the speaker focused on specific areas for which new experimental data is needed. These areas were identified as needed for steady-state analysis due to needs to improve the validation of models for fuel densification, swelling and fission gas release in restrained and unrestrained pellets, as well as the evolution of intragranular bubble size distribution. Moreover, these areas were identified as needed for transient conditions (fission gas release and microstructure evolution) and to improve fuel thermo-mechanical and thermochemical properties.

4.2.4. *Jinzhaio Zhang (Tractebel-Engie, Belgium)*

The speaker raised several items (central to the workshop themes) related to a challenging question: How can progress in fuel modelling be valued in safety analysis, or what is the link between progress in advanced modelling and safety analyses? After recalling the definition of safety margins (based on a definition recently proposed by Tractebel-Engie and EDF, building on a first definition provided in a NEA report published in 2007), the following items were introduced and further developed during a Q&A session:

- the necessity of distinguishing between safety margins controlled by the regulator and those available to the operator and the fuel/reactor vendor;
- new challenges associated with emerging advanced techniques (including multiscale/multi-physics methods) for fuel modelling, for example:

- how to approach the validation phase, which is likely to require new experiments and/or massive data analysis, associated with progress in reactor instrumentation;
- the need to develop the regulatory framework accompanying the progress in M&S tools (i.e. current standards or safety limits based on “old” 1D simulation that might not be applicable to “new” multiscale/multi-physics M&S);
- how to quantify uncertainties in multiscale/multi-physics M&S (with links to ongoing activities within the NEA Expert Group on Uncertainty Analysis in Modelling, www.oecd-nea.org/science/wprs/eguam/);
- the key role of multiscale/multi-physics M&S in providing new insights in the understanding of detailed physical mechanisms at lower scales and in particular at the mesoscale.

4.3. Overall summary of Session 3

Session 3 provided relevant illustrations of the different aspects mentioned in the introduction.

Much work has been performed on fuel microstructure and fission gas release, which evidently has created a proper field for co-operation. Further normal operation issues could be of interest, such as:

- how to improve departure from nucleate boiling ratio (DNBR) margins (for example, more fitting critical heat flux [CHF] correlations, improved fuel assembly design, etc.)?
- how to ensure the prevention of generic failure modes (fretting wear, stress corrosion cracking that may affect the structural components, etc.)?
- failed fuel as an additional initial state that is taken into consideration for accidental transients’ analysis (an issue that was explicitly raised by the French Safety Authority);
- cladding corrosion and hydriding in normal operation.

On the matter of code validation, the duration of the process emphasises the interest of co-operation in that area.

5. Overview of Session 4: Workshop Wrap-up

Co-chairs: Kemel Pasamehmetoglu (INL), Marc Petit (IRSN), Theodore Besmann (USC)

The discussions in the wrap-up session were animated by the workshop co-chairs and NEA Secretariat. The main objective of this session was the formulation of recommendations on key items identified during the workshop. Special attention was paid to the cross-cutting issues between safety and economic performance and to the update of requirements for experimental validation. The roles of the NEA and the IAEA in the existing frameworks for collaborative activities were reviewed and possible new activities or means for co-operation in nuclear fuel modelling were discussed.

The session generated some conclusions and identified questions for further discussions, including that:

- collaboration within the modelling and simulation (M&S) community is very encouraging;
- problems are being tackled that would not have been attempted over five years ago;
- observations of the models gave rise to new insights, though it is unclear if these insights are being used to drive design decisions;
- there are questions of how close a potential paradigm shift is in the use of M&S.
- “Design a fuel on a computer, validate the design with a few integral experiments leading to fuel qualification without any trial and error”.
- Mindset: M&S driving experiments versus experiments driving M&S.
- Is there an impact being made?
 - how experimentalists view their role and are challenging themselves in new and different types of experiments;
 - vendors adopting the tools;
 - regulators accepting a paradigm with predictive modelling in the core.
- The focus/priorities:
 - highest impact with longer and greater effort?
 - an important problem, where the maturity is the highest in order to get to the end faster?
 - adequate critical mass?
- What is the right collaboration mechanism for resolving a few of these problems?

5.1. Session 4 Summary

The closeout of the meeting was an opportunity to hear a presentation on the various NEA activities related to nuclear fuel modelling that could offer support to national and commercial efforts, as well as opportunities to participate in future developments in this area. These programmes fall under the various NEA standing committees. The Working Group on Fuel Safety, which comes under the Committee on the Safety of Nuclear Installations, has produced several reports containing modelling and code-related

information. The Nuclear Science Committee hosts Working Parties on Scientific Issues in the Fuel Cycle, Multi-Scale Modelling of Fuels and Structural Materials for Nuclear Systems, and Scientific Issues of Reactor Systems. These, together with the Expert Groups on Multi-Physics Experimental Data, Benchmarks and Validation and on Accident-Tolerant Fuels, and the joint project on the Thermodynamics of Advanced Fuels-International Database have all had, and continue to have, relevant activities.

In his closing remarks, the meeting co-chair, Kemel Pasamehmetoglu, posed some questions for the group to consider as they move forward:

- Is there an impact being made?
 - how experimentalists view their role and are challenging themselves in new and different types of experiments;
 - vendors adopting the tool;
 - regulators accepting a paradigm with predictive modelling in the core.
- The focus/priorities:
 - highest impact with longer and greater effort?
 - an important problem, where the maturity is the highest in order to get to the end faster?
 - adequate critical mass?
- What is the right collaboration mechanism for resolving a few of these problems?

Finally, Theodore Besmann raised the possibility of assessing priorities and needs as a group. Below are the questions that would need consideration in order to generate, for example, a table of needs and priorities. Although there was some discussion about starting such a table, the activity was regarded as too extensive to be addressed at the end of the workshop.

- modelling needs:
 - a greater development of physics;
 - new or improved computational approaches;
 - the improvement of data/parameters;
- priorities – assess the importance of needs with respect to:
 - the development of physics: a model form, framework and implementation;
 - the development/improvement of computational approaches;
 - data for determining/refining parameters or verification and validation [V&V]/benchmarking;
 - scale 1-5, with one as highest priority and five the lowest;
- the identification of potentially useful co-operation/connection opportunities between NEA and other committees.

The meeting concluded with an apparent consensus on the substantial value in sharing efforts and information, alongside an understanding that addressing all issues of interest is beyond the capability of single organisations or national programmes. The desire was expressed to find additional opportunities for co-operation on the fundamental issues of modelling and simulation of nuclear fuel.

6. Conclusions and recommendations

The workshop focused on nuclear fuel modelling and simulation (M&S) as at least a first step towards:

- the identification of which topics/developments are considered to be key by the international community in a short/medium time schedule (five-eight years);
- the identification of major challenges for the experimental validation of advanced M&S methods (methodological developments, the availability of experimental infrastructures and cost of experimental programmes) in order to optimise the interaction between M&S and the qualification process;
- providing an ultimate benefit to the design of new products (fuels and reactors), which facilitates the industrial implementation of these products by nuclear operators that require licensing by regulators;
- the identification of major hurdles and possible bottlenecks throughout the process that transfers research and design developments into licensed industrial products;
- forging a common understanding of the possible role of the NEA in tackling these challenges through effective multilateral collaboration.

Eighty participants from eighteen NEA member countries (Belgium, Canada, Czechia, France, Germany, Hungary, Italy, Japan, Korea, the Netherlands, Russia [suspended], Finland, Slovenia, Spain, Sweden, Switzerland, the United Kingdom and the United States), plus the European Commission and the IAEA attended the workshop.

The majority of participants came from R&D organisations (the majority were experts and modellers of nuclear fuel), with good participation also from nuclear utilities and fuel vendors, but lower than expected participation from regulators and experimentalists.

Four technical sessions were held over two and half days. The opening session was devoted to the status of the development of advanced fuel modelling, perspectives from nuclear utilities, fuel vendors and regulators. This was followed by two sessions, one on modelling in off-normal conditions and the other on modelling in nominal conditions, comprising 13 presentations and two panel discussions. The workshop ended with a wrap-up session.

The major outcomes can be summarised as shown below.

- M&S is driving experiments (rather than experiments driving M&S) that tackle problems and provide insights that would not have been attempted five or more years ago.
- The assessment of whether an enhanced use of advanced M&S in the design and licensing of new products is having an impact led to the observation that progress has been achieved in this direction, but that the impact is not yet major. There is some limited evidence that the fuel and/or experimental designers are using advanced M&S tools to develop fuel and experimental procedures. The key focus of regulators is dealing with convincing safety cases that are based on reliable (experimental) validation and not with M&S tools per se. However, advanced M&S tools may be used by the regulators to challenge the historical safety cases analysis provided by the designers.
- It must be noticed that most of the current “historical” design/safety limits are not adapted to approaches based on multi-physics tools.

- Some needs were identified: further progress on instrumentation to accompany the progress achieved on M&S tools; smaller-scale experiments (as opposed to integral and/or power reactor) for the validation of individual models and quantification of uncertainties; and the development of a methodology for assessing uncertainties in fuel performance codes (licensing).
- Collaboration mechanisms aiming to resolve a few of these issues are recommended as useful and effective, if they are not too formal and not too large; gathering modellers and experimentalists is one key to progress.
- Some areas for future collaboration were identified as follows: fuel densification and fission gas swelling; ballooning and fuel relocation in accident conditions; fuel restructuring during normal operation; microstructure/properties in high burnup region; interaction between fission-product and fuel microstructure; investigation of which mechanism drives fuel fragmentation; cladding failure and the modelling for design of accident-tolerant fuels.
- The presentations by international organisations (the NEA and IAEA) underlined the importance of international benchmark exercises for the validation of fuel behaviour codes using common databases. It was concluded that the development of accident-tolerant fuel concepts could also profit from advanced modelling that is carried out through international co-operation.
- The possibility of assessing priorities and needs as a group was raised. It is therefore recommended to build a table of needs and priorities.

Overall, advanced modelling was seen as contributing to fuel design. However, its direct application in the licensing process is not currently established (regulators may nevertheless use advanced M&S tools to challenge the “historical” design/safety approaches). The NEA Working Group on Fuel Safety (WGFS) will continue discussions on this issue to identify further areas where advanced techniques for fuel modelling could be utilised from the viewpoint of fuel safety.

Annexes

Annex A. Workshop programme

OECD Nuclear Energy Agency Workshop

Nuclear-Fuel Modelling to Support Safety and Performance Enhancement for Water-cooled Reactors.

7-9 March 2017

OECD Conference Centre, 2 rue André Pascal, Paris, room CC10

Table A.1. Final programme

7 March 2017 (9.00-18.00)	
8.00-9.00	Arrival formalities: security clearance, collection of badges, etc.
9.00-9.15	NEA Welcome <i>D. Iracane (NEA Deputy Director-General)</i>
9.15-9.30	Welcome from the Workshop Co-Chairs: review of the programme, objectives <i>K. Pasamehmetoglu (INL), M. Petit (IRSN), T. Besmann (USC)</i>
9.30-9.45	Introduction of attendees
9.45-12.35	Session 1: Recent developments and future challenges for nuclear fuel Co-Chairs: K. Pasamehmetoglu (INL), M. Petit (IRSN), T. Besmann (USC)
9.45-10.10	Recent developments in advanced modelling applied to nuclear fuel <i>C. Stanek (LANL), M. Freyss (CEA)</i>
10.10-10.35	Utility perspective on needs related to nuclear-fuel operation <i>N. Waackel (EDF), J. Zhang (Tractebel-Engie), K. Yueh (EPRI)</i>
10.35-10.50	Coffee break
10.50-11.50	Fuel-vendor perspectives on current trends and future needs for improvements <i>Four talks 15' each:</i> • Expectations from progress in fuel modelling in order to optimise fuel design and safety analysis, <i>N. Murakami (MNF, Japan)</i>. • Current and upcoming issues for fuel modelling, <i>P. Mailhe (AREVA, France)</i>. • Modelling accident-tolerant fuel concepts: gaining a mechanistic understanding to aid licensing, <i>S. Middleburgh (Westinghouse, Sweden)</i>. • Current issues and future needs for fuel modelling in LWRs, <i>J.S. Yoo (KEPCO-NF, Korea)</i>.
11.50-12.05	Safety and regulatory aspects related to nuclear fuel and activities within CSNI Working Group on Fuel Safety <i>M. Petit (IRSN), T. Fuketa (NRA)</i>
12.05-12.20	Link with NEA Innovation 2050 initiative <i>M. Deffrennes (NEA)</i>
12.20-12.35	IAEA activities on fuel performance <i>M. Veshchunov (IAEA)</i>
12.35-13.45	Lunch break
13.45-18.00	Session 2: Nuclear-fuel modelling in support of performance and safety improvements under off-normal conditions Co-Chairs: A. Alvestav (SSM) and B. Wirth (ORNL/UT)

13.45-14.00	Introduction and objective of the session <i>A. Alvestav (SSM) and B. Wirth (ORNL/UT)</i>
14.00-16.30	Keynote presentations: G. Guillard (IRSN, France), Computational analysis of multi-rod ballooning and fuel relocation during LOCA using the multi-physics DRACCAR code. M. Amaya (JAEA, Japan), Key issues in fuel safety studies on the modelling of fission-gas behaviour inside fuel pellet under normal and off-normal conditions. - H.C. Kim (KAERI, Korea), Development status of the fuel module for simulation of LOCA and RIA in KAERI. V. Ozrin (IBRAE, Russia), Modelling of irradiated oxide-fuel behaviour and fission-product releases under transient and severe-accident conditions by the fuel performance and safety code SFPR. K. Govers (SCK CEN, Belgium), Granular simulation of fuel relocation and dispersal in LOCA conditions.
16.30 – 16.45	Coffee break
16.45-18.00	Panel discussion moderated by session Co-Chairs T. Forgeron (CEA, France) T. Valentine (ORNL, US) N. Waackel (EDF, France) K. Yueh (EPRI, US)
8 March 2017 (9.00-17.45)	
9.00-10.00	Session 2 wrap-up <i>Co-Chairs: A. Alvestav (SSM) and B. Wirth (ORNL/UT)</i>
10.00-10.30	Discussion
10.30	Closure of session 2
10.30 – 10.45	Coffee break
10.45-17.45	Session 3: Nuclear-fuel modelling in support of performance and safety improvements during normal operating conditions <i>Co-Chairs: M. Moatti (EDF) and G. Rossiter (NNL)</i>
10.45-11.00	Introduction and objective of the session <i>M. Moatti (EDF) and G. Rossiter (NNL)</i>
11.00-16.15	Keynote presentations: C. Durand (EDF, France), Fuel assembly bowing during normal operation. G. Khvostov (PSI, Switzerland), On effects of high-temperature fuel restructuring during the steady-state irradiation in the context of the selected fuel design criteria. B. D. Wirth (ORNL/UT, US), Multiscale modelling of fission-gas bubble evolution in UO₂ under nominal operating conditions.
12.30 – 13.45	Lunch break
	L. Aagesen (INL, US), Modelling Fission Gas Bubble Swelling in Silicide Fuel using Marmot. P. van Uffelen (EC-JRC), Current meso-scale modelling developments for TRANSURANUS. G. Pastore (INL, US), Recent Developments in Modelling Fission Gas Behaviour for BISON. J. Julien (CEA, France), ALCYONE calculations of GONCOR experiment for the kinetics of gaseous swelling during a power transient. P. Demianov (JSC Bochar Institute, Russia), A model of irradiation-induced densification of oxide nuclear fuel.
16.15 – 16.30	Coffee break

16.30-17.45	Panel discussion moderated by session Co-Chairs F. Nagase (JAEA, Japan) C. Stanek (LANL, US) M. Veshchunov (IAEA) J. Zhang (Tractebel-Engie, Belgium)
17.45	<i>Adjourn for the day</i>
18.00-19.30	Cocktail, Roger Ockrent room
9 March 2017 (9.00-12.30)	
9.00-10.00	Session 3 wrap-up <i>Co-Chairs: M. Moatti (EDF) and G. Rossiter (NNL)</i>
10.00	Closure of session 3
10.00-12.15	Session 4: Workshop Wrap-up <i>Co-Chairs: K. Pasamehmetoglu (INL), M. Petit (IRSN), T. Besmann (USC)</i>
10.00-12.15	Discussion animated by workshop Co-Chairs and NEA Secretariat • recommendations on key items identified during the workshop; • key cross-cutting issues between safety and economic performance; • new requirements for experimental validation.
11.00 – 11.15	<i>Coffee break</i>
	• existing frameworks for collaborative activities (NEA, IAEA) and possible new activities or means for co-operation; • other issues (regulatory, IP, ...).
12.15-12.30	Conclusion of the workshop <i>Workshop Co-Chairs, NEA</i>
12.30	<i>Workshop adjournment</i>

Annex B. Abstracts for Session 1, Recent developments and future challenges for nuclear fuel

Recent developments in advanced modelling applied to nuclear fuel

C.R. Stanek (Los Alamos National Laboratory, United States) and M. Freyss (CEA/DEN, Centre de Cadarache, France)

Extended Abstract

The fuel element under irradiation is submitted to a wide variety of coupled phenomena involving among others temperature, mechanical load, radiation damage, chemical interaction between the material constituents and fission products. Recent developments in advanced modelling applied to nuclear fuel have improved both the understanding of the phenomena involved during irradiation and the capability to predict the fuel behaviour.

It is nevertheless still a challenge for R&D to refine the laws and models used in fuel performance codes by a more mechanistic and physically-based description of the fuel materials. It requires the development of improved mechanistic and predictive models for fuel performance using hierarchical, multiscale modelling. In particular, basic research on fuel materials focuses on the evolution under irradiation of the microstructure, the thermal conductivity, the transport properties of defects, fission products, helium, as well as their thermochemistry.

In France and the United States, advanced fuel modelling is developed within the BISON and the PLEIADES fuel performance codes, respectively.

Examples are given here in the framework of the MOOSE-BISON-MARMOT toolset [1,2] which provides an advanced, multiscale fuel performance capability and the PLEIADES / ALCYONE fuel performance software environment [3,4].

Development of a mechanistic thermal conductivity model

A primary source of uncertainty in fuel performance codes is the thermal conductivity model, and optimised fuel utilisation may be possible if existing empirical models were replaced with models that incorporate explicit thermal conductivity degradation mechanisms during fuel burn up. This approach would be able to represent the degradation of thermal conductivity due to each individual defect type, rather than the overall burnup measure typically used, which is not an accurate representation of the chemical or microstructure state of the fuel that actually governs thermal conductivity and other properties. To generate a mechanistic thermal conductivity model, molecular dynamics (MD) simulations of UO₂ thermal conductivity including representative uranium and oxygen defects and fission products have been carried out. Importantly, physical insights from the resonant phonon-spin-scattering mechanism due to spins on the magnetic uranium ions [5] are introduced into the treatment of the MD results, with the corresponding relaxation time derived from existing experimental data. Although much work remains to generate a truly predictive model, important steps have been taken to perform more accurate MD calculations [6], and subsequently translate those results in to models resident in an engineering scale fuel performance code (BISON) [7].

Development of a micromechanics-based modelling approach

A micromechanical approach taking into account the influence of the microstructure on the fuels properties has been developed, using a representative elementary volume (REV) of the material to represent the fuel microstructure geometry [8,9]. In particular, an example is given to model the fuel fragmentation under accidental LOCA conditions, taking into account the pressurised fission gas bubbles and the microstructure of the UO_2 pellet.

This micromechanical approach is a multi-scale process which considers the fuel microstructure and consists in:

- gathering information to represent the fuel microstructure geometry in a representative elementary volume (REV) of the material;
- achieving full-fields computations with the finite-element method (FEM) in order to define a crack pattern snapshot for UO_2 fuel;
- establishing a homogenised failure model for the fuel pellet scale, to access the fragment size;
- validating the failure model and implementing it into a fuel performance code at the fuel rod scale.

This approach has been applied to model crack initiation and growth in UO_2 fuels [8]. The results show that the first cracks initiate at a pressure of 120 MPa from fission gas bubbles where the stress concentration is higher. Such an approach can thus give a better insight into crack initiation and fuel fragmentation mechanisms.

Integration of thermochemistry in fuel performance codes

Thermochemistry has a high impact on irradiated fuel behaviour, it governs in particular the speciation of fission products which are involved in stress corrosion cracking (SCC). To better take into account thermochemical interactions in irradiated fuels, the coupling between thermochemical codes and the fuel performance code ALCYONE has been recently developed [10]. The integration of thermochemistry into fuel performance code can help optimise fuel for a better resistance to pellet cladding interaction (PCI) and stress corrosion cracking (SCC). It has been recently applied to the study of iodine-SCC [10].

The coupling proceeds as follows:

Fuel performance codes provide input conditions for thermochemical codes, such as:

- the temperature and internal (hydrostatic) pressure distribution in the pellet;
- the burnup, which defines the quantity of fission products in the pellet.

The thermochemical code can then determine such data as:

- the chemical state (speciation) and distribution of fission products;
- the oxygen potential (O/M).

These data can be used, for instance, to understand the behaviour of FP such as I, Cs and Te, which are involved in SCC. The combination of thermomechanical and thermochemical calculations can thus be used to define criterion to determine if the necessary conditions for SCC initiation are met.

Challenges for the future

The challenge of advanced nuclear fuel modelling is to support the design, manufacturing, performance and safety optimisation of existing and innovating fuels, through the coupling of modelling and simulation with analytical experiments and basic research characterisations.

Particular focus should be given to:

- the best use of modelling/simulation and analytical experiments to define critical irradiation tests and contribute in their interpretation to help industry in product licensing and safety requirement;
- the further development of uncertainty and sensitivity analysis in nuclear fuel behaviour modelling.

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Utility perspective on needs related to nuclear-fuel operation

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Extended Abstract

Introduction

Currently, nuclear energy is at a crossroads. All utilities will have to reduce their operating costs in a changing environment, and more and more nuclear power plants need to be under intensive flexible operations (i.e. load following, power modulation, extended low power operation, variable cycles).

One efficient way to reduce the cost is to improve the fuel design and operation margin management. This first needs a clear definition of the margins and limits.

Three areas of innovation can be identified around fuel modelling and fuel safety design to enhance safety or to restore licensing or design margins:

- Advanced modelling and simulation to quantify margins (e.g. safety, design and operational margins);
- Advanced techniques to better analyse data (e.g. big data algorithms to value in-reactor and in-pile tests massive data);
- New concepts of fuel to simplify fuel core safety analysis while maintaining a high level of operational reliability (e.g. Enhanced Accident-Tolerant Fuels or EATFs).

Of course, these three axes are strongly interdependent: new types of fuels cannot be developed without appropriate calculation and simulation tools, and those tools cannot be validated without using new ways of collecting and analysing data.

This keynote paper will address the utility's needs and challenges in fuel design and operation margin management.

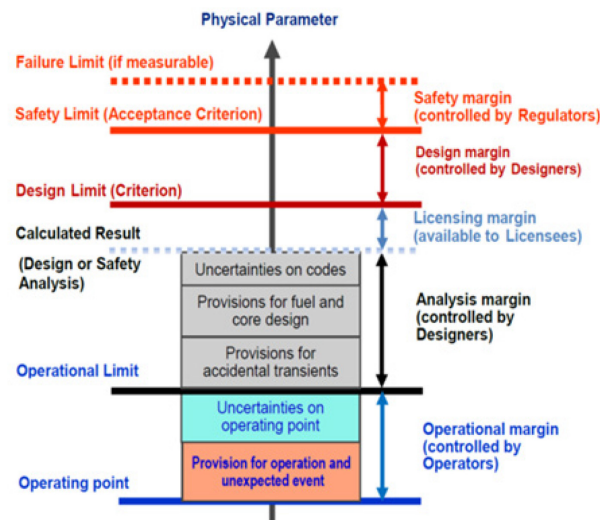
Improved fuel design and operation margin management

Safety margin is an important concept in nuclear power plant design and operation, and a key element of defence in depth (DiD): adequate safety margins shall be ensured at each of the levels of DiD, which must be demonstrated in the Safety Assessment. However, its definition is rather fuzzy and sometimes confusing: It is different for each organisation/country (IAEA², OECD³, Industry¹), divergent for each specialty/discipline (mechanics, neutronics, thermal-hydraulics, deterministic safety analysis [DSA], probabilistic safety assessment [PSA], designer, operator), and changing with advances in safety standard and technology.

There is no clear and unique definition of fuel design and safety limits and margins in the IAEA safety rules, requirements and guides and NEA documents, but these terms are widely used and closely related to provisions, uncertainties, conservatism and failure mechanisms. The margins are associated with various limits/criteria: operational limits and conditions, design limits, safety limits, acceptance criteria³, which can be quantified in a deterministic and probabilistic safety assessment.

To quantify the margins, we need first a clear definition. A simple and practical definition is proposed, based on the OECD/NEA definition⁴ and Tractebel-Engie⁵/EDF margin models (Figure B.1).

Figure B.1. A simple and practical definition of fuel design limits and margins



In the deterministic FSAR accident analysis, for a given physical parameter, a safety margin must always be maintained between the safety limit (or acceptance safety criterion) and the failure limit. The safety margin is controlled or imposed by the regulators; it includes uncertainties in the test data and the approach used to establish the safety limits.

The *design margin* may be maintained between the design limits and the safety limits (or acceptance criteria). The design margin is controlled and managed by the designer (fuel vendors or utilities); it is defined such as to ensure that, if preserved, the safety limits are met in all applicable plant states. A design limit (or criterion) can be proposed by the designers (fuel vendors or utilities). In practice, for normal operation and anticipated states the design limit is more restrictive than the safety limit, while for accident conditions the design limit is usually identical to the safety limit (or acceptance criteria). The licensing margin is defined as the difference between the calculated maximal value for the related physical parameter during the analysed transient and the design criterion. It is controlled and managed by the designers (fuel vendors or utilities).

The *analysis margin* is the difference between the operating limit and the maximal value calculated for the related physical parameter during the analysed transient. It is controlled by the designer, under the agreement of the utilities. The analysis margin consists of the conservatism on the following assumptions:

- the values of the physical parameters characterising the operating point at the beginning of the transient should bound all the normal operating conditions;
- the actual performances of the plant safety related systems (in particular, the protection systems and the safeguard systems) which are involved in the analysed transient;
- the design provisions on the physical data characterising the reference core and the reference fuel (design provision), which can be (re)allocated to justify different core and fuel designs or mixed cores;

- and the uncertainties related to the analysis (by performing conservative calculations or by performing best-estimate calculation plus uncertainty (BEPU) evaluation):
 - individual modelling or overall code uncertainties;
 - representation uncertainties, numerical inadequacies; user effects, computer / compiler effects; and
 - data uncertainties on the analysis of an individual event.

The *operational margin*, including the provision for operation and unexpected events and uncertainties on the operating point, has to be included in the safety analyses to ensure plant operation flexibility and reliability. This margin is controlled and managed by the operators.

The quantification of fuel design/operation margins depends on the advances in the following fields:

- best-estimate codes for realistic modelling of physical phenomena;
- better understanding of the design limits through careful design experiments and analytical analysis;
- better quantification of the uncertainties in the codes based on a wide range of experimental data;
- better knowledge of the plant operating conditions through realistic 3D modelling of the core and fuel behaviours;
- best estimate plus uncertainty analysis (BEPU) design methodology by removing unnecessary conservatisms.

The use of advanced multi-physics, multi-scale modelling provides opportunities, but also challenges for efficient margin management.

Advanced modelling and simulation tools to quantify margins

Advanced modelling may help reduce the need for costly tests:

This “Holy Grail” might be found in the long term, after all physical mechanisms / phenomena have been well-identified and characterised, but it will require a lot of time and effort. To achieve this goal, experimental validation of the calculation tools (V&V UQ) is inescapable and might be a serious issue, depending on the level of sophistication of the models. For instance, multi-scale, multi-physics calculations tools require developing new ways of ensuring proper validation. That may include developing dedicated advanced R&D tests and instrumentations and might turn out to be a real challenge.

Advanced modelling may help gain design margins (to be released to the designer, to the safety authorities or to the operators):

However, utilisation of advanced modelling (i.e. multi-scale, multi-physics coupled approaches) is not always adapted to improve fuel core safety analysis or generate safety margins because current standards have been defined based on former decoupled 1D static method. In other words, the following questions are still pending and prevent us from moving forward, with a good vision of the potential gains:

- Does it make sense to try to improve reactor system safety by simulating physical mechanisms at nano- or meso-scales?

- Are the current Specified Acceptable Fuel Design Limits (SAFDLs) still adapted to multi-scales calculations which provide results at the atoms or grain size scales?
- Is it possible to design relevant experiments to validate multi-scales tools (sine qua non condition for using them in a safety analysis)?

These questions are not trivial to address and the link between refined modelling and safety analysis still needs to be defined.

Multi-scale modelling is well suited to define mechanistic scenarios and help analyse complex in-pile tests:

As an example, multi-scale mechanistic approaches which have been developed recently at CEA and EDF6 to simulate the thermochemical behaviour of the fuel pellets during a power ramp are well suited to identifying and characterising stress corrosion cracking (SCC) key physical phenomena which occur in the fuel in case of strong pellet-cladding interaction (PCI).

It must be noted that such a mechanistic approach is too sophisticated to assess core wide SCC-PCI available margins (a fuel core contains more than 60 000 fuel rods, or about 19 million pellets, each of them having its own power history). That is why only simplified approaches are used to assess core wide SCC-PCI margins. Nevertheless, a mechanistic approach is relevant to improve, confirm or validate the simplified models implemented in the commercial fuel performance codes requested by the SCC-PCI design methods. In addition, a good understanding of the physical mechanisms, which occur during a power ramp, will help to develop and justify innovative SCC-PCI resistant fuels.

Advanced techniques to better analyse data

Innovation in nuclear power energy may also concern massive data analysis, which could be significantly improved by using advanced techniques. Data of interest include physical parameters recorded online in any in-pile experiments. In-pile experiments are usually considered as separate effect tests aiming at investigating one phenomenological scenario at a time. Despite high-quality instrumentation, in-pile measurements are often heavily scattered. Data are then analysed “by hand”, using ordinary tools (e.g. mean values, standard deviation, or least squares regression) but often fail at defining robust phenomenological correlations. In case data do not fit with hypothetical scenarios, it is tempting to reject the test, with no further investigation. Over the years, countless in-pile experiments have generated a deluge of data, which have not always been cross-processed. These unexploited data should be considered as a potential gold mine that should be valued.

As in other scientific fields, “big data” approaches and algorithms might be used to cross-analyse a bigger number of data and experiments. These digital analyses might be very beneficial to diversify the identification strategy of key parameters, to detect “weak signals” and phenomenological trends, to suggest new scenarios, hypothesis or correlations. A similar approach could be used to analyse thoroughly all the information recorded online in any commercial power plants. Such analysis could help characterise the specific behaviour of the plant (as compared to others) and anticipate any abnormal behaviour or events.

Of course, there is room for valuable synergies between multi-scales simulations, massive in-reactor data and experimental data, and “big data” analysis. It is noted however that “big data” approaches do not prevent the licensees from developing relevant experiments to verify the hypotheses derived from such approaches.

Innovative fuel concepts to simplify design while maintaining a high level of operational reliability

The current UO₂-zirconium alloy fuel system is a mature technology and meets all performance and safety requirements. The goal of enhanced accident-tolerant fuel (EATF) development is to identify alternative fuel system technologies to further enhance the safety margins, competitiveness and economics of commercial nuclear power.

Key attributes for a fuel system demonstrating enhanced accident tolerance include reduced steam reaction kinetics (reaction rate and heat of reaction), lower hydrogen generation rate (or generation of other combustible gases), and reduction of the initial stored energy in the core (to delay core meltdown).

The desired behaviours should be obtained while maintaining or improving cladding and fuel thermo-mechanical properties, fuel-clad interactions, fission-product behaviour and fuel rods thermo-hydraulic properties. A set of qualitative guidelines and metrics derived from these desired attributes across all fuel performance regimes (versus specific quantitative targets for each property) has been defined⁷ to facilitate the optimisation and prioritisation of candidate fuel system designs.

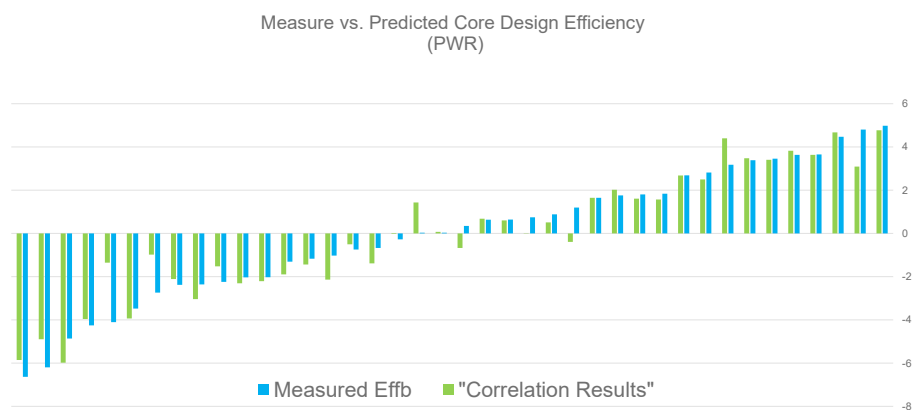
By definition, a nuclear operator is conservative and is usually reluctant to implement new types of fuel that may generate (bad) surprises during normal operation. In fact, nuclear utilities prefer proven fuel systems with a good safety and operational record, rather than testing unknown fuel concepts with no or little in-reactor experience.

The incentives to switch from a proven fuel system to an innovative fuel system should be well founded. Usually, a utility's motivation for a new fuel are focused on safety margin restoration and fuel cycle cost reductions, both aspects being closely linked.

US utility perspective

Like many utilities worldwide, the US nuclear industry is also under tremendous pressure to reduce operating costs to stay competitive with low natural gas and alternative energy prices. In deregulated markets, several plants have closed due to financial reasons and many more are on the profitability borderline. While sweeping changes are being made to reduce cost under the Nuclear Promise Initiative (NPI), the near-term efforts have been focused on plants' operational cost. The need to optimise fuel cycle efficiency is a topic of interest in response to the NPI as it makes up to 1/3 of a plant's operating budget. A core design benchmark composed of nearly half of the US fleet (Figure B.2) indicates an efficiency gap of more than USD 15M between the least and most efficient plants.

Figure B.2. Ranking of select US plants by operating efficiency (each Effb unit is worth ~USD 1.5M)

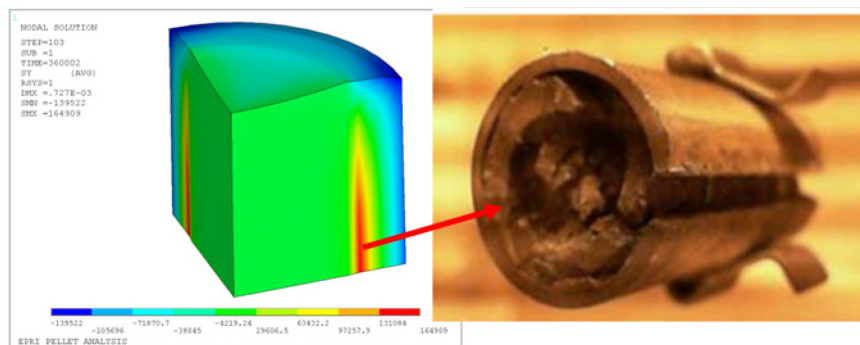


Part of the gap could be explained by core size, power density, core design goals/practices/strategies, etc., but in order to significantly narrow the gap key constraints that prevent efficient core designs must be overcome. Research and development to resolve these longer-term technical constraints/issues to improve core design efficiency is gaining attention and could benefit from improved modelling techniques. Three key constraints have been identified by the industry: (1) Crud induced power shift (CIPS), (2) burnup limit, and (3) enrichment limit.

For plants with low thermal margin, CIPS is a pressing issue as core designs are being detuned to meet design guidelines. While the formation of crud is a complex issue and models are continuously being refined to improve prediction capability, the current state of the art is limited to channel flow models. With advances in computing technology, the ability to predict local phenomenon from core wide 3D models could substantially improve phenomenon understanding and reduce uncertainty. In conjunction with model development, the industry is also exploring new approaches/technologies to improve reactivity control, such as poison enrichment and integration of the poison into the fuel rod.

The regulatory burnup limit is a constraint for approximately 1/3 of the fleet. In light of the current financial difficulties, there is a renewed effort to pursue burnup extension. Fuel safety research in the last 20 years has addressed many of the issues/questions associated with high burnup but the research has generated an unexpected concern with fuel fragmentation⁸. The fuel fragmentation phenomenon is being studied extensively via experimentation but mechanistic understanding is still lacking and being debated. A combination of experimentation and models will be needed to efficiently address the issue (Figure B.3). Currently, most of the effort has been focused on the impact of fission gas/grain structure on fuel fragmentation but it needs to be modelled holistically to include other factors affecting the fuel pellet and rod condition. Fuel pellet internal stress due to temperature gradient reversal in a LOCA, shown below, is an example of other factors that needing consideration.

Figure B.3. FEA model showing localised stress that matches fuel fragmentation pattern



Although mechanistic models, if possible to develop, are desirable for empirical relationships, past experiences have shown great difficulty in modelling in-core material behaviour. While trying to develop models from the basic principle is a noble effort, the lack of mechanistic understanding and complexity of the phenomenon entails many assumptions/compounding assumptions that may result in misleading conclusions and hinder research. It is important that modellers engage experimenters to have a balanced view of the feasibility of active mechanisms and to help experimental design.

Greater than 5% enrichment has been a topic of interest for a number of years. The issue is gaining renewed attention, not only to support longer cycles/higher burnups, but also to support enhanced accident-tolerant fuel (EATF) concepts. Many of the EATF concepts

need higher enrichments to overcome neutronic or fuel rod geometry penalties. The various proposed changes taken together will require extensive modelling capability to optimise energy output. Some model development will be needed to address some of the issues but much of the evaluation could be performed with existing codes. As changes could be made to different aspects of the fuel cycle, an integrated code with active coupling would be ideal to evaluate many of the scenarios and their impacts on the fuel cycle efficiency.

Conclusions

Utilities worldwide are facing difficulties and need to cut costs. Advanced modelling will be relied on to reduce research and operating cost. Therefore, we need:

- better understanding of phenomena;
- better integration of data/codes/synergistic use of existing modelling capabilities;
- improved margin and uncertainty management.

Advanced fuel modelling and/or calculation techniques help improve the safety and economics of flexible operation but need to be compatible with fuel and core design requirements (i.e. standards and methodologies).

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Expectations from progress in fuel modelling in order to optimise fuel design and safety analysis

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Extended Abstract

Introduction

After the TEPCO Fukushima Daiichi Accident in 2011, new regulations were established and enforced in order to prevent such serious accident from occurring again, and to manage and mitigate an accident if it occurs in the worst case. New regulations mainly focus on how to prevent and/or mitigate design-basis accident (DBA) and how to manage to control at design extended condition (DEC), and at severe accident (SA). Fuel is the key component in most of the events. Therefore, conventionally, fuel design is based on conservative models to protect the core. On the other hand, conservative results of fuel performance will lead excessive conservatism in DBA/SA analysis. In order to increase safety margins of safety analysis, it is important to establish more precise, best-estimate models to evaluate fuel behaviours / performances. Based on the current Japanese activity and situation, expectations from the point of optimising and improving current fuel design and related safety analysis are described. (This document mainly focuses on PWR fuel unless addressed specifically.)

Background in Japan

1) High burnup fuel trend in Japan (before 2011)

The development of high burnup fuel has continued with the aim of efficient use of uranium resources, as well as the enhancement of the fuels integrated with power plant. Mitsubishi has developed programmes to increase the licensed discharge burnup from 39 000 MWd/t to 48 000 MWd/t in the 1980s, and the 48 000 MWd/t fuel (Step 1 fuel) was put into commercial use in the early 1990s. In 2004, the licensed discharge burnup was raised from 48 000 MWd/t to 55 000 MWd/t (Step 2 fuel). In addition to UO₂ fuel, licence of MOX fuel Usage (up to 45 000MWd/t Assembly burnup) is also permitted with step1 fuel and step 2 fuel.

2) Improving nuclear safety trend (after 2011)

After 2011, safety improvement has become the most important and focused-on topic as a result of lessons learnt from the accident. In order to increase safety margins, it is important to establish more precise, best-estimate models to evaluate fuel behaviours/ performances. In addition, from the point of view of improving nuclear safety, the relationship between safety requirements (considering new regulations in Japan) and fuel design criteria has been reviewed and compared with regulation in several countries. The result of the review is summarised as technical reports, AESJ-SC-TR009: 2015 (in Japanese), by Atomic Energy Society in Japan (AESJ).

In these reports, several items are listed from the point of improvement of safety, and the listed topics are mainly divided into two categories. One is “Quantification of safety margin”; the other is “Approach to new, recent findings”. In the following section, major topics and expectations are summarised.

Topics and expectations

Quantification of safety margin

1) Cladding failure under transient conditions

Fuel cladding must keep its integrity during normal operation (NO) and anticipated operational occurrences (AOOs). Stress and strain are the main parameters to assess failure of cladding, and are applicable to slow, middle transient condition. On the other hand, for very fast transient conditions, thermal parameters, like fuel temperature, enthalpy rise rather than stress and strain are selected for specific analysis. Improvement of the evaluation method of cladding failure under transient condition is expected in order to evaluate cladding failure precisely in order to quantify and clarify the safety margin. In addition, embrittlement by neutron and hydrogen is considered in the evaluation.

Expectations:

- a) Update failure evaluation models from slow to very fast transient condition.
- 2) Safety assessment for seismic condition.

After 2011, the seismic hazard is one of the most important issues in Japan. The condition of ground motion acceleration for safe shutdown increases over 800 gals. For this condition, accurate evaluation models of required fuel safety functions during a seismic event are necessary in order to quantify safety margins.

Expectations:

- a) Optimisation of evaluation models for fuel assembly strength at seismic condition.
- b) Study of deformed components from point of thermal-hydraulics.
- c) Irradiation effects (materials, function) modelling for seismic point of view.
(In Japan, consideration of irradiation effects is already required in regulations)
- d) Optimisation of vibration analysis models inside core.

3) Long-term coolability

After 2011, more attention was put on long-term coolability after a LOCA event. At the moment, the assessment of long-term coolability is qualitative, and further discussion on how to treat the topic is necessary. This topic relates both to fuel design and safety analysis. Fuel designers should reflect and work together with safety analysts.

Expectations:

- a) Models related to fuel for long-term coolability
- b) Models to evaluate fuel condition after LOCA
- c) Models to evaluate fuel performance and behaviour after LOCA

Approach to recent findings

1) LOCA fuel fragmentation, relocation and dispersal (FFRD)

For high burnup fuel, the onset of fuel pulverisation, fragmentation, and relocation and/or dispersal outside the cladding ballooning/burst point during LOCA event for high-temperature transient condition should be further investigated. In current studies in Halden and Studsvik tests, threshold burnups of 60-70 GWd/t are investigated. FFRD is likely to be determining coolability assessment under/after LOCA event for high burnup fuel.

Therefore, an evaluation needs to be done of models of fuel fragmentation, relocation and dispersal and also of coolability of dispersed, relocated fuel.

Expectations:

- a) Models to evaluate amount of fragmentation and dispersal of pellets (as function of burnup)
- b) Coolability evaluation method considering relocated, dispersed pellet.

General expectations

1) Test programme for model verification and validation (V&V)

For the development of models, an appropriate test programme to verify and validate models should be also considered. In principle, the purpose of modelling is generally the same for each fuel vendor, utility and regulator. Thus, generally, international collaboration, such as Halden, SCIP, is important. In addition, for specific areas of modelling, discussion among interested organisations is expected.

2) Benchmarking activity

In addition to test programmes, an evaluation model benchmarking activity is important. This kind of activity will contribute to reaching a consensus on the specific evaluation area.

Current and upcoming issues for fuel modelling

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Extended Abstract

1) Introduction

The purpose of this presentation is to provide an overview of the current and upcoming issues for fuel modelling in LWRs at AREVA NP. These issues are determined by the following main drivers for a fuel vendor:

- improvement of predictive capabilities in order to justify increased fuel performances for improved fuel managements, fuel manoeuvrability and safety margins;
- development and licensing of new fuel products;
- compliance with new rules and requirements from safety authorities.

The next sections will illustrate with some representative examples how these different drivers impact the current trends and future needs for fuel modelling.

2) Current trends

One main feature of the current framework for fuel modelling at AREVA NP is that the company is currently ending its process of extension, integration and rationalisation of its numerous legacy codes. This is a global process which is implemented in various domains such as neutronics, thermal-hydraulics and thermal-mechanics. It is illustrated here with an example for fuel rod design codes where AREVA, starting from different codes previously developed in the United States (RODEX4, BWR), Germany (CARO-E, PWR & BWR) and France (COPERNIC2, PWR), has developed one global fuel rod code (GALILEO™, PWR & BWR) able to fulfil all the AREVA market needs. This global code capitalises the best practices in terms of fuel modelling from the previous codes, encompasses advanced models gained from recent R&D programmes and is validated on an extended database arising from various horizons.

Fuel modelling at AREVA NP is also supported by active R&D programmes. Many of these programmes are carried out within the French tri-partite institute (I3P) gathering means and competencies from the CEA (research institute), EDF (French utility) and AREVA NP (fuel vendor). Examples of some recent and significant R&D achievements are provided in the presentation. We can quote the development of the CARACAS fission gas behaviour model or the RACHEL helium balance model for MOX fuel. CARACAS and RACHEL are both very mechanistic models that have been implemented in the GALILEO™ industrial fuel rod code. Another example is related to a multi-D modelling of a fuel element during a power ramp by considering the coupled effects of thermal fuel creep and gaseous swelling. This multi-D approach contributes to enrich the 1.5 mechanical modelling in the industrial fuel rod design codes. Then a close-up is performed on the CARACAS model which is one of the more recent and significant developments within the I3P. This development has begun by the identification of the elementary mechanisms based on detailed experimental observations such as metallography, fuel fractography or SEM-FIB (coupled Scanning Electron Microscope and Focused Ion Beam) and TEM

(Transmission Electron Microscope) examinations at a microscopic scale. Then the CARACAS models derived from these elementary mechanisms have been formulated and coded. At the end of the process, the CARACAS models are validated against experimental results, including EPMA (Electron Probe Micro-Analysis) and SIMS (Secondary Ion Mass Spectrometry) radial gas concentration profiles within the pellet. The CARACAS model which has been design at the departure to be integrated in industrial codes, provides mechanistic fission gas release (FGR) and gaseous swelling assessments. It also gives very detailed local gas concentrations, which are required for relevant pre-accidental initial fuel condition calculations.

Another aspect of the current trends in terms of fuel modelling is the ongoing process at AREVA NP of multi-physic coupling. Previously, in the 90s, neutronics, thermal-mechanic, thermal-hydraulic and reactor system analysis were performed sequentially. Nowadays and by taking advantage of largely increased computing power, these calculations are fully coupled in new generation code systems. One example is provided here with the ARCADIA®, the new AREVA NP code system for PWRs. ARCADIA® is an advanced 3D coupled code system for steady-state and transient core design. The new software architecture allows for nodal and pin-by-pin calculations. ARCADIA® encloses the following main sub-systems: spectral code APOLLO2-A, core simulator ARTEMIS™, core thermal-hydraulics code COBRA-FLX™, Fuel Rod Module (FRM) fully consistent with the fuel rod performance code GALILEO™ and LADON™, a comprehensive user environment. The same kind of approach of extended multi-physic coupling is also ongoing at AREVA NP for BWR reactors. These new code systems provide gain in margin and robustness by avoiding unrealistic assumptions and decoupled approaches. They enable to manage fuel design and safety criteria evolutions while keeping the operational flexibility.

The current trends for fuel modelling as described above are necessarily accompanied by some evolutions in terms of methodologies. The development and generalisation of statistical methodologies is one of these evolutions. Some examples are provided here such as the GALILEO™ thermal-mechanical realistic methodology, which aims at analysing the fuel rod performance during normal operation, and anticipated operational occurrence conditions. The GALILEO™ realistic methodology is based on a Monte Carlo type random sampling of all the relevant input variables, i.e. inputs related to reactor operation conditions, fuel rod manufacturing and thermal-mechanical models uncertainties. Then the best-estimate GALILEO™ code in conjunction with non-parametric statistics is used to evaluate the propagation of these uncertainties to the design analysis results. Another example is the calculation of the internal fuel rod pressure distributions in pre-accidental conditions used in the AREVA CATHSBI (CATHare Statistique Brèches Intermédiares) methodology for intermediate break LOCA analysis in PWRs. These statistical methodologies have some consequences on fuel modelling. They require first a best-estimate modelling, i.e. nominal responses of the different models without significant bias or under/over prediction trends otherwise some model decalibration effects can be induced by the statistical sampling. Then the model uncertainties are taken into account through relevant model parameter distributions that are identified based on benchmarking processes carried out on the corresponding model validation databases. One example is provided here with the lognormal distribution of a multiplicative factor applied to the Xe diffusion coefficient of the GALILEO™ fission gas release model that is considered in its realistic thermal-mechanical methodology. Statistical methodologies require also efficient, stable and robust numerical schemes. This is a significant issue for a fuel vendor which has to perform intensive calculations without non-convergence, instability or crash even in case of simultaneous combination of extreme values for input variables that can occur in statistical methodologies.

3) Upcoming issues

In a next future, AREVA NP will carry on improving the predictive capabilities of its fuel models by capitalising in its industrial codes some forthcoming R&D achievements. One example is the adaptation of the GALILEO™ mechanical modelling based on 3D R&D mechanical simulations (ALCYONE) in order to improve the prediction of power ramps with different pellet Length/Diameter (L/D) ratios. Another example will be the adaptation of the CARACAS FGR model to simulate fuels with complex microstructures such as heterogeneous MOX fuels.

Improvement of the transient and accidental fuel modelling is another axis for further developments at AREVA NP. Taking advantage of detailed local gas concentrations as provided by the CARACAS FGR model, a mechanistic fuel-grain decohesion modelling based on intergranular bubbles pressure is on the way to be developed to address FGR behaviour in RIA conditions. Micromechanical approaches will also contribute to better assess the potential fuel fragmentation and dispersal phenomena as observed in some integral fuelled LOCA tests at Studsvik laboratories (Sweden). Along with these local models, integral 2D gas flow models within the fuel rod, based on fuel permeability measurements, are going to improve the fuel rod internal pressure calculations. All these developments are necessitated by the current emphasis put on accidental fuel behaviour by the different regulators.

Nevertheless, the main issues for fuel modelling in the next years will be quite obviously triggered by new fuel product developments and licensing. AREVA NP is currently entering in Phase 2 of the US Department of Energy (US DOE) enhanced accident-tolerant fuel (EATF) programme. Cr coated cladding with Cr₂O₃ doped UO₂ pellet have been identified as the AREVA primary EATF fuel concept with an insertion in LWRs planned by 2019. Along with this primary concept, AREVA will continue the development of its SiC/SiC cladding concepts with the objective to have a feasibility demonstration for introduction into a commercial reactor by 2022. Cr₂O₃ doped UO₂ fuel is also already proposed to AREVA customers as an improved fuel product to be loaded in the current ATRIUM™ 11 (contract for a BWR reload in 2018) and GAIA (contract for a PWR reload in 2019) fuel assemblies. Cr₂O₃ doped UO₂ fuel is characterised by a specific fission gas localisation within the fuel microstructure, especially in transient conditions, with less fission gas than standard UO₂ on grain boundaries and more gas trapped in intragranular position within the large grains. This specific Cr₂O₃ doped fuel behaviour will naturally require some FGR modelling adaptations. We have also to mention the development on the midterm of the CHROMOX Cr₂O₃ doped MOX fuel with an increased grain size and enhanced homogeneity. These features for the CHROMOX fuel will induce a reduced fission gas release and high burnup structure (HBS) extension within the pellet. Therefore, new fuel product developments appear to be strong drivers for fuel modelling activities at AREVA NP in the next years. They will affect various models such as FGR, gaseous swelling, fuel fragmentation, pellet-clad interaction (PCI), HBS development, clad oxidation and SiC material behaviour.

4) Conclusions

This presentation has described some current and upcoming actions set up at AREVA NP in order to improve the predictive capabilities, validation and robustness of the fuel modelling. Fuel rod internal pressure (particularly for MOX) and PCI constraints (enhanced by renewable energy impact) still appear to be the most limiting fuel issues for the AREVA customers. Therefore, AREVA fuel modelling developments will stay focused on these critical items. Global code validation and robustness, particularly for statistical methodologies, are also at stake for a fuel vendor.

Post-Fukushima initiatives and evolutions of the regulatory framework have reinforced the needs for accidental fuel modelling. Taking the benefits from R&D programmes such as the ones carried out in the French I3P institute, more mechanistic models are being progressively introduced in industrial codes and will contribute to fulfil these new requirements.

Nevertheless, the main issues for fuel modelling in the next years will be quite obviously triggered by new fuel product developments. Among these new fuel products, we can mention the AREVA EATF fuel concepts, the Cr_2O_3 doped UO_2 fuel already on the way to be delivered as fuel reloads for commercial PWR and BWR reactors and also the CHROMOX Cr_2O_3 doped MOX fuel on the midterm. These new fuel products will require further modelling developments in various domains such as FGR, gaseous swelling, fuel fragmentation, PCI, HBS formation, clad oxidation and SiC material behaviour.

Modelling accident-tolerant fuel concepts: Gaining a mechanistic understanding to aid licensing

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Abstract

Accident-tolerant fuels are being developed to improve the safety and increase the economic benefit of nuclear power. Never in the last half-century has the entire nuclear energy industry focused so much attention on such revolutionary materials. Within Westinghouse, it is clear that this effort has the potential to provide both incremental improvements, having direct benefits to nuclear power generation in the short term, and long-term massive advances that will eventually become the standard product for nuclear energy generation. Westinghouse has two focuses: cladding materials – providing accident tolerance – and fuel materials – enabling the accident-tolerant claddings to be economically viable.

Uranium silicide and uranium nitride production methods are being investigated and techniques to produce pellets on an industrial scale are being developed. The manufacturing processes for both coated claddings and SiC-SiC are also being optimised. Current characterisation investigations have focused on the behaviour of the candidate materials in simulated reactor environments. Computer simulation methods are increasingly being used to aid the material selection process and to understand the mechanisms at play. These computer simulations will also provide a mechanistic understanding of the fuel to enable accurate and adaptable fuel performance codes to be developed – a key step towards the licensing and operation of these exciting new fuel concepts.

In addition to impacting the accident-tolerant fuels programme, computer simulation methods (from the atomic scale and higher) are being utilised to optimise and enhance our understanding of the current UO₂-Zr system and incremental developments thereof.

Current issues and future needs for fuel modelling in LWRs

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Abstract: Fuel rod design code developed by KEPCO NF, ROPER, is briefly described. As current issues of fuel modelling, fuel thermal conductivity uncertainty as well as crud deposition rate and its thermal conductivity are explained. And also, fuel behaviours and models that should be considered in developing fuel rod performance analysis code for PCI/PCMI analysis and accident analysis such as LOCA and RIA are addressed for future needs.

Keywords: fuel modelling, fuel rod design code, ROPER, PCI/PCMI analysis and accident analysis.

ROPER code

The fuel rod design code ROPER [1] has been developed by KNF (KEPCO Nuclear Fuel) to perform steady-state fuel rod performance analysis for PWR plants and to generate burnup-dependent fuel rod initial conditions for LOCA and Non-LOCA safety analyses. Moreover, it can be used to assist in-pile performance testing of fuel rod in research and commercial reactors. Major features of ROPER are the incorporation of 1) models and properties of UO₂ fuel rod with zirconium alloy claddings, 2) the burnup-dependent fuel thermal conductivity models, 3) semi-mechanistic steady-state fission gas release model, 4) cladding stress-strain analysis under generalised plane strain condition, 5) cladding oxidation and hydrogen pickup models, and 6) cladding fatigue, lift-off and plasticity analysis models. ROPER has been validated using the in-pile database such as Halden IFA data as well as the data obtained from domestic and oversea commercial reactors. For the evaluation of fuel rod design criteria, ROPER adopts a statistical approach such as SRSS (Square Root of the Sum of the Squares) method to give conservative prediction. The SRSS method takes into account the uncertainties of fuel manufacturing data and fuel performance models such as cladding creep, cladding corrosion, pellet densification, pellet thermal conductivity, etc.

Current issues in fuel modelling

Fuel thermal conductivity degradation and uncertainty

Since the fuel thermal conductivity is a critical factor for fuel temperature distribution and eventually fuel rod behaviour, it is important to determine the accurate value of thermal conductivity. Recently, it has been found that fuel thermal conductivity degradation (TCD) occurs as burnup increases and several TCD models have been suggested [2]. Fuel thermal conductivity uncertainty needs to be considered in fuel rod design analysis such as fuel centreline temperature calculation for power-to-melt evaluation by the SRSS design methodology.

Figure B.4 shows the measured fuel thermal conductivity data for unirradiated and irradiated conditions from open literatures [3-16] along with thermal conductivity models at unirradiated condition. And the statistical analysis results for the measured-to-prediction ratio for several thermal conductivity models are also given in Figure B.4. The statistical analysis on the entire data shows that the lower bound uncertainty is larger than 25% for

models considered, and thus resulting in an overly conservative fuel temperature calculation.

On the other hand, the thermal conductivity uncertainty may be determined using the conductivity integral to melt (CIM = $\int_{T_{ref}}^{T_{melt}} k dT$). Using available CIM values [10,17-18] of UO₂ fuel given in Figure B.5, lower bound uncertainty of thermal conductivity is evaluated to be less than about 5%. However, it should be noted that CIM values have been reported only for unirradiated and low burnup fuel, therefore CIM at high burnup are needed to support this approach.

Figure B.4. UO₂ thermal conductivity model uncertainties with measured data

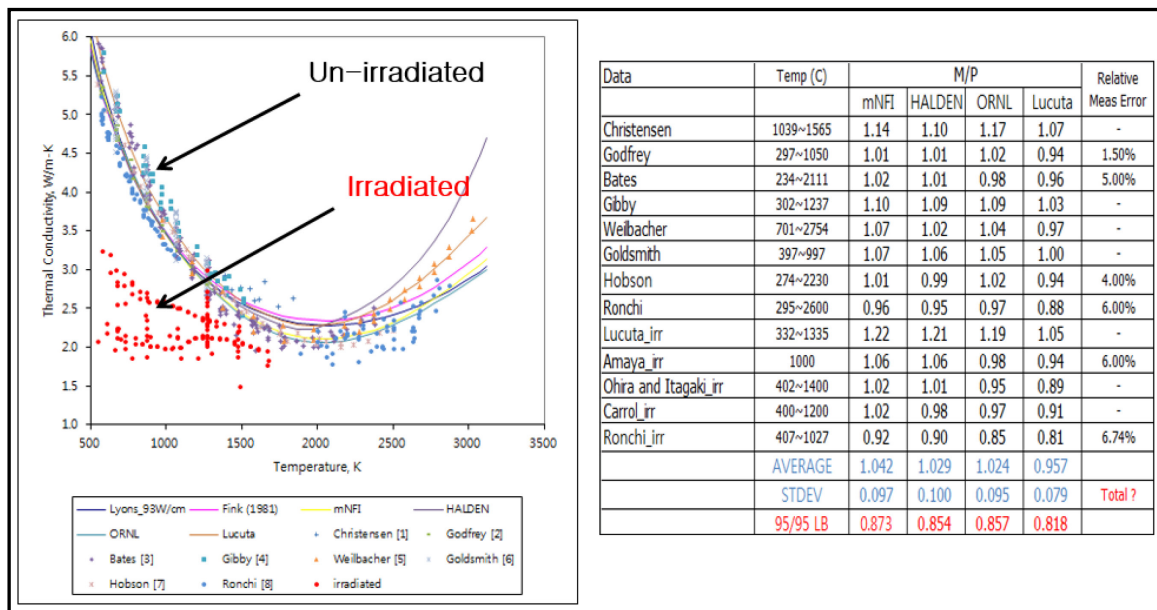
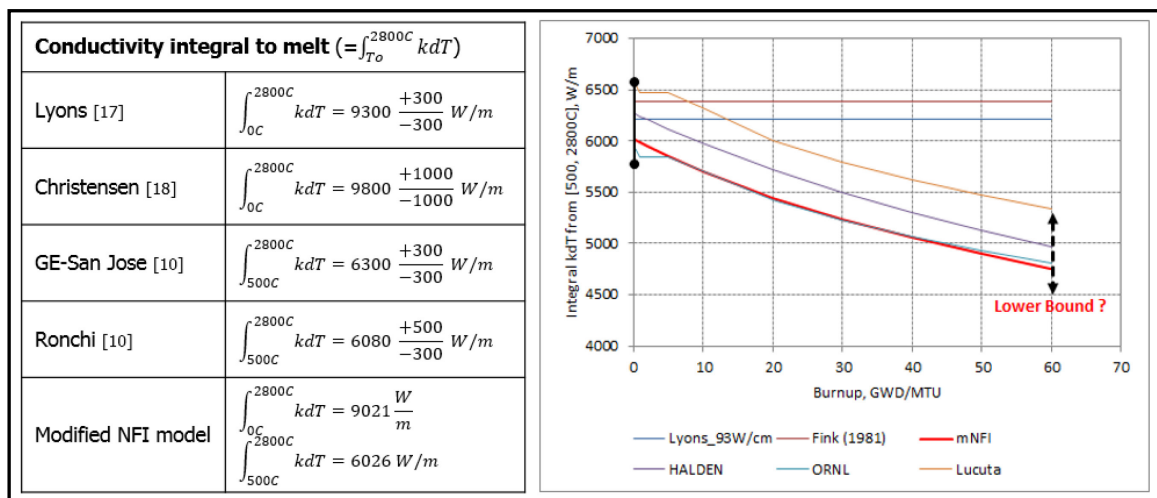


Figure B.5. Conductivity integral to melt (CIM) values of UO₂ fuel

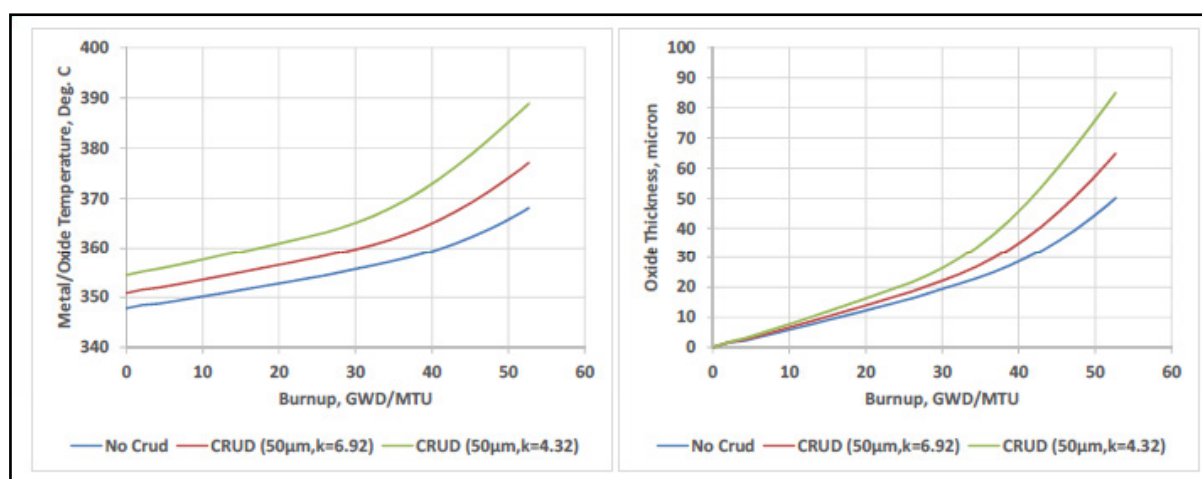


Crud deposition

It is known that undesired axial power change may be caused by deposition of crud on fuel rod in PWR core. Crud also affects the cladding oxide thickness and fuel temperature as a thermal barrier. Therefore, the effect of crud on fuel rod behaviour needs to be considered in fuel modelling. Figure B.6 represents the effects of crud thickness and its thermal conductivity on cladding metal-oxide interface temperature and oxide thickness evolution. It is seen that cladding corrosion is significantly affected by the crud thickness and its thermal conductivity.

To evaluate the effect of crud on fuel rod behaviour, it is necessary to identify the crud thickness and its thermal conductivity. According to a study [19], it has been found that crud deposition rate is strongly dependent on the heat flux above the flux required for onset of nuclear boiling. However, the accurate crud deposition condition and rate have not been fully identified. On the other hand, thermal conductivity of crud is difficult to determine because of the large variability. It has been found that a porous crud layer with high water content and low density could have thermal conductivity ten times higher than that expected from a deposited crud layer due to “wick boiling” [20]. Therefore, it is necessary to develop the appropriate crud deposition model and to determine the accurate thermal conductivity of crud.

Figure B.6. Effects of crud thickness and its thermal conductivity on (a) cladding metal-oxide interface temperature, and (b) oxide thickness evolution



(a)

(b)

Future needs for fuel modelling

PCI/PCMI analysis

KNF is developing a code to calculate the thermo-mechanical behaviour of the fuel rod using 3-dimensional finite-element method for PCI/PCMI analysis. Compared to steady-state analysis, we need to consider the additional fuel models such as 1) pellet cracking and relocation for accurate calculation of fuel temperature and eventually stress-strain state on a node basis, 2) pellet deformation by high-temperature creep under compressive stress due to pellet-cladding contact, hot pressing and gas swelling for consideration of pellet expansion at high-power condition, 3) cladding deformation by creep reversal due to power ramp up and down under daily load following operation, 4) pellet-cladding chemical bonding at high burnup affecting pellet-to-cladding gap heat transfer and local stress state,

and 5) well-defined cladding failure criterion (strain-based, or strain energy-based, or stress-based criterion) considering the irradiated cladding conditions.

Accident analysis

KNF is also developing a code to calculate the thermomechanical behaviour of the fuel rod during accident conditions such as LOCA and RIA. For accident analysis, the applicability of models used in steady state or mild transient should be reviewed and fuel models describing transient-specific phenomena need to be considered additionally. The major fuel models for accident analysis are 1) cladding-to-coolant heat transfer during transient considering that circumferential variation in coolant temperature and/or steam content at cladding surface may affect cladding temperature distribution, 2) axial gas mixing within fuel rod considering the significant transient fission gas release which affects the ballooning and fuel ejection after burst, 3) high-temperature mechanical properties of irradiated cladding such as creep for more exact calculation of mechanical integrity of cladding, and 4) simulation of post-failure phenomena such as gap gas ejection, fuel dispersal, fuel-coolant interaction and loss of axisymmetric geometry.

Conclusion

The fuel rod design code ROPER, developed by KNF for steady-state fuel performance analysis, is briefly described. Current issues and future needs for fuel modelling have been addressed. To enhance safety and performance margins of the fuel rod, it is required to elaborate the fuel models and properties for more accurate prediction of fuel rod behaviour during normal operation and transients such as PCI, LOCA and RIA. Meanwhile, the reduction of uncertainties, incorporated in the fuel rod design methodology, is necessary.

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Safety and regulatory aspects related to nuclear fuel and activities within CSNI Working Group on Fuel Safety

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Discussions focused on the work of the NEA Committee on the Safety of Nuclear Installations (CSNI) Working Group on Fuel Safety (WGFS). The reports done on RIA fuel behaviour; RIA code benchmarking; behaviour under LOCA, including spent fuel pool; fuel fragmentation, relocation and dispersal were highlighted. Recent activity on leaking fuel and impacts; SCC and PCI; oxygen and hydrogen in cladding; FP behaviour during transients; behaviour in spent fuel pools; and fuel assembly bow were described. It was noted that a number of topics related to fuel safety offer opportunities for advancing modelling, particularly in areas such as uncertainty evaluation which is increasing in importance with modelling sophistication. It was also mentioned that new fuel concepts such as ATFs may also benefit from advanced modelling.

Nuclear Innovation 2050

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Extended Abstract

Nuclear Innovation NI2050 is a broad NEA Initiative aimed at selecting and developing large-scale research, development and market uptake programmes of actions (projects and infrastructures), at seeking agreement of interested stakeholders (member countries, R&D organisations, industry, regulators) on their content and timelines, and at leading to international co-operation for their implementation, under appropriate legal frameworks and with adequate financing, in order to accelerate the readiness of innovative technologies and help them reach competitive deployment in time to contribute to the sustainability of nuclear energy in the short/medium term (2030) and longer term (2050).

The joint IEA/NEA Nuclear Technology Roadmap, issued in 2015 and based on the 2DS ETPs scenarios of the IEA (Energy Technology Perspectives scenario limiting the temperature rise to 2°C by 2100), already describes the main barriers to overcome and provides the main priorities for actions to have a role for nuclear energy in the future low-carbon energy mix. NI2050 is therefore not a new additional roadmap, but seeks to boost innovation as being the transfer of the outcomes of research towards industrial deployment. Indeed, in a number of countries, while nuclear research and development has for 15 years continued to be funded by national budgets at rather constant levels, what is mainly lacking is the uptake and deployment by industry of the outcomes of research. This is partly due to the difficult financial environment where nuclear industry finds itself today, and also due to the “increased rigidity” of the regulatory and licensing process, both aspects being non-conducive to innovation taking place.

In order to contribute, either through electricity generation or direct heat supply, to the decarbonisation of the energy system of the future (IEA, in the 2DS scenario, estimates the needed world nuclear power capacity in 2050 at 2.3 times the fleet in operation today), nuclear energy will need to be safe AND economic AND flexible – in line with the three pillars of sustainability: environment protection, economics, reliability of energy supply. Indeed, safety ensures the protection of the environment, cost control contributes to the economic viability, and flexibility will foster the integration with (variable) renewable energy sources while providing grid stability.

In concrete terms, NI2050 is about bridging the gap (also called valley of death) between research and market deployment, going from lower to higher technology-readiness levels (TRLs). At the centre of this process, beyond technology development, one finds testing and validation of technologies and their further qualification and licensing. A necessary condition for this to happen effectively in an accelerated way is to make sure that all stakeholders are involved and engaged as early as possible in the innovation process. This may be difficult at national level, where, in particular, the safety authority independence from industry is required, but might be more effective at international level. NEA is a framework where this effective interaction may be organised.

NI2050 is targeting three types of actions, applicable and useful in a large international framework, and all three being key to target at the same time for increased safety and market needs. The initiative aims to:

- *support common development of technologies*, before these technologies become industrial products with strong intellectual property (IP) limitations;
- *optimise the common scientific testing and validation* of these technologies, including in particular through extensive recourse to modelling and simulation, itself duly tested and validated, with proper assessment of uncertainties;
- *establish common qualification methods and processes* for these technologies and the resulting industrial products, including for licensing purposes.

Activities under the three axes mentioned above will require the use of research and demonstration infrastructures, tools and facilities. A number of them exist but their level of readiness, experimental perimeter and availability need to be checked. Additional facilities may be necessary, in particular since some existing ones have limited lifetime available. It makes full sense to work in common to establish a global picture of such infrastructures and to work together to optimise their use or the need to build new ones, fostering complementarities and avoiding duplications.

Beyond developing the concepts described above, the NI2050 Advisory Panel, established under the auspices of the Nuclear Development Committee (NDC), but interacting via the NEA Secretariat with all other concerned Committees (i.e. NSC, CSNI, CNRA, RWMC), has now selected a set of topical areas to develop concrete “10 years” Programmes of Actions along the lines of the three axis (Technology Development, Testing/Validation, Qualification and Licensing). These topical areas concern Accident-Tolerant Fuels, Severe Accident Knowledge and Management, Passive Safety Systems, Ageing Management, Advanced Fuels and Materials, Advanced Components, Fuel Cycle Chemistry/Recycling, Heat Production and Cogeneration, and some enablers: Modelling and Simulation, Digitalisation and Measurements, Infrastructures and Demonstrations. Selected experts, mainly from the research community, have started to draft the Programmes of Actions. Once developed, the Programmes of Actions will be discussed with industry and regulators, aiming at reaching a consensus on “what” needs to be done to foster technological evolution and innovation in the given topical areas. From there, interested stakeholders may come together, helped by the NEA, to discuss the ways and means, as the “how” for implementation, in particular the necessary legal and financial frameworks.

To conclude, reboosting the innovation process in nuclear technology is a necessary condition for having nuclear energy ready in time to play a role in the sustainable energy mix of the future. Sustainability is a combination of environment protection, security of energy supply and economics. To be part of the sustainable energy mix, nuclear will have to be safe AND affordable AND flexible, the three being cross-connected.

In this context, a multilateral approach of technological evolution and innovation, as developed in NI2050, may be a way to accelerate the process and create the robust and wide confidence necessary for the deployment and licensing in a worldwide market.

Nuclear fuel technologies (i.e. ATF and Advanced Fuels) are in the list of topical areas selected by the Advisory Panel, for which Programmes of Actions are presently being drafted.

IAEA activities on fuel performance

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Extended Abstract

The IAEA Sub-programme on Nuclear Power Reactor Fuel Engineering

While adhering to appropriate safety margins, effective design and manufacturing technologies, and optimised in-pile fuel performance are required to ensure reliability and economic efficiency in nuclear fuel utilisation. To support this, the IAEA sub-programme on Nuclear Power Reactor Fuel Engineering assists interested Member States in organising an adequate R&D programme by transferring information and sharing experiences. The sub-programme covers the following topics of expertise:

- development, design and engineering;
- fabrication: manufacturing techniques, nuclear safety and radiological protection in fuel fabrication;
- behaviour, analysis and modelling:
 - behaviour during normal and overpower operation;
 - behaviour under postulated and severe accident conditions;
 - properties of zirconium alloys and other core materials relevant to performance;
 - corrosion and hydrogen effects;
 - post-irradiation examination;
 - inspection, reconstitution and repair;
 - relationship with back-end requirements.
- utilisation and management;
- MOX, alternative fuels and advanced fuel technologies and materials;
- economic and other aspects, e.g. environmental issues;
- quality assurance and control.

In order to assist Member States in planning for and using nuclear science and technology for peaceful purposes, the International Atomic Energy Agency (IAEA) plans, implements and manages co-ordinated research projects (CRPs), which are essential for the IAEA to foster collaboration between Member States and improve nuclear techniques worldwide.

A co-ordinated research project (CRP) is designed to encourage the acquisition and dissemination of new knowledge from the use of nuclear technologies and isotopic techniques. By bringing together research institutions in both developing and developed countries and sharing resources and expertise, CRPs help foster the exchange of scientific and technical information while achieving a particular research agenda. This also helps improve capacity building in Member States, which is especially important for developing countries that would otherwise be unable to undergo such extensive research projects.

Several examples of CRPs currently supported by the IAEA subprogramme on Nuclear Power Reactor Fuel Engineering are presented below.

CRP T12028 on Fuel Modelling for Accident Conditions (FUMAC)

Summary

The CRP supports the Member States in their efforts to analyse and better understand the behaviour of water-cooled power reactor fuel in accident conditions through sharing of experimental data and best practices in application of fuel modelling computer codes.

Background situation analysis

Fuel modelling is a recurrent priority in the IAEA sub-programme “Nuclear Power Reactor Fuel Engineering”. Development and verification of computer codes are possible only on the basis of good experimental data that requires very durable and expensive in-reactor and post-irradiation studies. That is why international co-operation in this area is highly desirable, and the IAEA traditionally supports interested Member States in their efforts to enhance capacities of their computer codes used for prediction of fuel behaviour. Since the early nineties a series of four CRPs D-COM (1982-1984), FUMEX (1993-1996), FUMEX-2 (2002-2007) and FUMEX-3 (2008-2012) targeted fuel modelling in normal operational conditions. Those projects were highly appreciated by Member States, and the proposed CRP “Fuel Modelling in Accident Conditions” (FUMAC) continues the series with the focus on fuel behaviour in design basis and severe accidents that is particularly demanding nowadays.

CRP FUMAC is planned under the IAEA Nuclear Safety Action Plan with the well-proven organisational approach used in the CRP FUMEX-3, which presumes cross-comparisons of computer codes used in different Member States and close collaboration with the NEA/OECD and the joint NEA-IAEA International Fuel Performance Experimental (IFPE) Database. Selected sets of accident simulation experimental results, provided by CRP members, will be integrated into the IFPE Database and used for codes verification.

In the light of the Fukushima accident, the 2012 meeting of the IAEA Technical Working Group on Fuel Performance and Technology approved FUMEX-3 results and recommended IAEA to launch a new fuel modelling CRP FUMAC focusing on accident conditions. Preliminary ideas of FUMAC were initiated at the Technical Meeting “Fuel Behaviour and Modelling under Severe Transient and Loss of Coolant Accident (LOCA) conditions” in Japan in October 2011 and agreed with NEA/OECD in 2012, with more detailed discussion on its objectives at the Technical Meeting “Modelling of Water-cooled Fuel Including Design Basis and Severe Accidents” in China and the 20th International QUENCH Workshop in Germany in 2013.

Participants: 24 organisations from 18 countries (+ 2 observers)

Planned duration: 2014-2017

- The first Research Coordination Meeting (RCM) was held 11-14 November 2014 in Karlsruhe.
- The second RCM was held from May 30 to June 2, 2016 in Vienna.
- The third RCM is planned to be held in November 2017.

CRP overall objectives

Better understanding and enhanced safety of nuclear fuel behaviour in accident conditions.

Nuclear component

Nearly the entire hazard from an accident at a nuclear reactor stems from the nuclear fuel. Computer modelling allows the prediction of the key aspects of the performance of fuel materials and components (temperatures, dimensional changes of fuel components, release of fission gases, etc.), and the development of acceptable safety limits of operational parameters. The subject of CRP FUMAC fully corresponds to the aim of the IAEA Nuclear Safety Action Plan at enhancing safety of nuclear reactor operations.

CRP T12030 on Analysis of Options and Experimental Examination of Fuels for Water-Cooled Reactors with Increased Accident Tolerance (ACTOF)

Summary

Nuclear fuel is a highly complex material that has been subject to continuous development over the past 40 years and has reached a stage of development where it can be safely and reliably irradiated up to 65 GWd/tU or more in commercial nuclear reactors. During this time there have been many improvements to the original designs and materials used. However, the basic design of uranium oxide fuel pellets clad with zirconium alloy tubing has remained the fuel of choice for the vast majority of commercial nuclear power plants.

Severe accidents, such as those at Three Mile Island and Fukushima Daiichi have shown that under such extreme conditions, nuclear fuel will fail and the high-temperature reactions between zirconium alloys and water will lead to the generation of hydrogen with the potential for explosions to occur, damaging the plant further.

Recognising that the current fuel designs are vulnerable to severe accident conditions, there is renewed interest in alternative fuel designs that would be more resistant to fuel failure and hydrogen production. Such new fuel designs would need to be compatible with existing fuel and reactor systems if they are to be utilised in the current reactor fleet and in current new build designs, but there is also the possibility of new designs for new reactor systems.

Globally, there is a great deal of experience with the performance of reactor fuel in off-normal conditions. Theoretical studies and experiments have been performed and there have been excursions from normal operating conditions in a few power reactors. During such an excursion, the difference between an incident of limited or no consequence and a severe accident, such the one at Fukushima, depends on the conditions in the reactor and the performance of the fuel under those conditions. The CRP T12030 “Analysis of Options and Experimental Examination of Fuels for Water-Cooled Reactors with Increased Accident Tolerance” (ACTOF) explores the potential to design and operate advanced fuel types that are intended to be more tolerant of severe accident conditions while retaining the capability of current fuel designs for safe operation under normal operation and anticipated transient conditions.

Participants: 14 organisations from 11 countries and 1 observer.

Planned duration: 2015-2018

- The first RCM was held from 2 to 4 November 2015 in Vienna (12 participants from 11 Member States and 1 observer from OECD-NEA).
- The second RCM was held from 20 to 22 June 2017 in Vienna.

Main objective

To support options for the development of nuclear fuel with an improved tolerance of severe accident conditions:

- to acquire data through experiments on new fuel types and cladding materials to support their use for fuel with improved accident tolerance;
- support modelling of new fuel designs with advanced cladding or fuel.

Expected outcomes

- Provision of information to Member States to support decision-making on the choices available to improve the safety of Nuclear Power Plants under severe accident conditions.
- Provision of data, analyses and advanced techniques to understand and predict the behaviour of the components and the integral performance of accident-tolerant fuel designs under normal and transient conditions.

Expected results

- well checked experimental data on the behaviour of candidate materials for Accident-Tolerant Fuel designs;
- new models of materials behaviour in fuel modelling codes;
- results of computer modelling of advanced fuel types under normal and accident conditions.

New CRP on Fuel Materials for Fast Reactors

A new CRP on Fuel Materials for Fast Reactors is planned to be launched in 2018.

Main objective

Bringing together specialists from the Member States with active fast reactor programmes for a co-ordinated support of their national efforts in the R&D areas:

- traditional (MOX) and innovative "dense" non-oxide fuels, including ceramic (carbides and nitrides) and metallic (U-Pu alloys) fuels;
- thermomechanical properties and irradiation behaviour of fuel cladding materials (austenitic, ferritic-martensitic, high-nickel alloys, ODS steels);
- compatibility of stainless steels with heavy liquid metals (also for ADS);
- validation, verification and benchmarking of FR fuel performance codes.

A preliminary discussion on the scope and objectives of the new CRP is foreseen to take place during the International Conference on Fast Reactors and Related Fuel Cycles: Next Generation Nuclear Systems for Sustainable Development (FR17).

Conclusions

- The performance of nuclear fuel is key to the safe operation of nuclear power plants.
- Development and modelling of advanced fuel types that can better withstand the extreme conditions found in severe accident conditions will improve safety margins.
- The subject of CRPs FUMAC and ACTOF supports realisation of the IAEA Nuclear Safety Action Plan to enhance safety of nuclear reactors' operation.

Annex C. Abstracts for Session 2, Nuclear-fuel modelling in support of performance and safety improvements under off-normal conditions

Computational analysis of multi-rod ballooning and fuel relocation during LOCA using the multi-physics DRACCAR code

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Extended Abstract

In the framework of its research activities related to loss-of-coolant accident (LOCA) the French Institut de Radioprotection et de Sûreté Nucléaire (IRSN) is developing a multi-rod computational tool named DRACCAR.

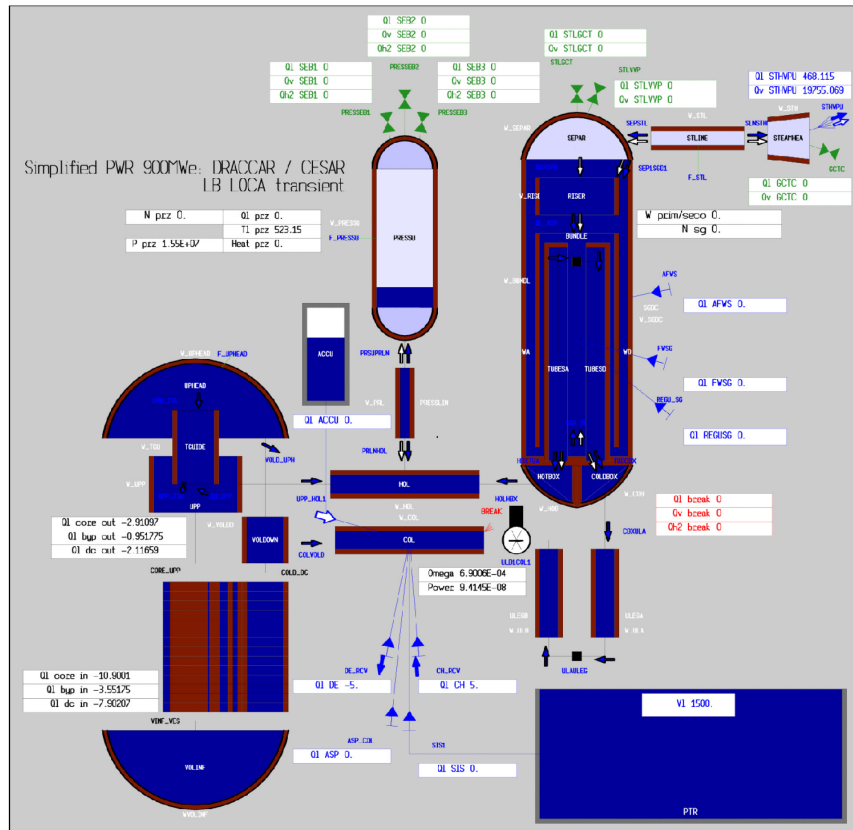
In order to realistically describe the behaviour of the reactor core during a LOCA, modelling has to take into account many coupled phenomena. This implies complex computations involving multidimensional two-phase flows, coupled with heat transfers (electrical heating or decay heat, conduction, convection and radiation), chemical reactions (oxidation, hydriding, nitriding), mechanical strain (creep behaviour, thermal expansion), material relocation (balloons filling up with fuel pellet fragments, associated with a possible power profile modification) and contact between structures which modifies all physical phenomena (conduction instead of convection, oxidation and radiation).

Changes in the core geometry, as well as the ability to cool down the core are addressed and analysed. This analysis is essential for a detailed understanding of all the circumstances that can lead to assemblies quenching even in case of a large flow blockage ratio due to clad ballooning.

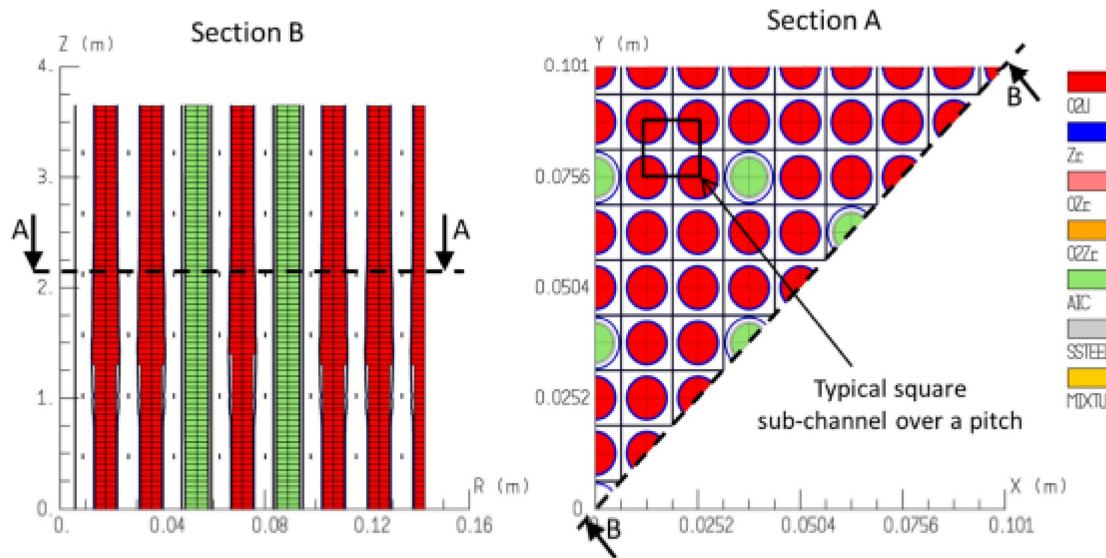
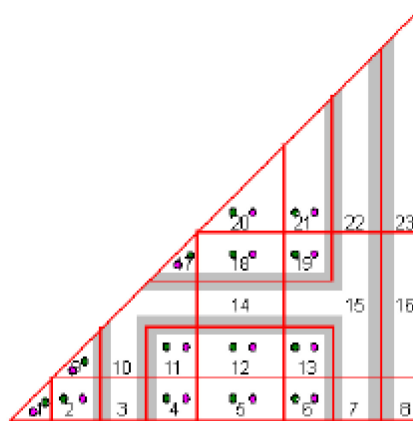
The flexibility of the DRACCAR code allows to model from a simple fuel rod up to a full core connected to all systems of a Pressurised Water Reactor (primary and secondary circuits, safety systems – see Figure C.1) or a full experimental device. It is thus possible to simulate any LOCA transient from the initial event till the fuel rod reflooding.

The code uses a 3D non-structured meshing: the horizontal discretisation defines subchannel thermal-hydraulics while the axial discretisation leads to analyse quasi-independent 2D thermal-mechanical problems. Each structure (rod, grid or shroud) can be precisely defined (geometry, composition and location). It is also possible to model representative structures to simulate the average behaviour of a large number of structures. Moreover, DRACCAR allows the mixing of the two modelling scales: definition of a precise assembly (each rod is modelled) surrounded by assemblies using representative rods.

Figure C.1. Modelling of a full PWR 900MWe with DRACCAR coupled to CESAR



Even if DRACCAR computations benefit from OpenMP parallelism, the use of symmetries is available to reduce the size of the system to compute and thus the CPU time. Therefore, the reasonable target for fuel assembly calculations is to model precisely 1/8th of a fuel assembly including fuel rods (stack of fuel pellets, cladding), control rods (absorber, cladding), guide tubes, instrumentation tube and spacer grids (see Figure C.2). Each structure is axially and azimuthally discretised by the meshing; it is moreover possible to refine the azimuthal discretisation of any structure inside sub-channels (see Figure C.3). Each structure is in mechanical and thermal interaction with others: the main variables of DRACCAR are the geometry, the material composition and the temperature of each piece of structure.

Figure C.2. Modelling of 1/8th of a fuel assembly with DRACCAR (vertical and horizontal cuts)**Figure C.3. Modelling of 1/8th of a spent fuel pool rack with DRACCAR**

An Application Programming Interface (API) has been developed to allow an efficient implicit coupling between the structure code DRACCAR and any thermal-hydraulics code. It leads to a deep coupling of codes to solve the Newton-Raphson method over a same time step. The DRACCAR code is currently coupled to the IRSN two-phase flow module CESAR of the ASTEC code as well as to the CEA-EDF-AREVA-IRSN two-phase flow CATHARE 3 code. Important modelling such as pellet eccentricity, heat transfers (within the solid and through the fluid), material properties evolutions (oxidation layer, phase changing,...) or contact between structures (with local modification of heat transfers and chemical reactions amplifying azimuthal temperature gradients) can thus be taken into account. Cladding integrity and structure coolability issues, which are essential points to conclude on LOCA transient effects, can only be addressed by a multi-pin code coupled with an efficient thermal-hydraulics code.

Many results have already been obtained with the DRACCAR code with respect to a substantial validation matrix based on tests from experimental programmes EDGAR, HALDEN IFA 650, REBEKA, MT, PHEBUS SFD, PHEBUS LOCA, MARGO-R, SFP, PERICLES, ROSCO, FEBA, SEFLEX, ACHILLES and THETIS.

Key issues identified in fuel safety studies at JAEA on the modelling of fission gas behaviours inside fuel pellet under normal and off-normal conditions

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Extended Abstract

Fuel failure phenomena under accident conditions have been extensively studied at JAEA up to the very high burnup region. Recently, experimental analyses on fuel-grain separation, gas communication inside fuel rod, gas-induced fuel deformation and fuel/coolant thermal interaction under reactivity-initiated accident conditions have been performed using the fuel performance code RANNS and the steam explosion simulation code JASMINE. The results show that some fission gas behaviours are likely to dominate both fuel deformation and the intensity of destructive force at fuel failure. Specifically, the timing of gas release to the free volume in fuel rod, gas communication in the axial direction of fuel rod, and the mixing of the fission gas released by fuel failure with coolant water have been identified as elementary processes that should be clarified to reflect the knowledge obtained from experiments into safety criteria properly.

In terms of the analyses of fission gas behaviours under accident conditions, the state of fission gas inside fuel rod under normal operation condition is also recognised as one of the most important sources of uncertainty. While the importance of proper modelling of fission gas behaviours under normal operation condition has long been noticed, the current fission gas release (FGR) model implemented in our fuel performance code FEMAXI-7 supports only a very simple description of intragranular processes with single bubble size, assumption of equilibrium bubble state, and the gas atom diffusion coefficient tuned by in-pile FGR data, and its applicability is considered to be limited for the irradiation conditions out of supported range by validation database. Hence, motivated mainly by the above-mentioned accident analyses, a new FGR model has been incorporated into FEMAXI-7 to cover both normal and off-normal conditions with consistent model structure, with focusing on the most fundamental part of fission gas release, i.e. intragranular fission gas behaviour so far: the model is much more flexible and expected to be versatile owing to its treatment of bubble size distribution and the dynamic descriptions of bubble nucleation, diffusion, coalescence and re-resolution processes and interaction between bubbles and point defects. In this paper, the characteristics of some typical FGR models are introduced and the key issues on the modelling of FGR behaviour are described through the comparison between these FGR models.

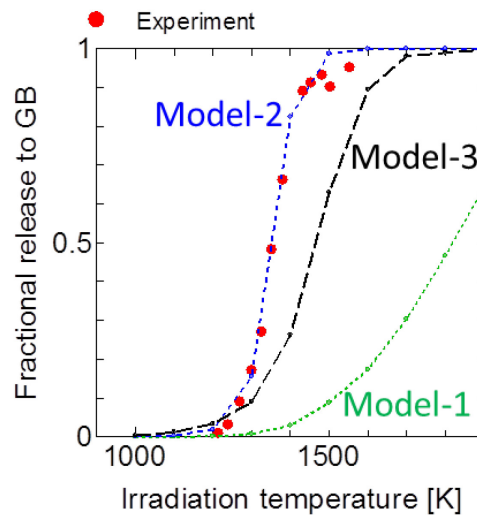
Some preliminary calculations to determine the configuration of component models were performed in the framework of the development of new FGR models and compared with the results of the previous studies [1,2] where FGR models with essentially common structure were employed: the concept of rate equation is mainly applied in these models. As a sensitivity study in terms of the FGR model, FGR under a steady-state irradiation condition at 4% burnup, originally reported by the Hanford Engineering Development Laboratory (HEDL) and analysed in both preceding studies [1,2], was calculated by using three configurations of component models given in Table C.1. Here, Model-1 and -2 were intended to reproduce the calculations, which correspond to the previous studies [1] and [2], respectively.

Table C.1. Sensitivity study matrix

Component models	Model-1	Model-2	Model-3
Bubble nucleation	Nelson type [1]	Nelson type [2]	Turnbull type [1] with nucleation volume of $1.1 \times 10^{-18} \text{ cm}^3$
Gas atom diffusion	Matzke [1]	Matzke'+Turnbull [2]	Matzke+Turnbull [1,2]
Gas bubble diffusion	Buescher and Mayer [1]	Mikhlin [3]	Buescher and Mayer
Coalescence between gas atoms/gas bubbles	Equal to collision rate between gas atoms/bubbles [1]	Coalescence rates of large bubbles are suppressed [2]	Coalescence rate of gas atoms and gas bubbles are suppressed
Gas atom re-solution	Turnbull type [1]	Nelson type [2]	Turnbull type [1]

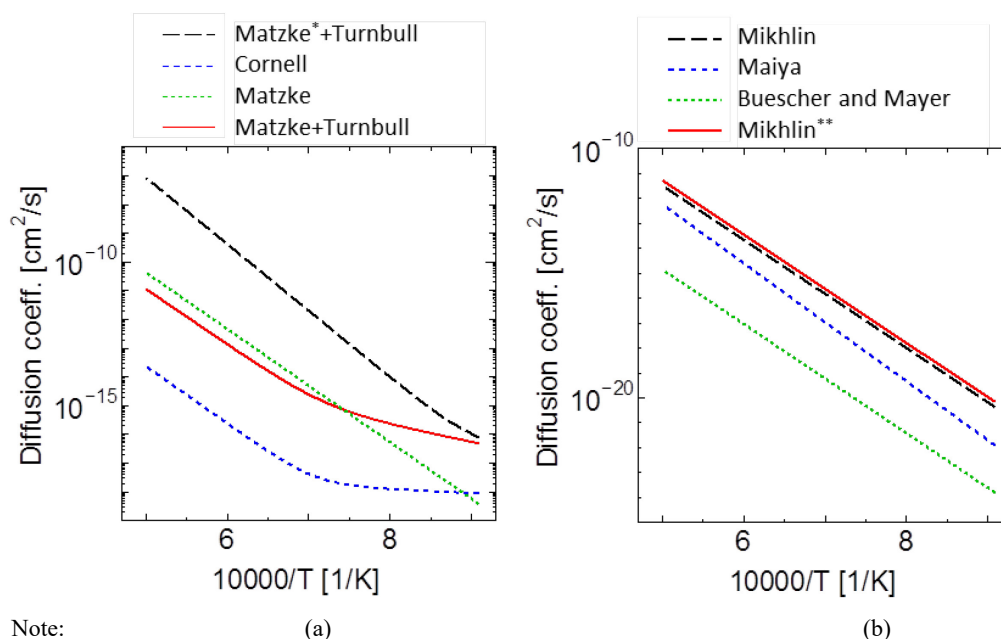
Note: (* The term of thermal diffusion given in [2] is different from that given in [1] (and Model-1 and -3), though both citing Matzke's results (see Figure C.5(a)).

Figure C.4. Fractional fission gas releases from intragranular region to grain boundary (GB) as a function of irradiation temperature after 4% burnup from HEDL data, and simulation results obtained by using Model-1, -2 and -3.



As an example, Figure C.4 compares the fractional FGRs from intragranular region to grain boundary as a function of irradiation temperature after 4% burnup from HEDL data and the simulation results obtained by using Model-1, -2 and -3. Although rather lower bubble diffusion coefficient than the original work [2] was adopted simply due to the reason of numerical stability, Model-2 agrees quite well with the experimental data. On the other hand, while a model equivalent to Model-1 was claimed in the original work [1] to give good agreement with the experimental results, our simulation with Model-1 is biased to give significantly lower FGR than the original work [1], in spite of almost the same model selection. We hence need to keep in mind that the complexity of the model of fission gas behaviour may result in some implicit bias in any implementation in [1] or [2], and/or ours. In consideration of the reproducibility of simulation seen in Figure C.4, our current implementation appears close to that of the preceding study [2]. Hereafter, based on our implementation and Model-1 to -3, key issues which should be considered in the modelling of FGR are discussed by comparing the properties of components used in these FGR models.

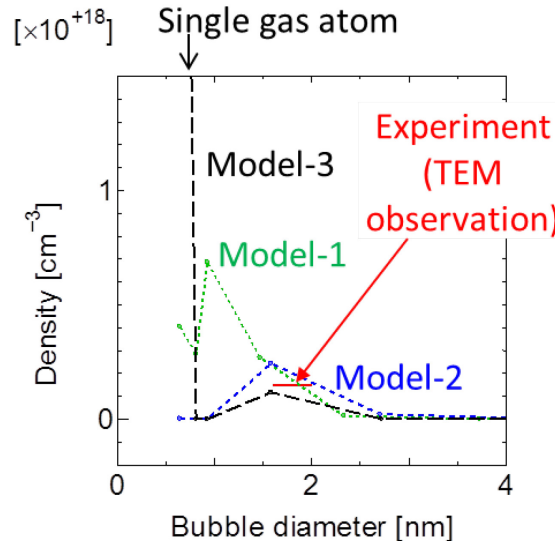
Figure C.5. Diffusion coefficients for (a) single gas atoms and (b) gas bubbles containing two gas atoms employed in Model-1, -2 and -3. A few other correlations are plotted together for comparison.



The important difference between Model-1 and -2 is in the diffusion coefficient. As shown in Figure C.5, the correlations adopted in Model-2 give 2-4 order higher diffusion coefficients than those usually adopted as intrinsic diffusion coefficients. A Model like Maiya's or Mikhlin's gives high bubble diffusion coefficients mainly because they assumed significant contribution of bubble migration via surface diffusion mechanism in bubble. This point seems a drawback of Model-2 from a physical point of view, because the surface diffusion mechanism which drives bubble migration has not been confirmed well by experimental studies.

Model-3 was intended to reproduce the results obtained by HEDL as much as possible without adopting surface diffusion mechanism. While Model-3 shows a reasonable prediction as seen in Figure C.4, the diffusion models used are quite similar to those used in Model-1. Instead, the coalescence rate in Model-3 was assumed to be lower than those in Model-1 and -2, and a model parameter of bubble nucleation model was tuned within its uncertain range [1]. This alternative configuration was validated by performing additional simulations of other irradiation tests where bubble size distribution had been identified by TEM observation [4]. Figure 3 shows bubble size distribution in a fuel specimen after pre-irradiation up to 2.5×10^{25} fission/m³ followed by annealing at 1 500 °C for 6 hours and irradiation at 1 200 °C for 2 hours. After final irradiation process, it was observed that small fraction of produced fission gas was retained as bubbles with diameter of about 1.8 nm and other part of fission gas was believed to be re-solved in the fuel matrix. In these three models, only Model-3 captured the feature found in the experimental observation; it gives a small peak at about 1.5 nm and a large peak of single gas atom density in Figure C.6.

Figure C.6. Bubble size distribution in a fuel specimen as a function of bubble diameter after pre-irradiation up to 2.5×10^{25} fission/m³ followed by annealing at 1 500 °C for 6 hours and irradiation at 1 200 °C for 2 hours [4], and simulation results obtained by using Model-1, -2 and -3.



We have proposed an alternative configuration of component models for the new FGR model as a valid option that reasonably explains the experimental results without assuming predominant contribution of bubble migration by surface diffusion. However, there seem to be limitations in terms of the modelling of FGR only by the concept of rate equation in order to maintain consistency with experimental results, etc. For establishing more physics-based modelling, it is considered that the contribution of meso- and/or micro-scale studies is important: they will be able to provide key information to support the above discussion. As a basis of FGR model configuration for a fuel performance code, it may be proper to use such microscopic properties of fission gas as the mobility of single gas atoms and gas bubbles and influential factors on the effective rate of coalescence between single gas atoms and gas bubbles.

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Development status of fuel module for simulation of LOCA and RIA in KAERI

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Extended Abstract

Introduction

The study of fuel behaviour under accidental conditions is a major concern in the safety analysis of the pressurised water reactors (PWRs). In particular, the consequences of reference accidents (or design-basis accidents, DBA) such as loss-of-coolant accident (LOCA) and reactivity-initiated accident (RIA) have to be investigated and quantified in comparison to the related safety criteria already defined, in order to prevent from severe core damage that could result from fuel rods failure, fuel ejection into coolant, loss of core coolability and fission products release into the primary circuit. Those criteria have been established in the 70s on the basis of several experimental programmes performed with fresh or low burnup irradiated fuel.

However, since the early 90s, economic concerns led utilities to consider the increase of the average burnup of the fuel subassemblies and the use of new types of fuel and cladding materials, in view of optimising the fuel management. At the present time, the increased industrial competition and constraints result in more aggressive conditions for the fuel (higher burnup, higher power, load follow...) and create incentive conditions for the development of advanced fuel designs with improved performance (new fuel types with additives, cladding material with better resistance to corrosion...). These long-anticipated developments involved the need for new investigations of irradiated fuel behaviour under reference accidents in order to check the adequacy of the current criteria, evaluate the safety margins, provide new technical bases for modelling and allow an evolution of these criteria.

Recently, revision of ECCS acceptance criteria (10CFR50.46c) will be performed in Korea. In the revised criteria, safety analysis code system should calculate fuel behaviour models. For LOCA, the fuel behaviours to be considered in safety analysis code system can be cladding material properties as function of burnup, inner-side oxidation of cladding, breakaway oxidation, FFRD (fuel fragmentation, relocation and dispersion) and thermal resistance of oxidation and CRUD layer. For RIA, the related criteria also will be revised with fuel behaviour models.

Therefore, KAERI has been developing new methodology of safety analysis code system that incorporates the best-estimated fuel module for rule revision. For LOCA, we are developing a fully coupled safety analysis code system with fuel module. As the first step, the modified FRAPTRAN (so-called S-FRAPTRAN) will be embedded into safety analysis code system (MARS-KS). As the following step, KAERI's fuel module based on finite-element method (FEM) will be developed and the developed fuel module in multi-dimension also will be implemented into the three-dimensional thermal-hydraulic code system of KAERI (CUPID).

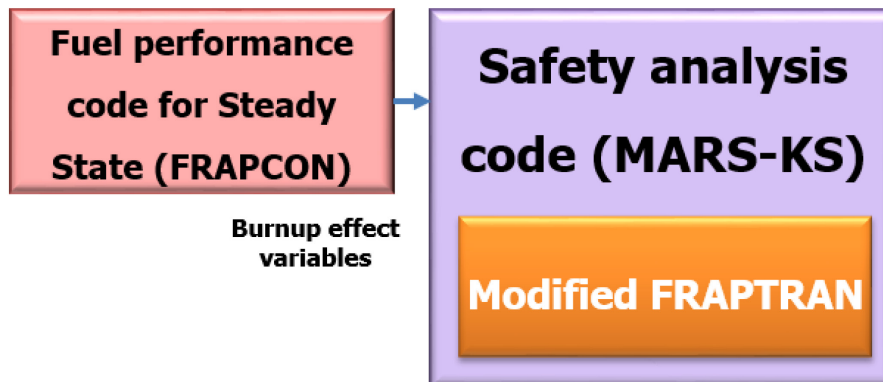
In the case of RIA, the development of the fuel module will begin late in comparison with LOCA because fuel behaviours during RIA are not fully understood and more in-pile experiments for RIA should be made first. Difficulties of fuel-behaviour simulation leads to more effort to develop the fuel module. One of the failure mechanisms of fuel during RIA is known as pellet-cladding mechanical interaction (PCMI), so-called NUFORM3D, for PCMI simulation since 2013. The NUFORM3D which KAERI developed based on

three-dimensional FEM was implemented into FRAPCON3.4 to simulate the stress and strain with in-reactor conditions.

Development of the coupled FRAPTRAN with MARS-KS

To apply fuel behaviour into safety analysis code system, fuel code and thermal-hydraulic code should be coupled. So far, a few coupling methods such as one way coupling, two way based on script has been tried. However, the previous coupling methods faced inherent limitations. To overcome previous methods, fuel models should be embedded into safety analysis code system. For the fully coupling, FRAPCON results should be applied into the coupled code system because the burnup effects of fuel should be considered when the fuel models for transient are calculated. Therefore, the coupled MARS-KS, which is audit code system owned by KINS, with FRAPTRAN take an input which FRAPCON calculates in same manner as stand-alone FRAPTRAN methodology. Instead of heat structure in safety analysis code system, best-estimated fuel module, modified-FRAPTRAN, will be called by main subroutine. It will be expected that the modified-FRAPTRAN calculate the thermos-mechanical behaviour of fuel with the given T/H boundary conditions at current time step as shown in Figure C.7. In addition, all variables of modified-FRAPTRAN can be shared with safety analysis code system.

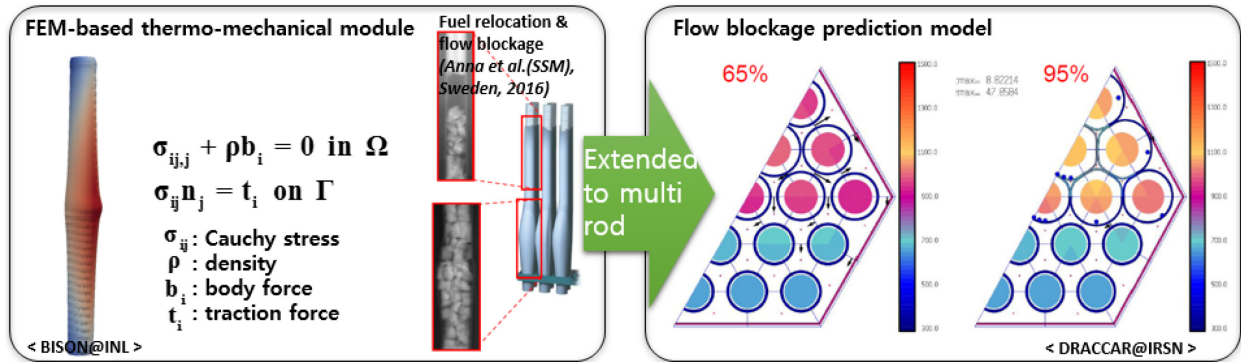
Figure C.7. Schematic diagram of the coupled safety analysis code with fuel module



Development of new fuel module with cupid

Thermomechanical models of existing fuel performance code employ the lumped methodology, which has limitations for the simulation of fuel behaviour. Therefore, recently the performance codes have been developed based on FEM in multi-dimension. We are going to develop the fuel modules based on FEM to simulate the fuel behaviour during LOCA and the developed fuel module will be implemented to thermal-hydraulic (T/H) code system (CUPID). In KAERI, three-dimension T/H code system, so-called CUPID, has been developed. As shown in Figure C.8, for the first phase, fuel module of single rod in multi-dimension will be developed and implemented into CUPID. And then, for the next phase, fuel module of multi-rods will be developed to simulate the flow blockage when the ballooning occurs. Concurrently, out-of-pile experiments are also planned in order to validate fuel models in multi-dimension such as ballooning/burst and FFRD.

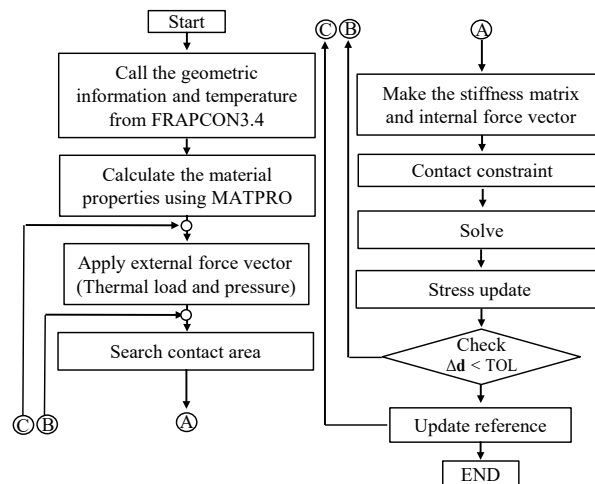
Figure C.8. Development plan of FEM fuel module for LOCA



Development of NUFORM3D for PCMI simulation

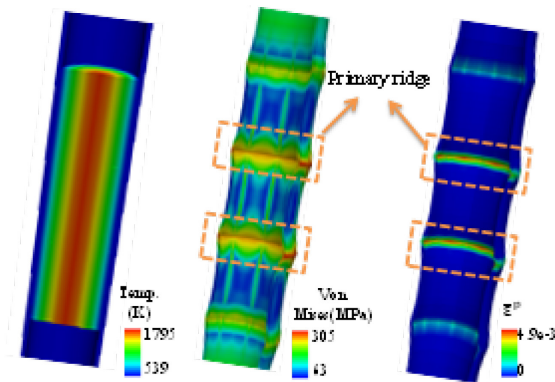
In KAERI, NUFORM3D has been developed to calculate the stress and strain in three-dimension for the simulation of a PCMI. In this module, the deformation of the fuel rod includes the elastic, plastic and thermal strain. In terms of elasto-plasticity, it is assumed that the isotropic hardening von-Mises yield condition (J-2 flow) applies to the cladding, and the deformation of the pellet has an elastic behaviour.

Figure C.9. The coupled NUFORM3D calculation flow



As shown in Figure C.9, the NUFORM3D calculates the thermal strain and contact between the pellet and cladding considering plastic deformation. For this reason, NUFORM3D could show the effect of thermal strain and plastic deformation of the cladding as a three-dimensional description instead of FRAPCON-3.4. Therefore, the NUFORM3D module calls the geometric information from the FRAPCON-3.4 code except for the plastic strain and thermal strain to calculate the thermal expansion and elasto-plastic deformation.

Figure C.10. Temperature of the fuel rod, von-Mises stress and effective plastic strain of the cladding



In Figure C.10, it was found that the NUFORM3D simulates PCMI in three-dimension with FRAPCON-3.4 successfully. Due to the hourglass deformation of pellet during a power ramp, the primary ridge of cladding occurs, as shown in Figure C.10. In addition, the maximum stress and plastic strain can be observed near the primary ridge region. NUFORM3D, which is able to calculate the elasto-plastic and contact behaviour in three-dimension.

Modelling of irradiated oxide fuel behaviour and fission-product releases under transient and severe accident conditions by the fuel performance and safety code SFPR

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Extended Abstract

The SFPR code [1] for mechanistic, multi-scale modelling of single fuel rod behaviour under various regimes of light water reactor operation (normal and off-normal, including severe accidents), has been developed at IBRAE during the last decade. The code was designed by coupling of the two stand-alone codes MFPR [2] (for mesoscale modelling of irradiated UO₂ fuel behaviour), developed in co-operation with IRSN (France) and SVECHA/QUENCH [3] (for macro-scale modelling of Zr cladding thermo-mechanical and physico-chemical behaviour), developed in co-operation with KIT (Germany).

Basic processes in irradiated fuel simulated by the code

The code includes the following models describing behaviour of irradiated fuel:

- An advanced model for actinide and FP transformations based on so-called two-component representation of reaction rates which more accurately takes into account reactions with resonance neutrons.
- Thermochemical model of oxide fuel.
- Intergranular FP diffusion with the boundary conditions determined by local thermochemical equilibrium at the 'solid solution – intergranular bubbles' interface.
- Interaction of FP with crystal defects (vacancies, interstitials, dislocations) and intragranular bubbles; evolution of the fuel defect structure.
- Formation of solid (condensed) phases – precipitates at the 'solid solution – intergranular bubbles' interface; molecular composition of the gas phase (in the intergranular bubbles).
- Evolution of intergranular porosity.
- Model for coalescence of grain face bubbles.
- Model of formation and evolution of grain edge channels and FP release to open porosity.
- Effects of radioactive transformations on FP transport and release.
- Oxygen diffusion through a fuel pellet in temperature and fission rate gradients.
- Fuel oxidation/reduction in various gas environments (in accident conditions); FP and fuel evaporation and releases from the pellet surface.
- FP release to the fuel-cladding gap and their partial condensation in the gap; FP release from defective fuel rod (during normal operation conditions).

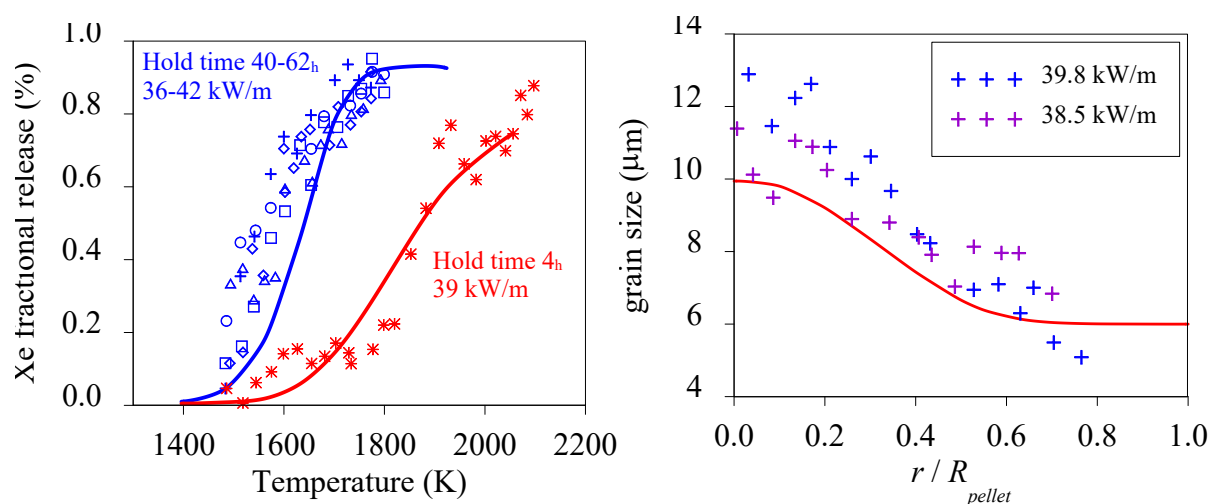
The main feature of the code is self-consistent consideration of the listed problems to take into account their interference and mutual impact.

Validation of the SFPR code under off-normal conditions

Transient conditions (by example of Bagger's test, 1994)

The power ramp tests [7] have been carried out in Risø Project to explore UO₂ fuel performance at increasing burnup levels (~4.7% FIMA) for power increases (transients) late in life. In these tests the transient terminal power ranged from 16.9 to 44.7 kW/m, the fuel centreline temperature and the fission gas pressure in the plenum being simultaneously measured. Post-test examinations of the specimens allowed plotting fractional gas releases and grain growth as functions of terminal local fuel temperature. The SFPR simulations are illustrated in Figure C.11.

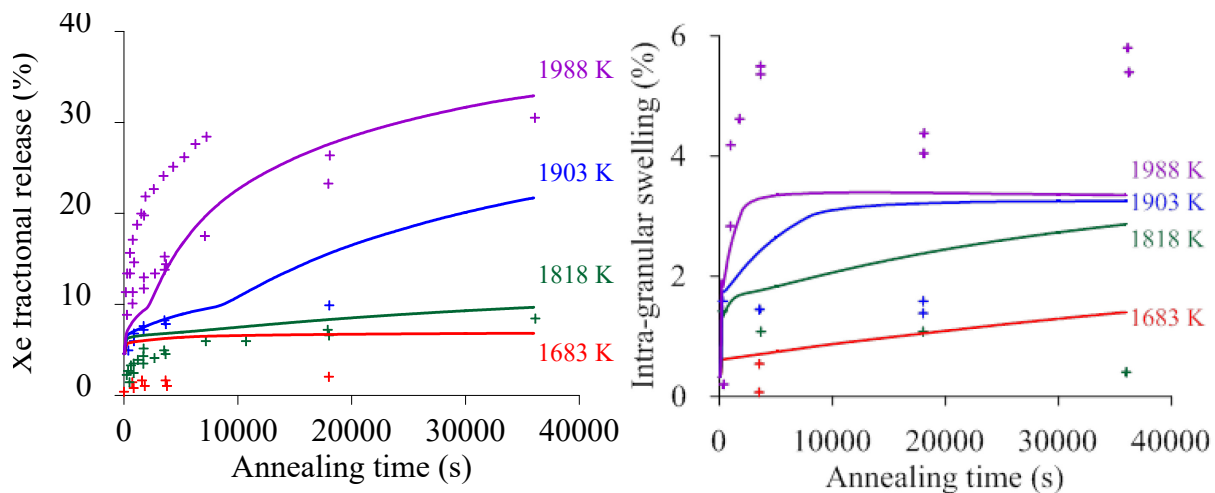
Figure C.11. SFPR simulation of Xe release and grain size radial profile under transient conditions of the Risø reactor ramp tests; markers are the data from Ref. 7 (C. Bagger et al, 1994)



Annealing conditions (by example of Zacharie's test, 1998)

In the experiments [6] the UO₂ samples irradiated in PWR up to burnup of 25 GW d t⁻¹ were subjected to thermal treatment in a laboratory furnace at temperatures from 1 403 K to 1988 K for duration between 5 minutes and 10 hours. The time dependence of fission gas release and fuel swelling were measured at each temperature. Comparison of SFPR results with the experiment is given in Figure C.12.

Figure C.12. SFPR simulation of fission gas release (the left panel) and intragranular swelling (the right panel) under annealing conditions; markers are the data from Ref. 6 (Zacharie et al, 1998)



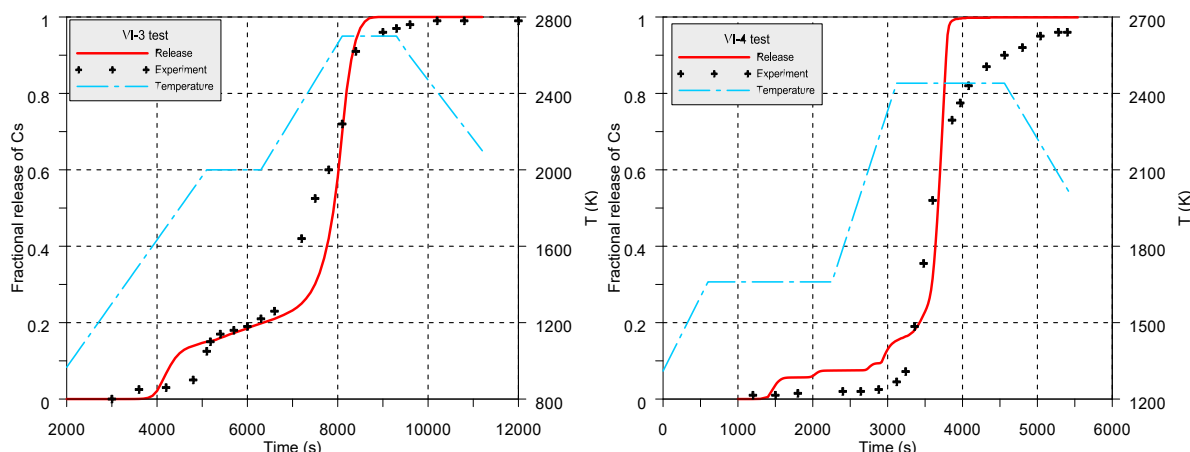
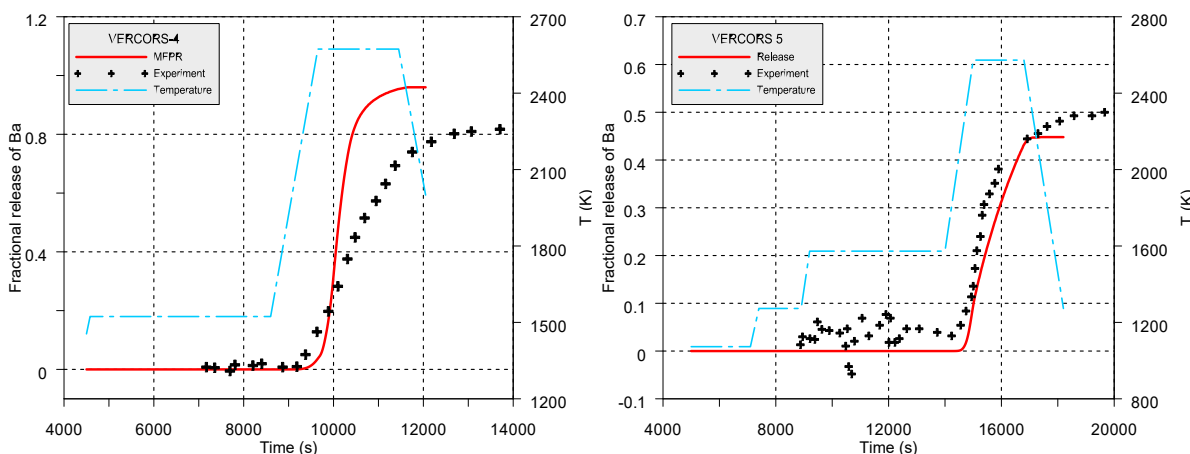
Modelling of the release kinetics of chemically-active elements under severe accident conditions

The SFPR performance is illustrated by modelling of annealing tests VI 1–6 and VERCORS 1–5.

A series of annealing tests were conducted in vertical induction (VI) facility at ORNL [8] with the high burnup LWR fuel. In these tests the fuel specimens consisted of 15-cm sections cut from full-length rods. The temperature history of the tests included heating with the rate of ~ 0.3 – 1 K/s (with intermediate plateaus $T \sim 1700$ – 2000 K in VI-3–VI-6), annealing at the high-temperature plateau with T varied from 2300 K to 2700 K in different tests. In tests VI 1–3, annealing was performed in oxidising conditions of H_2O/He mixtures, while tests VI-4 and VI-5 used reducing atmosphere of hydrogen; in VI-6, the H_2O/He mixtures was changed to H_2/He approximately at the middle of the high-temperature plateau.

The VERCORS test series of annealing experiments was carried out at CEA-Grenoble [9] in order to investigate the release behaviour of fission products in the conditions of great fuel deterioration at high temperature. For each test the fuel sample comprised a small section of a spent PWR fuel rod consisted of three pellets in their original Zr cladding. During the tests the fuel temperature was increased with the rate of about 1 K/s through a series of plateaus to the highest value ranged from 2100 to 2600 K. The test was made under total pressure of about 1 atmosphere at a gas flow of steam/hydrogen mixture with the following compositions at the high-temperature plateau: mixture H_2O/H_2 in VERCORS-1,2,3 and 5, H_2/He in VERCORS-4.

In the both series of experiments, the release kinetics and total releases of wide set of fission products were measured. The results of SFPR modelling of FP release kinetics in comparison with experimental data are illustrated in Figure C.13 – release of caesium in oxidising VI-3 and reducing VI-4 tests, and in Figure C.14 – releases of Ba in VERCORS-4, 5.

Figure C.13. SFPR modelling of Cs release kinetics in VI-3 (the left panel) and VI-4 (the right panel) tests**Figure C.14. SFPR modelling of Ba release kinetics in VERCORS-4 (the left panel) and VERCORS-5 (the right panel) tests**

Comparison of calculations of total FP releases with the experimental data through both set of tests is presented in Table 1 which shows the order of magnitude deviation (OMD) between measured and calculated fractional release:

$$OMD = \log_{10} (\text{Calculated Release} / \text{Measured Release})$$

Table C.2. Order of magnitude deviations between calculated and measured values of relative FP releases in tests VI and VERCORS

Element	VI-1	VI-2	VI-3	VI-4	VI-5	VI-6	VR-1	VR-2	VR-3	VR-4	VR-5
Xe	0.12	–	-0.06	-0.09	-0.06	-0.03	0.09	0.27	0.01	-0.02	-0.03
Cs	0.04	-0.03	0.00	0.02	0.00	0.02	-0.20	-0.05	-0.01	0.03	0.03
I	0.31	0.38	0.10	0.03	0.15	0.16	0.38	0.27	0.12	0.05	0.02
Mo	0.21	-0.06	0.09	-0.47	0.19	0.56	–	0.01	0.26	0.03	0.01
Ru	–	–	0.43	–	–	–	–	–	1.08	-0.97	-0.04
Ba	–	-0.24	0.21	0.55	0.12	-0.12	-0.48	-0.50	0.21	0.08	-0.09
Sr	–	–	0.52	–	0.47	-0.86	–	–	–	1.09	-0.21
Zr	–	–	–	–	–	–	–	–	–	-1.02	-0.23
La	–	–	–	–	–	–	–	–	-0.36	-0.95	-0.11
Ce	–	–	1.45	0	0.39	–	–	–	–	-0.79	-0.11
Eu	–	–	2.75	-0.06	0.24	-2.31	–	–	-0.53	0.05	-0.10
Sb	0.25	-0.03	-0.06	1.00	0.65	-0.10	1.12	0.06	0.03	-0.12	-0.08
Te	–	–	-0.04	0.29	0.06	0.13	1.23	0.22	0.04	-0.04	-0.04

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Granular simulation of fuel relocation and dispersal in LOCA conditions

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Extended Abstract

Summary

The occurrence of extended fuel relocation and dispersal at high burnup was evidenced in the Halden in-pile LOCA tests – IFA-650 series. Several experimental programmes have been launched worldwide in the wake of these observations, to better understand the mechanisms leading to fuel relocation and dispersal. Achieving representative experimental conditions remain challenging: while separate effect studies may be performed on small quantities of active material, integral out-of-pile tests relying on mock-up materials fail to catch the entirety of the mechanisms at play. The complexity of the fragmentation pattern and that of the cladding deformation requires integral in-pile tests!

The fall of fuel fragments and their collisions are, conceptually, simple events, which can be modelled analytically; the complexity lies in the amount of particles – and collisions – involved and requires computer simulations. Discrete element methods (DEM) simulations at the granular level may therefore provide an alternative insight on the phenomena underlying fuel relocation and dispersal during LOCA accidents. Using such techniques, we modelled the fall of fuel fragments in a rapidly expanding cladding (balloon zone). We evaluated the packing density in the ballooned area in the range 50 to 60%, in good agreement with the most recent experimental measurements. The methodology adopted has also shown the capabilities of addressing fuel dispersal through the burst and opens the way for linking the amount of dispersed fuel to the balloon and burst geometrical characteristics.

Methodology

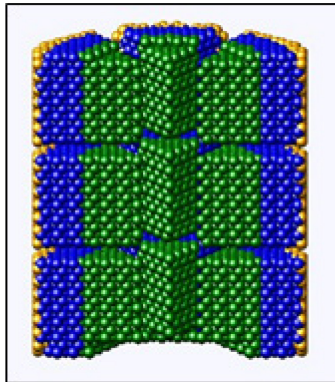
The material is discretised as a set of (spherical) particles whose trajectories are followed as collisions occur. A granular simulation algorithm is present in the LAMMPS code [1], known in the atomistic simulation community for molecular dynamics applications: indeed, except for the length and time scales, atom and granular particles interaction show high similarities and the system evolution can be tracked with the same algorithms. Interactions between two spherical granular particles are typically pairwise; the Hertz model is used in this work. It is based on elastic theory of deformation, so that the force between two spherical particles is not simply a linear function of their “overlap” but rather depends on the overlap area [2]. Some specificities have to be added, which are usually not present in atomic-scale simulations: friction forces.

The simplest particle shape consists of spheres; more complex shaped bodies can be considered by building them as rigid agglomerates of these simple elements. These agglomerates have, as a whole, only translational and rotational degrees of freedom; the total force and torque are computed from the forces acting on each individual particle, excluding internal interactions which have no resulting effect. Various descriptions were investigated [3]; the final model consisted of a coarse pellet fragments shape combined with small particles, cf. Figure C.15, to simulate the high burnup structure (HBS) region generally observed at high burnup in the pellet periphery [4]. The fuel fragments are discretised on the basis of a hexagonal close packed (hcp) arrangement of 0.05 cm diameter spheres. The choice for the size was the results of a compromise between geometrical representativeness of the HBS particles and the computing time.

The cladding may be described through simple plane and cylindrical wall implemented in LAMMPS; however, these simple models are not sufficient to reproduce the complex shape of the balloon. The complex wall geometries needed to describe the balloon and the burst can be approximated by a configuration built from spherical elements, in the same way as the fuel fragments were constructed. Overlapping of the spheres was considered, in order to smooth as much as possible the cladding wall roughness. This flexible approach was also further exploited to create “moving walls” and to model explicitly the cladding deformation during the process of ballooning. Burst is then simulated by removing particles, creating an opening in the cladding wall.

In the simulations reported here, a burst opening of 0.5 cm x 2 cm is considered, as shown on Figure C.16. Fuel pellets are described as 36 coarse fragments in the central part (6 radial cracks; 1 circumferential crack and 2 horizontal cracks); loose particles are considered in the periphery in order to simulate the HBS structure.

Figure C.15. Granular model of a pellet as coarse fragments (green and blue) and small isolated particles (yellow) to model the peripheral high burnup structure³

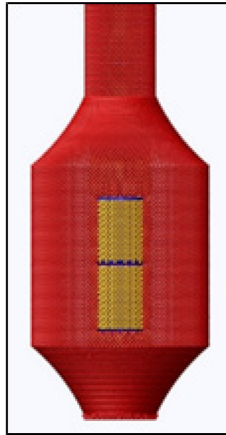


Note: Only half a pellet is shown for clarity. For the fragments, one assumes 6 radial fractures (centre to periphery), one circumferential fracture (separation between green and blue fragments) and two transversal cracks. A single pellet then contains around 7 500 spheres of 0.05 cm diameter.

Reproduced from [3] with permission.

³ All figures in the abstract “Granular Simulation of Fuel Relocation and Dispersal in LOCA Conditions” are reprinted from the Journal of Nuclear Materials, Vol 478, K. Govers and M. Verwerft, “Discrete element method study of fuel relocation and dispersal during loss-of-coolant accidents”, Pages 322-332, Copyright 2016, with permission from Elsevier, www.sciencedirect.com/journal/journal-of-nuclear-materials.

Figure C.16. DEM model for the cladding (red spheres) and the fuel (blue / green spheres for the coarse fragments; yellow spheres for the loose HBS particles).

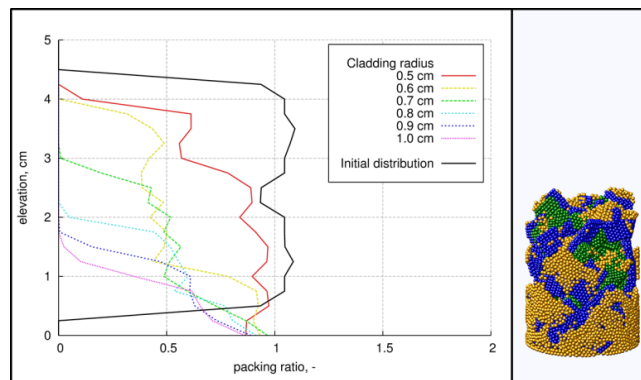


Note: The view shows the cladding deformation in the balloon area and the burst opening in the cladding. Reproduced from [3] with permission.

Results

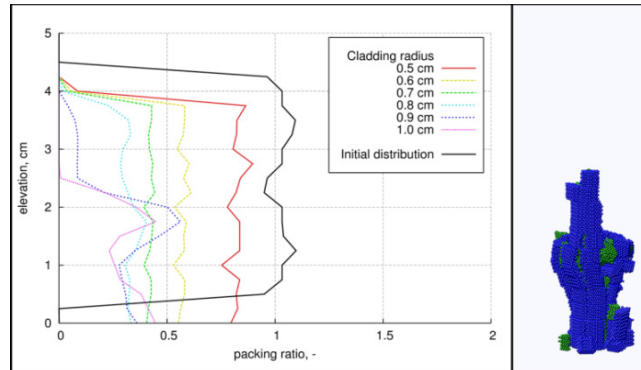
The packing ratio following to relocation in the balloon zone was investigated. Relocation is initiated by modelling the fall of the fuel stack – here, limited to 4 pellets to accumulate a sufficient amount of fuel in the balloon, while limiting the computation time – over a height of 0.5 cm. The influence of fall height, which might affect the relocation pattern, was not studied. When only pellet fragments were considered (no HBS), little is observed besides a global drop of the column: the fragmented fuel column does not collapse, but keeps more or less its original shape after the fall, as can be observed in Figure C.18. The influence of the HBS region is then clearly seen in Figure C.17: a full collapse of the column is observed, even at small cladding deformation, which is quite in line with experimental observation at low to medium burnup [5] and high burnup [6]. The packing ratio in the balloon seems to converge to a value between 50 and 60 %, in good agreement with experimental observations [6, 7].

Figure C.17. (left) Packing fraction of the fuel fragments in the balloon in presence of a HBS-like structure



Note: Balloons larger than 0.7 cm show extensive relocation, with a packing ratio between 0.5 and 0.6. (right) Snapshot of a simulation for a clad radius of 1 cm (100% hoop strain). Reproduced from [3] with permission.

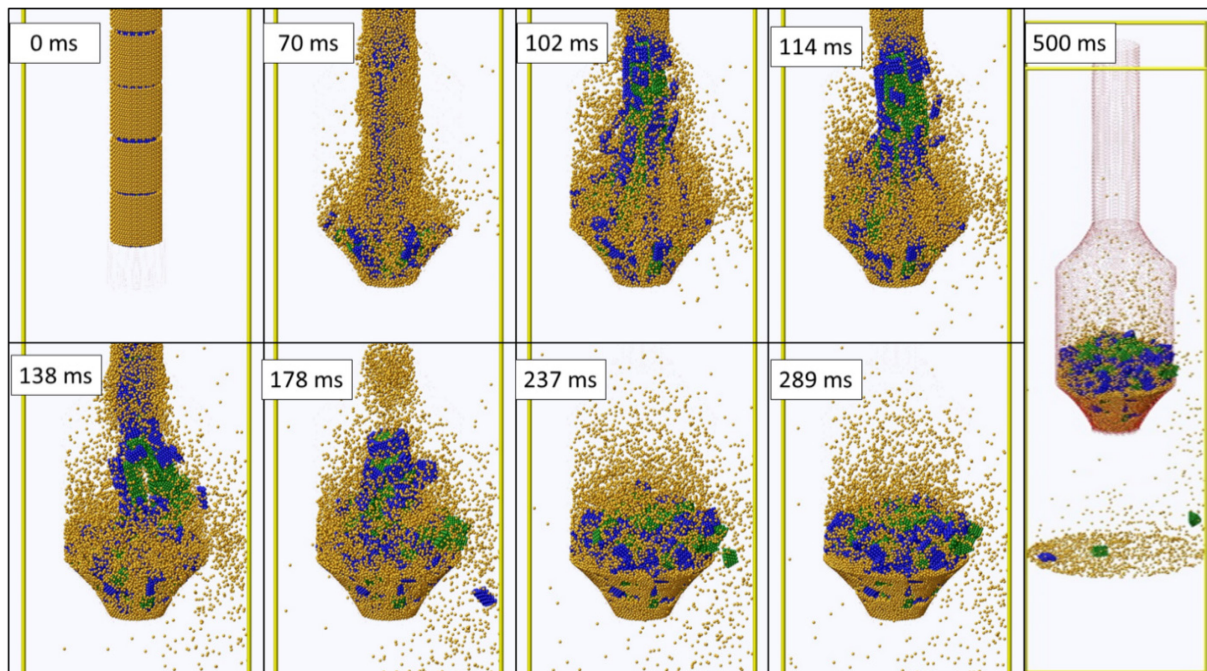
Figure C.18. (left) Packing fraction of the fuel fragments in the balloon in absence of HBS-like structure



Note: The decrease of the packing ratio with increasing cladding radius translates the balloon volume change. (right) Snapshot of a simulation with a balloon radius of 1 cm (100% hoop strain).
Reproduced from [3] with permission.

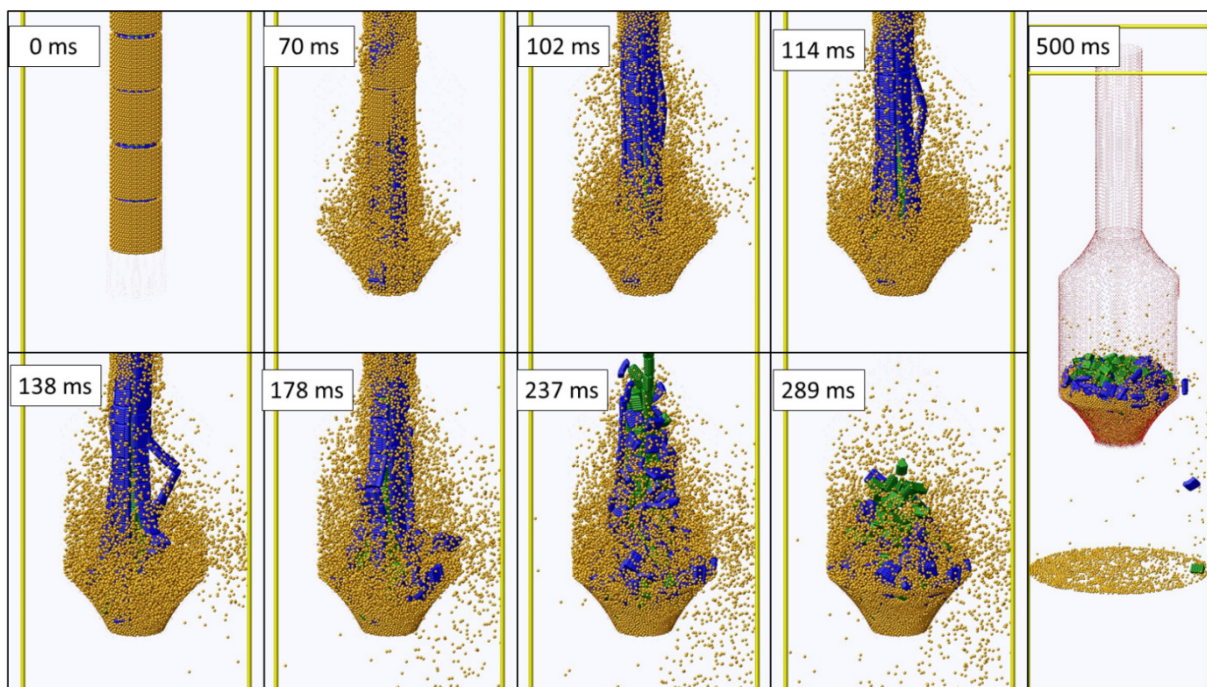
Simulations were then performed to investigate dispersal through the cladding burst. We report here preliminary simulations where, on the one hand, rough fragment surfaces are implemented (no overlap of the base elements in the rigid bodies) and, on the other, smooth surfaces are obtained by allowing overlap of the particles constituting each rigid body, then at the expense of computing time. During the course of the simulation (see Figure C.19 & Figure C.20), fragments and HBS particles progressively fill the balloon. A small amount of types of fragments can be seen escaping through the burst, of which a relatively larger fraction of finer particles. The amount is affected by the length of the falling fuel stack, to the burst dimensions and its location. A burst located at the bottom of the balloon, as well as a longer fuel stack, favour dispersal of larger fragments. Further analyses will be needed to derive a relation between the dispersed-fuel amount and the balloon and burst geometrical parameters.

Figure C.19. Snapshots at different time intervals of the simulation with rough fragment surfaces (non-overlapping spheres). Fuel relocation and dispersal are observed for a falling 8 cm long fuel stack.



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Figure C.20. Same series of snapshots for the simulation with smooth surfaces



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Annex D. Abstracts for Session 3, Nuclear-fuel modelling in support of performance and safety improvements during normal operating conditions

Fuel assembly bowing during normal operation

C. Durand (EDF, France)

The DAMAC tool operated by EDF provides easy and complete measurements of the bowing of all fuel assemblies during the core unloading. The measurement data clearly illustrate the main impact of hydraulic flows in the core, leading to symmetric deformation core phenomena. However, in the top of the core, in the direction not impacted by the hot legs suction, an asymmetric deformation can be observed due to contact forces between neighbouring assemblies; that situation can induce significant increased rod drop times and difficulties of assemblies handling. The ability of the structure to resist to creep under irradiation can lead to lower residual deformations. Deployment of reloads of suitable fuel assembly design shows encouraging results.

On effects of high-temperature fuel restructuring during the steady-state irradiation in the context of selected fuel design criteria

G. Khvostov (PSI, Switzerland)

Extended Abstract

It has been well known for a long time [1][2] that a high-temperature irradiation of uranium-dioxide fuel results in local restructuring of the fuel in the central pellet zone, where certain temperature is exceeded, viz.: 1 350-1 400 °C for equiaxed-grain growth, and 1 600-1 700 °C for columnar grain structure formation. These processes are accompanied by sweeping-out of as-fabricated pores and increase in local fuel density, which eventually results in a formation of the void in the centre of the pellet.

The occurrence of high-temperature restructuring, resulting in considerable effects on fuel rod behaviour, is unlikely during commercial irradiation in LWRs, because of a relatively low linear-heat-generation rate (LHR) at normal operation. Consequently, these effects are often neglected by industrial fuel performance codes. For example, corresponding simulation was, until recently, out of the scope of the fuel behaviour analysis by the advanced FALCON code, available at PSI [3].

However, licensing calculations for justification of fuel reliability usually deal with a hypothesised challenging power history, referred to as Thermo-Mechanical Operational Limit (TMOL), for which the high-temperature fuel restructuring and its consequences are expected. Corresponding calculations would be more adequate given the effects in question are taken into account. Specifically, the presence of a central void and the increase in local density will result in a decrease in peak fuel temperature and mitigation of the PCMI.

The GRSW-A model, integrated into the FALCON code, includes a model for high-temperature fuel restructuring, which was used as basis for evaluation of the central void volume/diameter as function of time during assumed high-power irradiation:

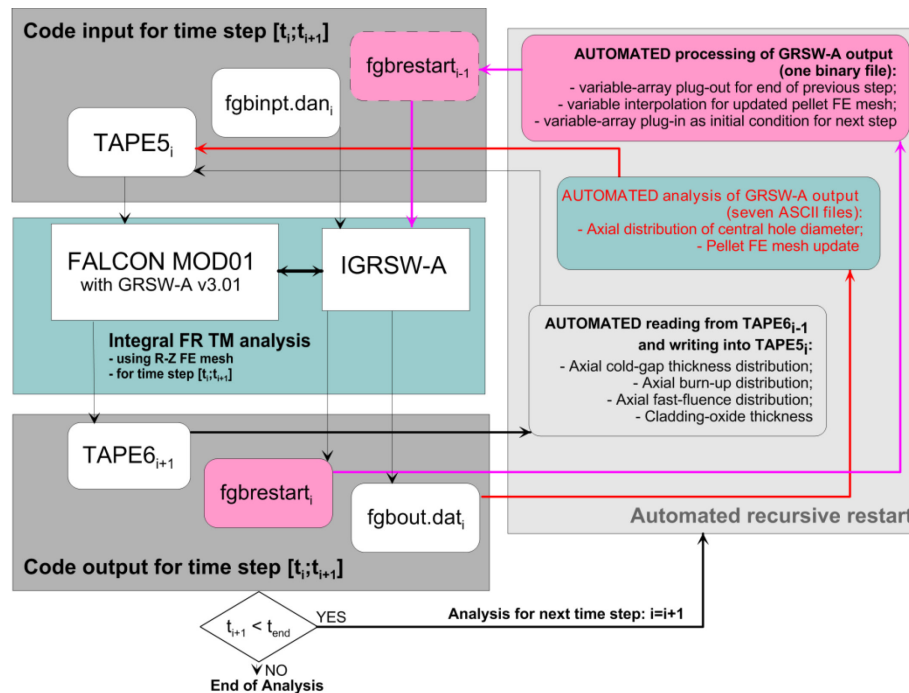
$$R_{hole} = R_{pellet} \left[k_a P_{as-fb} \sum_{i=1}^{N-zones} \varepsilon_i f_{i-rstr} \right]^{1/2}$$

where R_{hole} is the hole radius, R_{pellet} the pellet radius, P_{as-fb} the stable as-fabricated porosity, ε_i the relative volume ascribed to the i -th node of the radial pellet mesh, f_{i-rstr} the local fraction of the restructured fuel, k_a the anisotropy coefficient.

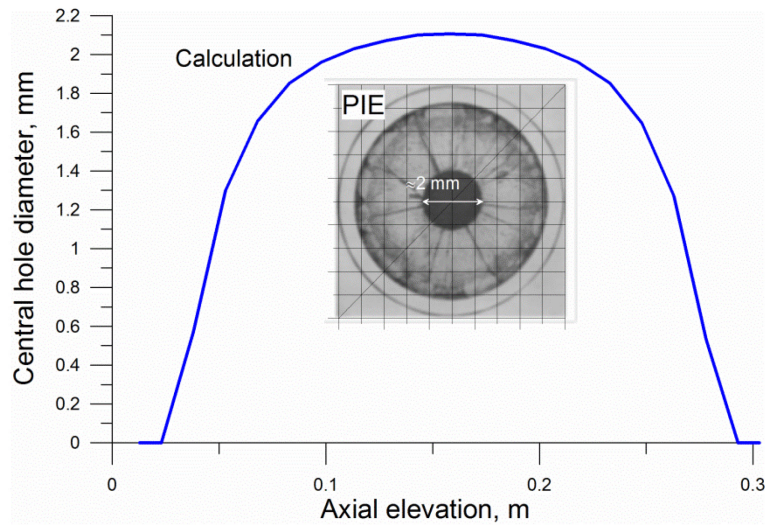
A FALCON-based methodology was developed [4] using a special procedure of the recursive restart of calculation with a periodic update of the finite-element mesh in the pellet, based on the GRSW-A predicted evolution of fuel micro-structure (see Figure D.1). The methodology was verified against the data of a special experiment [2]. In this experiment, a rod with the low-density (82 %TD) MOX (UO_2 - 20% wt PuO_2) fuel was irradiated under high-power conditions (a peak local LHR up to 56 kW/m), which resulted in a formation of the significant central void, as shown in Figure D.2.

Considerable effects of the predicated phenomena on important variables of fuel state, such as fuel temperature, fission gas release, rod internal pressure, stresses and strains in the cladding, are shown as applied to a BWR fuel rod operated along a hypothetical “typical” TMOL to a peak pellet burnup of ~80 MWd/kgU (see selected results in Figure D.3 through Figure D.5).

Including these effects into licensing analysis would suggest a reduction of its conservatism. Moreover, it may eventually result in alternative approaches to optimisation of parameters of rod design and fuel cycles.

Figure D.1. Calculation flow-chart for simulation of integral effects of fuel restructuring**Table D.1. Nomenclature:**

TAPE5	ASCII file containing all input for standard FALCON MOD1
fgbintpt.da	ASCII file containing supplementary input for Integrated GRSW-A analysis, e.g.: parameters of numerical methods, restart mode, GRSW-A model parameters, etc.
fgbrestart	Binary file containing the whole array of time-dependent GRSW-A variables for all integration points of pellet mesh and all time steps.
TAPE6	ASCII file containing all output results of standard FALCON MOD01.
fgbout1.dat ... fgbout7.dat	Seven ASCII files containing extended output results of Integrated GRSW-A for all integration points of pellet mesh and selected time steps, e.g.: spatial distribution of retained gas, grain-size distribution, porosity fractions, etc.
FE	Finite Element
FR	Fuel Rod
IGRSW-A	Version of GRSW-A integrated into FALCON MOD01

Figure D.2. Calculated diameter of central-hole in a MOX-fuel pellet against the PIE data [2]

Reproduced from [5] with permission.

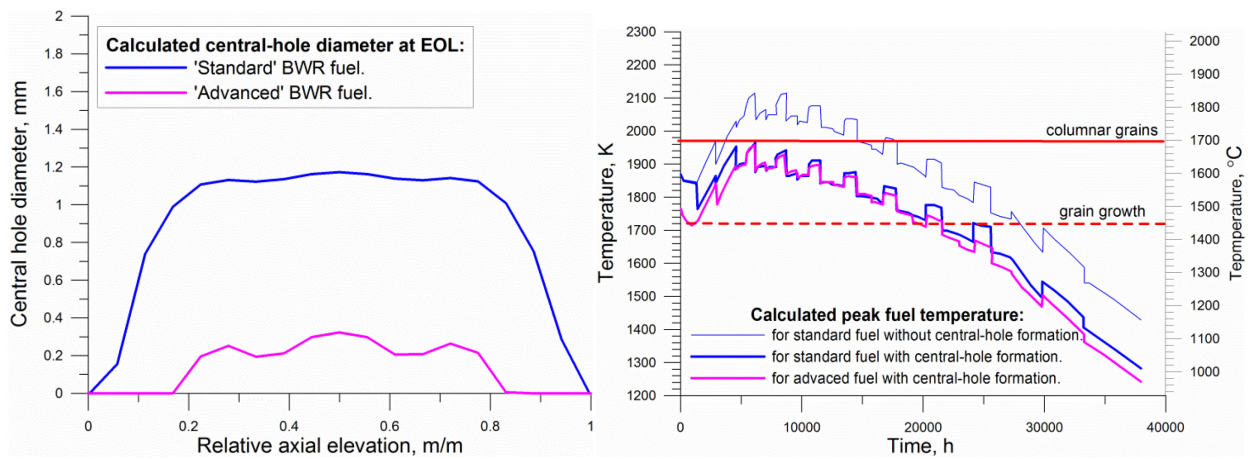
Figure D.3. Effect of the predicted central void (left) on calculated temperature (right) in a high-power irradiated BWR fuel

Figure D.4. Effect of central void on calculated FGR (left) and rod pressure (right) in a BWR fuel rod during high-power irradiation

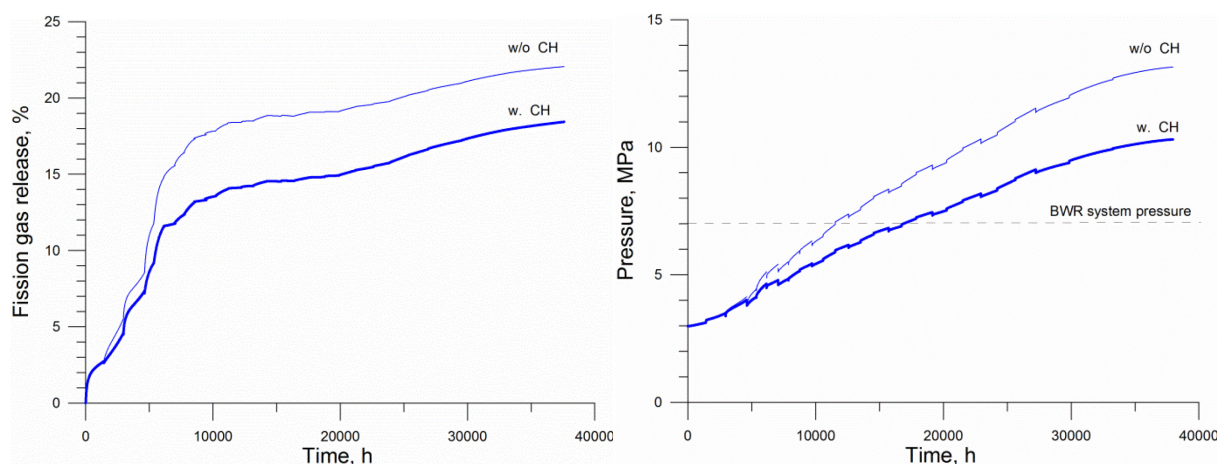
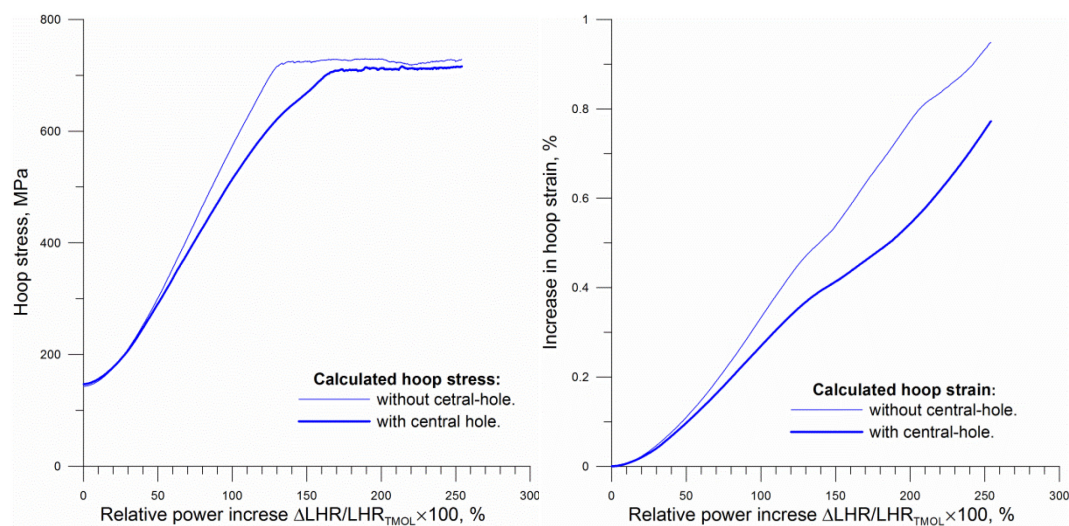


Figure D.5. Effect of central void on calculated cladding- stress (left) and strain (right) during a power ramp from the TMOL level at a burnup of 78 MWd/kgU



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Multiscale modelling of fission gas bubble evolution in UO₂ under nominal operating conditions

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Extended Abstract

The behaviour of xenon (Xe) in nuclear fuel is of critical importance to nuclear fuel performance because the diffusion and precipitation of Xe in fission gas bubbles influences both the amount of fuel swelling and the quantity of fission gas released to the fuel rod plenum [1]. Despite decades of investigation, significant uncertainties exist regarding the underlying mechanisms controlling Xe diffusion, precipitation and release that impact predictions of fission gas swelling and release during both normal operation and transient conditions in accidents. Such uncertainties limit the accuracy of integrated fuel performance models [2]. Most fission gas behaviour models used for fuel performance calculations trace back to the 1957 formulation by Booth [3], the mid-to-late 1960's formulation by Speight and co-workers [4,5]; or the slightly more recent work by Turnbull [6], White and Tucker [7], and Forsberg and Massih [8,9]. These models typically rely on a small number of spatially-independent partial differential equations, or even a single partial differential equation, along with the concept of an effective diffusivity to account for the effect of intragranular fission gas bubbles on the bulk diffusion rate [4]. These models are clearly over-simplifications of the actual behaviour of noble gas within the fuel. Indeed, the dynamics of fission gas bubbles, which form both within the grains (intragranular) and on grain boundaries (intergranular), affects the rate of fission gas diffusion and release, and also determines the fission gas swelling [1, 7,10]. Despite being a key determinant of fission gas effects, which control fuel performance, accurate physically-based models of intragranular bubble evolution are still lacking in current models. Indeed, a recent engineering scale study to assess the impact of the uncertainty associated with fission gas behaviour by Pastore et al. [11] indicated that there is at least a factor of two uncertainty in the current engineering predictions of fission gas release. Also, this uncertainty, combined with the uncertainty in fission gas induced fuel swelling, had a significant impact on predicted fuel-clad deformation. Pastore et al. concluded that “a better characterisation of the parameters through experimental and theoretical research may reduce the uncertainty in fission gas behaviour calculations and in the multiple related aspects of fuel performance analysis” [11]. Thus, there is a critical need to both identify and characterise the diffusive behaviour of Xe on the atomic scale and then use that as the foundation of higher-level models that can integrate that array of competing mechanisms, which in turn depend on irradiation conditions (temperature and fission density), to predict the gas bubble formation and evolution.

This presentation will first introduce a multiscale modelling approach to simulate the behaviour of fission gas and intragranular fission gas bubble populations. We will then review the current status of understanding of Xe diffusion mechanisms, and our recent results to investigate the re-solution behaviour of fission gas bubbles as a function of bubble size and xenon concentration (pressure), and finally show initial results of our cluster dynamics model for xenon bubble density. Our approach to multiscale modelling is based on an information-passing paradigm, which allows us to attack the complex fission gas behaviour problem from both a “bottom-up” atomistic-based approach, as well as from a

“top-down” continuum perspective that focuses on kinetic models of intragranular gas bubble evolution. Simultaneously attacking such complex and interrelated diffusion and gas bubble evolution processes from both an atomistic and a continuum approach will minimise the risk of using just a single approach and further the prospects for scale bridging, or multiscale integration. Our multiscale approach relies on using both large-scale MD simulations, as well as accelerated MD (AMD) simulation techniques and selected DFT calculations to investigate specific mechanisms of Xe and Xe cluster diffusion, as well as Xe re-resolution from fission gas bubbles as a function of size, gas pressure and mass of the fission fragment, which control noble gas diffusion in UO_2 . We then model the spatially-dependent nucleation, growth, possible re-resolution and coarsening evolution kinetics of fission gas bubbles, and ultimately the fission gas release from nuclear fuel, using our Xolotl-fission code. Xolotl is based on the classical reaction-diffusion kinetic theory that defines a defect/cluster by its character, atomic configuration and size (or, more specifically, the number of gas atoms and vacancies contained within the cluster), but not by its spatial position since the theory assumes that the concentration of each cluster is homogeneous through the volume of the sample. Xolotl establishes a partial differential equation for each and every cluster size of Xe, and then models the resulting nucleation, growth and coarsening evolution of the clusters based on defining the governing physics of reaction-diffusion theory, with input on diffusion and gas re-resolution from atomistic modelling.

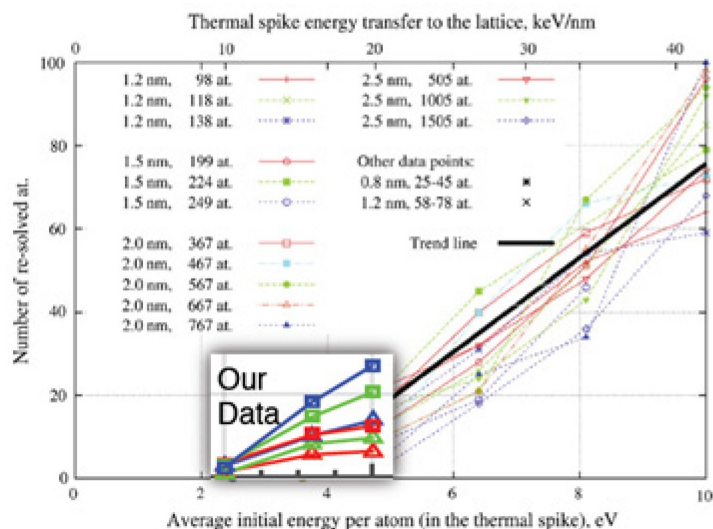
Recent studies have extensively investigated the diffusion mechanisms associated with Turnbull’s model of Xe diffusion through density functional theory and atomistic modelling [12-16]. However, while these studies have shed new light on the behaviour of Xe at the atomic scale, both the thermal/intrinsic and irradiation-enhanced gas diffusion processes are complex and their aggregate behaviour is not easy to capture by atomistic simulations alone. This is because the concentration of radiation-induced defects, as well as the lattice position each Xe atom occupies, must be known to specify the diffusion mechanism and to quantify the Xe diffusivity. The high-temperature, or so-called intrinsic, diffusivity has been predicted with some success, but the lower temperature radiation-enhanced diffusivities have been more problematic [14,15]. The presumed reasons for the discrepancy between predication and Turnbull’s assessment of the experimental data relate to possible diffusion of Xe by a vacancy cluster mechanism. However, calculations indicate that these clusters are not sufficiently mobile to explain the observed diffusion rates. Likewise, interstitial Xe atoms, which can diffuse very rapidly, tend to quickly interact with vacancies and other sinks, and are thus believed to be present in concentrations too low to contribute to diffusion. This raises questions as to what other Xe-defect configurations may exhibit significant mobility at low temperature, and questions our knowledge of the fission-induced vacancy concentrations and the diffusivities of vacancies.

Small fission gas bubbles or extended clusters are known to be present in the fuel but are typically assumed to be immobile based on experiments involving out-of-pile conditions. Recent modelling work has indicated that the most likely diffusional pathway for Xe in the intermediate irradiation-enhanced temperature regime from about 600 to 1 100°C involves interaction and motion with an 8-Uranium, 10-Oxygen vacancy cluster. Likewise, recent molecular dynamics (MD) simulations [17] indicate that the lower temperature radiation-induced Xe diffusivity, which appears temperature-independent, results from the influence of electronic stopping of fission fragments, and the predicted noble gas diffusion coefficients are in good agreement with experimental observations [17].

MD simulations have also been used to investigate the mechanisms of Xe re-resolution from fission gas bubbles, which are believed to contribute to the spatial ordering of fission gas bubbles. Traditional fission gas re-resolution models assume that individual Xe atoms are ejected from the gas bubble as the result of a ballistic collision of a Xe atom with either a

fission fragment, or a recoiling uranium atom, which traverses the bubble. This is known as homogeneous re-solution. MD simulations confirm theoretical estimates that the magnitude of re-solution by homogeneous re-solution is on the order of 10^{-6} re-solved Xe per Xe gas bubble atom per second, whereas a heterogeneous re-solution mechanism, in which multiple gas atoms, or even the entire bubble, can be re-solved into the UO_2 matrix by the passage of a fission fragment depositing energy through electronic excitation. This heterogeneous re-solution mechanism has been shown [18] to produce much larger re-solution by at least three orders of magnitude (10^3 times). In our work, we have used MD simulations to further evaluate the threshold value of the electronic stopping (dE/dx_{elec}) for re-solution for smaller bubbles in the size range of 0.6 to 1.0 nm, and with a range of Xe concentrations corresponding to both equilibrium bubble pressures and slightly under- or over-pressurised. Figure D.6 shows our results, using an interatomic potential from Cooper [19], in comparison with literature data from Govers et al. [18]. The results are in generally good agreement, which shows that there is a critical electronic stopping energy a little above 2 eV/atom (normalised to the total number of atoms within a cylindrical electronic spike), and a fair amount of scatter in the data with respect to the number of Xe atoms re-solved. These results will ultimately provide a comprehensive model for heterogeneous re-solution that will be used in the Xolotl-fission code to predict intragranular bubble populations.

Figure D.6. MD simulation results of the number of re-solved Xe atoms from gas bubbles in UO_2 as a function of the average electronic energy loss (normalised to the number of atoms in the spike), and gas bubble size and pressure.

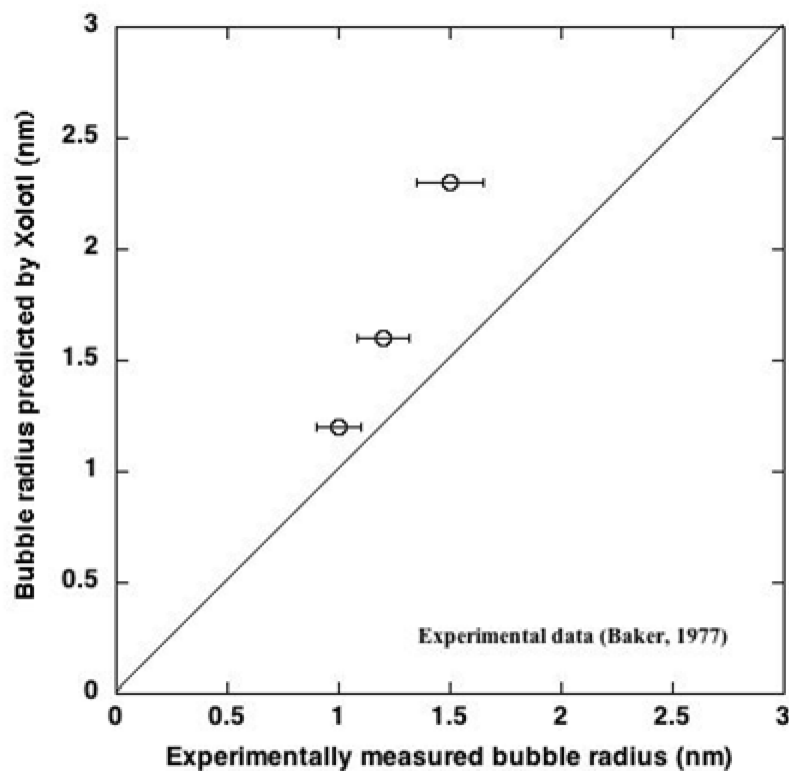


Note: The new results, shown in the inset, are in good agreement with literature data from Govers et al. [18]. Reproduced from [18] with permission.

Figure D.7 demonstrates the initial results of our Xolotl cluster dynamics model to predict the average intragranular bubble radius associated with the experimental results of Baker [20]. In these initial calculations, we have not yet incorporated Xe re-solution, and have taken our estimates for Xe gas diffusion from the experimental assessment of Turnbull and co-workers [6]. These experiments involved uranium dioxide fuel pins irradiated in the UK Atomic Energy Agency (AEA) Winfrith heavy water reactor to burnups of approximately 1% ($\sim 2 \times 10^{26}$ fissions/m³) at a power of approximately 8×10^{18} fissions/m³/s at irradiation temperatures from about 1 000 to 1 560°C [20]. We have simulated these conditions, to

predict the full Xe gas bubble size distribution, as well as the mean size and density. Figure D.7 compares the predicted Xe gas bubble average size to that measured by Baker [20]. Overall, the agreement in both size and number density (not shown) are quite promising, although the cluster dynamics model predicts larger bubble sizes than experimentally measured. Of course, these initial model predictions do not include a gas re-solution mechanism, and the current model only incorporates homogeneous gas bubble nucleation whereas the experimental results indicated a strong spatial correlation of bubbles at the lower irradiation temperatures that Baker interpreted as being caused by heterogeneous nucleation along dislocations or fission tracks. Future efforts will involve incorporating a more precise input of xenon diffusivity based on lower-length scale modelling, the heterogeneous gas re-solution mechanism and an evaluation of heterogeneous bubble nucleation. We also anticipate benchmarking to a larger range of experimental conditions, including higher irradiation temperatures where the intragranular fission gas bubbles take a strongly bi-modal size distribution.

Figure D.7. Xolotl-fission predictions of the mean fission gas bubble radius for 3 irradiation temperatures from 1 000 to 1 560°C at a burnup of approximately 1%, as compared to the experimental data of Baker [20].



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Microstructure-level modelling of fuel performance using a multi-scale approach

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Extended Abstract

Several factors have led to increased emphasis on computational modelling of nuclear fuels in recent years. Many currently operating UO₂-fuelled, water-cooled reactors are nearing the end of their original design lifetimes. If modelling and simulation can contribute to extending the operating lifetimes of these existing plants, it will provide significant economic and environmental benefits. At the same time, there is an increased desire for fuels that can withstand accidents such as a loss of cooling. Metallic fuels such as those based on the U-Si and U-Mo systems are considered good candidates for these applications due to their significantly higher thermal conductivity compared with UO₂ fuel. However, because of the lack of operating experience with these systems, their behaviour over extended operation is not well understood. Modelling of the microstructural evolution of fuels such as U₃Si₂ can provide insight into potential mechanisms of degradation that may be difficult to obtain experimentally.

Because the microstructure of nuclear fuel has a strong impact on performance in both UO₂ and metallic-U fuels, microstructure-level modelling techniques such as the phase-field method have been increasingly applied to nuclear fuels. A key advantage of phase-field models is that there is a clear link between model parameters and physical parameters of the system at the atomic length scale. Therefore, phase-field models of microstructural evolution can be parameterised based on a combination of existing experimental data and calculations from lower length scale techniques such as molecular dynamics (MD) and density functional theory (DFT). In this work, we will describe the development of a new phase-field model to simulate microstructural evolution of polycrystalline UO₂ and U₃Si₂ with fission gas bubbles. The UO₂ model is parameterised with a combination of existing data and MD calculations. In the less-studied material U₃Si₂, we have developed new interatomic potentials to enable the calculation of necessary parameters such as grain boundary energies and interfacial energies. In UO₂, the model will be applied to study the interconnection of intergranular fission gas bubbles along grain faces and grain edges. In U₃Si₂, the model will be applied to investigate swelling due to fission gas bubbles.

The phase-field model developed for these studies has been implemented in the MARMOT application, based on the MOOSE (Multiphysics Object-Oriented Simulation Environment) framework developed at Idaho National Laboratory. The model is unique in that it allows for an arbitrary number of phases, grain orientations of each type of phase, and chemical species. It is based on the grand-potential functional model of Plapp [1]. In this model, the total grand potential Ω of the system is used, rather than the total Helmholtz free energy F more typically used in phase-field models. The original model of Ref. [1] considered only a single order parameter and thus could only be applied to two phases with a single orientation of each phase, and only considered a single substitutional chemical component. By introducing a new grand-potential functional, we have extended the model to consider polycrystalline fuel microstructures with a gas bubble phase, and with gas atoms and vacancies considered as substitutional species on U lattice sites.

In our model, each orientation of a particular phase is represented by an order parameter $\eta_{\alpha i}$, where α indexes the phases and i indexes the grains or orientations of that phase. The order parameter has a value of 1 in that grain/phase and 0 in all other grains/phases, and the interface between grains/phases is represented by a smooth variation of the order

parameter. From the grand potential functional, a set of Allen-Cahn equations are derived to describe the evolution of each order parameter. An evolution equation for the concentration of each substitutional chemical species is written in terms of its chemical potential, and the Allen-Cahn equations and chemical potential equations are solved simultaneously.

This new model retains the advantages of the model in Ref. [1] in that the bulk free energy contribution is removed from the interfaces between phases. This allows the interfacial energies to be parameterised from lower length scale data in a straightforward manner. It prevents the spurious formation of a third phase at a two-phase interface that commonly plagues multi-order parameter phase-field models. It also allows the interfacial thickness to be set larger than the thickness of a physical interface, thus allowing a coarser mesh and improved computational efficiency.

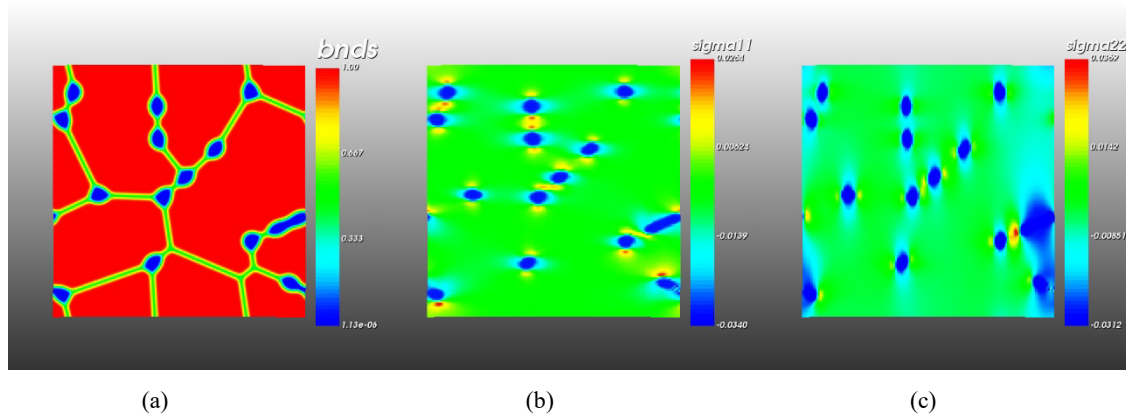
The grand potential model also allows incorporation of stress effects from the hydrostatic pressure within the gas bubbles. A new approach has been implemented to allow the bubble's hydrostatic pressure to be controlled directly in the weak form of the mechanical equilibrium equation. In contrast to previous approaches of calculating an equivalent eigenstrain to impose gas bubble pressure, the new approach allows a hydrostatic stress state in an intergranular bubble.

The multi-phase, multi-order parameter grand potential model was parameterised for the UO_2 system using a combination of existing data from the literature (bulk free energy densities, elastic constants, gas bubble pressure, interfacial energy) and MD calculations (grain boundary energy). The microstructure of a polycrystalline UO_2 fuel with intergranular fission gas bubbles was simulated in 2D to test the model's capabilities, as shown in Figure D.8. The stress state of bubbles at the intersection of both two and three grains is hydrostatic. In future work, 3D simulations will be used to investigate the interconnection of bubbles along grain edges (the intersections of three grains). It is believed that along these grain edges, interconnected bubbles form tunnels that can connect to a free surface, allowing a pathway for fission gases to escape from percolated grain faces that are far from the free surface. The microstructure of such tunnels will be investigated, and the results will be used to improve the fission gas release model used in BISON.

To parameterise phase-field simulations of U_3Si_2 fuel, data such as grain boundary energies, interfacial energies and elastic constants are required. To supply this data, interatomic potentials have been developed for use in MD calculations. The first is based on the Tersoff-type potential for the single element Si [2]. While focusing on the U_3Si_2 phase, a discussion of the transferability will also be presented so that the potential can be used to study secondary phases, such as $(\alpha, \beta, \gamma)\text{-U}$ and U_3Si . The potential predicts the cohesive energies well compared to experimental data for all these phases. It also matches reasonably well with previous experiments on the lattice constants and elastic constants for all these phases. The effect of Xe on the thermal expansion of U_3Si_2 fuels will also be presented.

Additionally, a potential for the U-Si system was developed using the Modified Embedded-Atom Method (MEAM). The potential accurately describes 0 K properties of U_3Si_2 , including formation energy, lattice constants, elastic constants and a variety of point defect properties. The potential can also reasonably predict properties of a variety of U-Si phases across the composition spectrum. The predicted thermal expansion compares excellently to reported experimental values. The advantages and disadvantages of this potential will be compared to those of the Tersoff-type potential.

Figure D.8. (a) Phase-field simulation of polycrystalline fuel microstructure with intergranular fission gas bubbles. Grains are in red, grain boundaries in yellow/green, and bubbles in blue. (b) Stress tensor component σ_{11} , (c) Stress tensor component σ_{22} .



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Current meso-scale modelling developments for TRANSURANUS

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Extended Abstract

The simulation of the cylindrical fuel rod behaviour in a reactor or a storage pool for spent fuel requires a fuel performance code. Such tool solves the equations for the heat transfer, the stresses and strains in fuel and cladding, the evolution of several isotopes and the behaviour of various fission products in the fuel rod. Thanks to a clearly defined mechanical and mathematical framework as well as a consistent modelling, the TRANSURANUS fuel performance code has been able to cope with normal, off-normal and accidental operating conditions right from the beginning. With the advent of advanced hardware and software along with more detailed experimental data in recent years, there has been a general trend to develop more mechanistic models in the fuel rod performance codes like TRANSURANUS.

The first model considered in this paper is that for the high burnup structure (HBS) formation and evolution. Following developments to describe the onset of the HBS on the basis of both local temperature and burnup values, more experimental data have become available at JRC-Karlsruhe for the more precise description of the hardness and Young's modulus of high burnup fuel, the HBS pore size distribution and its evolution during irradiation. Concerning the mechanical properties, the measured radial profiles suggest a close relationship between the hardness and the Young's modulus, and extend the range of available data in high burnup LWR fuels (60-110 GWd/tHM). The experimental data also hint at the possibility of using micro-hardness as local probe for the variation of the Young's modulus in the pellet periphery, where direct measurements by means of acoustic microscopy are challenging. The new data are used to modify the correlation for the fuel Young's modulus by accounting for the decrease due to burnup accumulation. The new correlation shows better agreement with the experimental results, extending its range of experimental validation from non-irradiated to irradiated UO₂.

As a second step towards the mechanistic modelling of the HBS in the TRANSURANUS code, a model is being developed to describe the pore size evolution in the HBS during normal operation and the corresponding progression of the mechanical properties. In parallel to this, we developed a semi-empirical model to describe the formation of the HBS, which embraces the polygonisation/recrystallisation process and the depletion of

intragranular fission gas, describing them as inherently related. For this purpose, we performed grain-size measurements on samples at radial positions in which the restructuring was incomplete. Based on these new experimental data, we inferred an exponential reduction of the average grain size with local effective burnup, paired with a simultaneous depletion of intragranular fission gas driven by diffusion. The comparison with currently used models indicates the applicability of the herein developed model within integral fuel performance codes like TRANSURANUS and BISON.

The more mechanistic modelling of fission gas behaviour is a second crucial aspect of nuclear fuel performance analysis, which can be particularly significant during transients. To accurately reproduce the rapid kinetics of the burst release process in fuel performance calculations, a model that accounts for non-diffusional mechanisms such as fuel micro-cracking is needed. For that purpose, we developed and assessed a model for transient fission gas behaviour in oxide fuel in the frame of collaboration between JRC-Karlsruhe, POLIMI and INL. The model is applied as an extension of conventional diffusion-based models to introduce the burst release effect. The concept and governing equations of the model are presented, and the sensitivity of results to the newly introduced parameters is evaluated through an analytic sensitivity analysis. The model is assessed for application to integral fuel rod analysis by implementation in two structurally different fuel performance codes; BISON and TRANSURANUS. The model assessment is based on the analysis of 19 light water reactor fuel rod irradiation experiments from the OECD/NEA IFPE (International Fuel Performance Experiments) database, all of which are simulated with both codes. The results point out an improvement in both the quantitative predictions of integral fuel rod FGR and the qualitative representation of the FGR kinetics with the transient model relative to the canonical, purely diffusion-based models of the codes. The overall quantitative improvement of the integral FGR predictions in the two codes is comparable. Moreover, calculated radial profiles of xenon concentration after irradiation are investigated and compared to experimental data, illustrating the underlying representation of the physical mechanisms of burst release.

The modelling of helium in nuclear fuel is the third mesoscopic model described in this paper. To begin with, its peculiar characteristics, i.e. higher mobility and solubility or Henry's constant in the fuel matrix in comparison with the other inert fission gases have been critically reviewed on the basis of previous experiments. The measured diffusion coefficients and Henry's constants have been classified depending on the technique used to introduce the helium in the samples (either by infusion, implantation or doping) and the characteristics of the sample itself (single crystal, poly-crystal or powder). This has revealed a high degree of clustering in the available data. Different correlations for both the diffusion coefficient and the Henry's constant have been inferred accordingly. The uncertainty associated with each specific correlation turned out to be less compared to the previously available correlations.

In a second step, the new set of correlations has been introduced in a new modal algorithm to efficiently solve the helium diffusion problem, applying it to the helium behaviour model proposed earlier at JRC-Karlsruhe. The adopted modal algorithm presents computational requirements in line with the needs of state-of-art fuel performance codes. The algorithm has been verified by comparing its results with those obtained by means of the reference finite element tool COMSOL Multiphysics on several typical temperature histories, using the diffusion coefficients fitted earlier on a specific set of experimental data. Subsequently, we have validated the model against experimental data coming from two measurements deeply different in terms of helium introduction technique and characteristics of the samples measured, using the new correlations for the helium diffusion coefficient. Finally, in order to investigate how the initial different percentage of bubbles could affect the helium release, we have also made a sensitivity analysis on the initial concentration of

helium both as single gas and bubbles and on their spatial distribution in the fuel grain. The analysis has pointed out that the fraction of helium precipitated in bubbles has a limited importance compared to the spatial distribution of the bubbles and the single gas atoms (uniform or not).

Following these three model developments, an outline is provided about the ongoing and planned activities, with a particular emphasis on design-basis accidents and transients. Despite the fact that the numerical solution techniques in TRANSURANUS enable handling of non-steady-state conditions, some of the phenomena important for design-basis accidents (DBA) were incorporated later in the code.

More recently, the safety criteria for DBA are being revised as well. One of them deals with the cladding oxidation and hydriding. Similarly to what happens during normal operation conditions during corrosion of the outer cladding surface, a fraction of the hydrogen accompanying the Zr-steam reaction in LWRs under DBA conditions is absorbed by the cladding, especially via inner-side corrosion following cladding failure. Hydrogen absorption is known to enhance cladding embrittlement. It takes place during the oxidation process or from a hydrogen-rich atmosphere under steam starvation conditions in a later phase of an accident. Experiments have indicated that the intensities of these two phenomena are different. In order to predict the hydrogen concentration in the cladding under both conditions, a simple stand-alone hydrogen uptake model has been developed for Zr1%Nb that considers steam oxidation and steam starvation conditions (or H₂ rich environment) separately. In line with the high-temperature oxidation model, the content of hydrogen uptake is computed incrementally with a quasi-stationary approach. Nevertheless, prior to implementation of the model in the TRANSURANUS code, a comparison with more recent publications is required. Only then a consolidated model can be implemented in the TRANSURANUS code.

The fission-product chemistry is another important aspect of the fuel behaviour during accident conditions (both in-pile and during storage) that is currently not considered. However, the models in the MFPR code of IRSN gives very detailed and reliable information on gas release, swelling, porosity evolution, fission-product speciation, fuel stoichiometry, extended defect behaviour which impact the thermomechanical fuel behaviour and are thus relevant for fuel performance code improvements. The coupling of both codes represents the true goal of a multi-scale approach that is to link the different scales by integration of basic data and insights coming from lower length scales. This has been only partially demonstrated up to now. The coupling of the two codes can therefore provide an improved fuel performance code more physically grounded for the prediction of the fuel rod behaviour under normal and off-normal or accident conditions in a reactor or a storage facility for fuel.

In addition to the models for fission-product behaviour, also the model for plenum temperature and pressure are being revised on the basis of detailed multidimensional and multi-physics calculations with the COMSOL software package in the frame of collaboration between JRC-Karlsruhe and NPIC. More precisely, in order to consider the heating of gas by the pellet surface and its impact on the gas temperature distribution, the plenum is divided into two sections according to 2D COMSOL simulations of various conditions. Analytic solutions for the two sections' temperature are obtained and incorporated in the TRANSURANUS and FUPAC codes. The validation of these models is demanding as it is difficult to directly measure plenum temperature distribution or its average value in a fuel rod during irradiation. Due to its interdependency with internal pressure, it is also impossible to validate the plenum temperature model from internal pressure and fission gas release measurements in integral tests. Therefore out-of-pile

experiments are being designed for the experimental validation of the plenum temperature modelling tools.

Finally, it is proposed that in the frame of the INSPYRE project of Euratom, we will extend the modelling of the mechanisms of fast breeder reactor MOX fuel restructuring at the beginning of life, the modelling of the gaseous fission product and inert gas behaviour at high burnup and in transient conditions and the modelling of creep and fracture. The resulting models should then also be transferred to various fuel performance codes (TRANSURANUS, GERMINAL, etc.).

Recent developments in modelling fission gas behaviour for BISON

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Extended Abstract

Overview

The behaviour of fission gases (Xe, Kr) is of critical importance to nuclear fuel performance, because fission gas diffusion and precipitation in bubbles influences both the amount of fuel swelling and the quantity of fission gas released to the fuel rod plenum. Fission gas swelling and release importantly affect the performance of uranium dioxide (UO₂) and also of other fuel materials such as uranium silicide (U₃Si₂), which is one of the leading concepts considered within the accident-tolerant fuel (ATF) programme of the US DOE Advanced Fuels Campaign [1]. It follows that accurate models of fission gas behaviour need to be developed for the calculation of fission gas swelling and release in fuel performance codes, such as the BISON code developed at Idaho National Laboratory (INL) [2,3]. In this framework, the fission gas behaviour model included in BISON is being extended, both for the improved modelling of UO₂ and to introduce a new U₃Si₂ capability.

Due to the extremely low solubility of Xe and Kr atoms in the fuel, the gas tends to precipitate out of the matrix in the form of bubbles. These include intragranular and grain boundary bubbles, both contributing to progressive gaseous swelling of the fuel and affecting the kinetics of fission gas release (FGR). In particular, the evolution of intragranular bubbles is coupled to gas atom diffusion to grain boundaries, which is the first and basic step of FGR. Also, fuel swelling associated with intragranular bubbles is important at high burnup and during power transients in UO₂, and may be more significant, even at low burnup, in U₃Si₂ [4,5].

Recent developments of the fission gas behaviour model in BISON include a new and improved numerical algorithm for the computation of gas atom diffusion to grain boundaries [6,7] as well as a new capability for transient behaviour at the grain boundaries that allows for the burst FGR effect [8]. Furthermore, developments have been accomplished in the modelling of intragranular fission gas bubble evolution. The latter are the main subject of the present paper.

Models for the evolution of intragranular fission gas bubbles in UO₂ applied in engineering-scale codes are still largely empirical, which includes the original capability in the BISON fission gas behaviour model [3,9,10]. Consequently, they can be applied to a limited range of conditions and cannot be transferred to fuel materials other than UO₂. As for U₃Si₂, the data available are rather limited, in particular for the temperature range where power reactors would operate. Such knowledge gap can be filled by calculations at lower length scale to derive unknown material parameters by investigating the basic physical mechanisms. However, in order to allow for scale bridging and apply such information to engineering-scale calculations, physically-based models in engineering codes are needed that can be informed with parameters extracted at smaller scales.

In this work, we develop a physically-based capability for intragranular fission gas bubble evolution that can be effectively applied to engineering-scale codes and also is able to use parameters from lower length scale calculations as input. Such capability is applied to both the improved modelling of bubble evolution in UO₂ and as the basis for a new multiscale

model of fission gas behaviour in U_3Si_2 . These developments are being incorporated in the BISON fuel performance code.

Intragranular bubble evolution model

The evolution of intragranular fission gas bubbles in nuclear fuel is controlled by the fundamental processes of bubble nucleation, gas atom trapping at the bubbles, and irradiation-induced gas atom re-solution from bubbles back into the lattice. Nucleation and re-solution may occur by different mechanisms, i.e. *heterogeneous* and *homogeneous* [11]. Heterogeneous nucleation and re-solution refer to the nuclei of the new bubbles being created as a direct consequence of the interaction of fission fragments with the lattice and the bubbles being destroyed *en-bloc* by passing fission fragments, respectively. The homogeneous mechanisms refer to bubbles being nucleated by diffusion-driven interactions of dissolved gas atoms and re-solution occurring gradually by individual-atom ejection. The dominant mechanisms depend upon the nature of the interactions between fission fragments and lattice (electronic or phononic). Based on the available knowledge, we consider the heterogeneous mechanisms of nucleation and re-solution for UO_2 [12], whereas we assume the homogeneous mechanisms to dominate in U_3Si_2 [13]. We develop a general modelling approach that embraces both the hetero- and homogeneous mechanisms, then we specialise the model for the two materials by selecting the appropriate mechanism and adopting the parameters specific to each material.

Bubble evolution can be tracked via a cluster dynamics approach where coupled partial differential equations are written for the evolution of each class of gas atom clusters (bubbles) from single atoms to the largest clusters. In this work, we seek a simplification to obtain a reduced-parameter model for the calculation of the bubble mean size and concentration, and the associated fuel gaseous swelling, that can be directly applied to engineering fuel performance calculations. More detailed calculations can then be used to inform such simplified model with improved parameters. The developed approach is outlined below.

Let c_n be the concentration of clusters containing n atoms (with c_1 being the concentration of single gas atoms). We define the total concentration of bubbles (i.e. clusters of size $n \geq 2$ atoms), N , and the mean of the size distribution, $\bar{n}$, respectively, as

$$N = \sum_{n=2}^{\infty} c_n \quad (1)$$

$$\bar{n} = \sum_{n=2}^{\infty} n c_n / N \quad (2)$$

Combining the classic cluster dynamics formulation of the master equations for $c_1 \dots c_n$ for either the heterogeneous or the homogeneous cases with Eqs. (1,2), and performing a first order Taylor expansion in the phase space, we derive a simplified cluster dynamics formulation with only two differential equations for the total bubble concentration and mean size. For the heterogeneous case, the obtained formulation reads

$$\frac{dN}{dt} = \nu - \alpha_{\bar{n}} N \quad (3)$$

$$\frac{d\bar{n}}{dt} = \beta_{\bar{n}} - (\bar{n} - 1) \alpha_{\bar{n}} \quad (4)$$

Where ν is the bubble (dimer) nucleation rate, and $\alpha_{\bar{n}}$ and $\beta_{\bar{n}}$ are the rates of re-resolution and trapping events, respectively, for a cluster of size $\bar{n}$. For the homogeneous case, an analogous mathematical form is obtained.

This model can be applied, with a suitable choice of the parameters describing nucleation, re-resolution, trapping (ν, α, β), to calculation of the total intragranular bubble concentration and mean size, and ultimately, intragranular gaseous swelling. In particular, for UO_2 we adopted parameters from either lower length scale modelling or experimental work, based on the extensive information available for this material. The model also opens to engineering-scale fission gas calculations in U_3Si_2 as it permits exploiting recent lower length scale modelling of the fundamental processes in a multiscale modelling approach. In particular, for U_3Si_2 we informed the model described above with recent density functional theory calculations for the gas atom diffusivity and trapping rate [14] and molecular dynamics calculations for the re-resolution rate [13].

Main outcomes

A new physically-based model for intragranular fission gas bubble evolution has been developed that relies on the concepts of cluster dynamics as well as lower length-scale modelling for the determination of the basic parameters, and ultimately provides calculations at the engineering scale. The model has also been interfaced with a newly developed numerical algorithm for gas atom diffusion [6,7], resulting in a comprehensive intragranular fission gas capability that computes bubble evolution and swelling coupled to gas diffusion to grain boundaries. We compared the results for UO_2 to experimental data of bubble number density and size, demonstrating a clear improvement compared to previous attempt to model bubble evolution with a mean, single size approach [11]. The application to U_3Si_2 was integrated with a description of grain boundary processes, leading to an initial engineering model for fission gas swelling and release in this type of fuel at power reactor temperatures. Given the considerable uncertainty that still exists in the parameters and the lack of experimental data, we also performed a sensitivity analysis of the model parameters that can help addressing future research on lower length scale modelling of fission gas behaviour in U_3Si_2 . The developed models are being incorporated in INL's fuel performance code BISON.

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ALCYONE calculations of GONCOR experiment for the kinetics of gaseous swelling during a power transient

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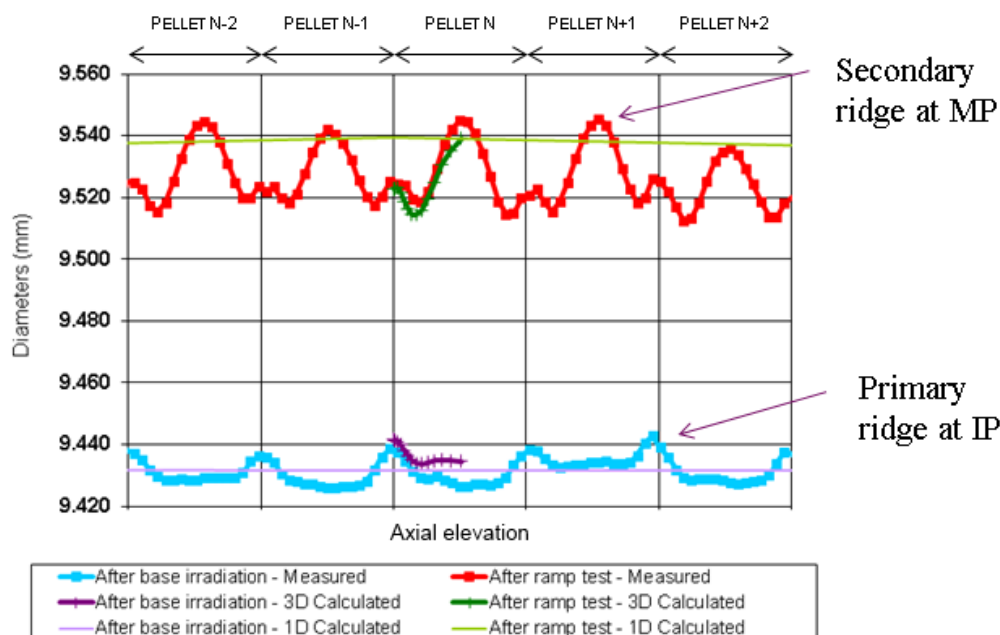
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Extended Abstract

Safety requirements in French nuclear power plants impose that no cladding failure by pellet-cladding interaction (PCI) should occur during normal operation and incidental situations such as Class 2 transients. The PCI fuel technological limit is based on interpretations of power ramp tests performed in experimental reactors (that include transient with or without holding time), such as OSIRIS, on rod sections irradiated in PWRs. Such experiments with extensive post-irradiation examinations have been performed on different types of fuel and cladding materials, including advanced doped fuels, and constitute a large experimental database for modelling. In order to study PWR fuel behaviour during incidental conditions, CEA, in collaboration with EDF and AREVA, have developed the multidimensional fuel performance code ALCYONE in the simulation platform PLEIADES [1].

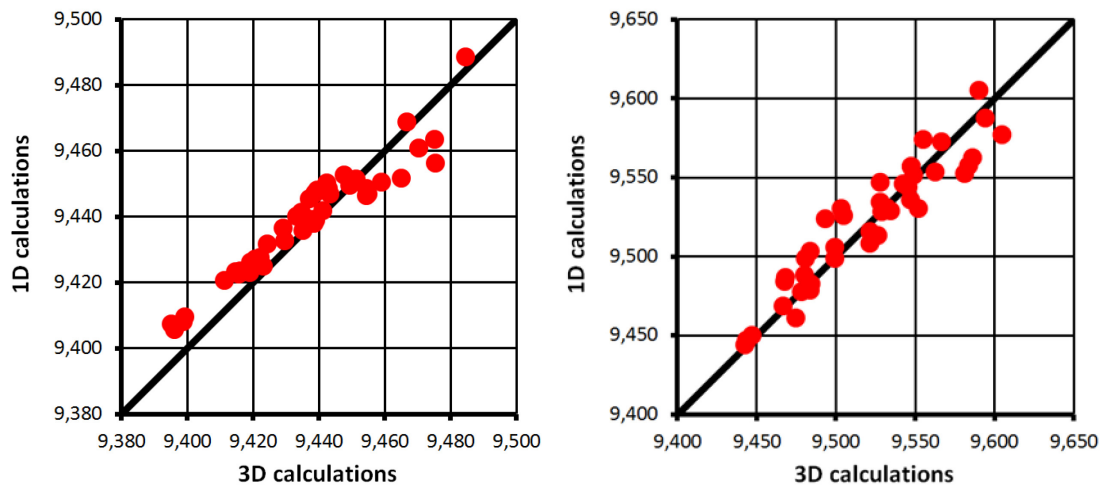
ALCYONE gives a good agreement between the calculations and the measurements for several various power ramps [2]. With 1D modelling, the aim is to estimate integral quantities (like fission gas release xenon/krypton for example) or local mean quantities (like external cladding diameters for example). With 3D modelling, studies focus on local quantities such as external cladding diameters, their increments during the power ramp or the height of ridges (primary ridge on Inter-Pellet plane or secondary ridge on Mid-Pellet plane). A comparison between 1D/3D calculations and measurements is shown in Figure D.9.

Figure D.9. Comparison between 1D/3D calculations and measurements for external cladding diameters after base irradiation and power ramp for a specific rod



It is important to remember that 1D modelling represents only Mid-Pellet planes, whereas 3D modelling gives information at pellet fragment scale. In the previous figure, the focus was on the profilometry of a specific rod but the 1D to 3D comparison has been extended to the validation database related to UO₂ rods [2] that includes more than 40 power ramps.

Figure D.10. Comparison between 1D and 3D calculations for the external cladding diameter after base irradiations (on the left) and power ramps (on the right) at Peak Power Node (Mid-Pellet plane)

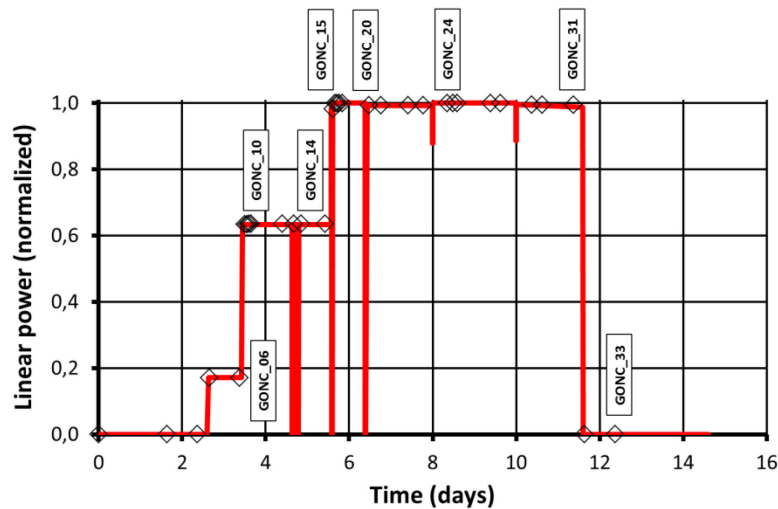


The two graphics gathered on Figure D.10 underline the close correlation between 1D and 3D modelling for the external cladding diameters at the Mid-Pellet plane for the end of base irradiation (on the left) and for the end of power ramp (on the right).

One stage further, efforts have been made to model the kinetics evolution of external cladding diameters impacted by the gaseous swelling throughout the ramp test. Recently, some focus has been put on the validation of the gaseous swelling kinetics with the fission gas behaviour advanced model CARACAS [3] that is used within ALCYONE to describe the several gas populations in the fuel, their precipitation, growing, migration and coalescence.

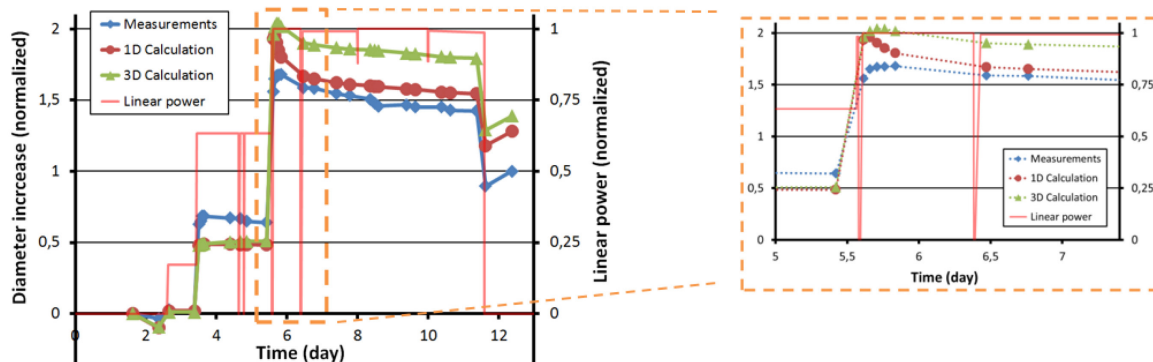
To investigate the impact of the gaseous swelling on fuel rod deformation at high burnup (around 50 GWd/tU), the GONCOR experiment carried out in 1993 in the SILOE Material Testing Reactor (Grenoble, France). This experiment benefited from online cladding diameter measurements during a transient whose maximal power was maintained for nearly 6 days (see Figure D.11) thanks to the DECOR device [4][5]. The power history and the measuring times are shown in Figure D.11.

Figure D.11. Power history for the ramp of GONCOR experiment (normalised to the maximum of the linear power)



In order to compare the results between calculations and measurements (Figure D.12), the evolution of the diameter of the Median-Pellet plane during the experiment is analysed at Peak Power Node (PPN, averaged on 3 pellets).

Figure D.12. Comparison between measurement, 1D and 3D calculations for the increase of the external cladding diameter (median-pellet) of GONCOR experiment (normalised to the final experimental measure)



In this Figure, at the beginning of the irradiation (during the so-called power conditioning level), the calculations (1D or 3D which are very similar) underestimate slightly the increase of the diameter. During the transient to the highest power, calculations show that the increase of the diameter is more important than the measurement. And during the holding time (6 days), the decrease of the diameter is rather well predicted, which means that the kinetics of the evolution of the radius due to the fission gas release are correctly modelled.

Regarding the transient stage that leads to the highest power, although the calculations (1D or 3D) overestimate the increase of the diameter, the shape of the diameter evolution is well reproduced during the first instants of the holding time with the 3D modelling. At the end of the irradiation, the calculated increase of the diameter is slightly greater than the measurement. This is probably linked to the initial overestimation of the diameter increase during this transient stage. Finally, the calculated value of the final diameter is the same

order of magnitude as the measurement, due to the counterbalances of under and over estimations between plateaus (4-6 days and 6-12 days).

To conclude, the GONCOR experiment allows study of the contribution of the gaseous swelling to the deformation of the fuel rod during a power ramp. Thanks to this first experiment with a holding time of 6 days, new results about online cladding diameter measurements were available and confronted to the calculations. These new comparisons underline the importance to have these kinds of experimental results in order to validate precisely fuel performance codes, as regards the kinetics of the cladding deformation throughout the irradiation. ALCYONE calculations have shown an overall good coherence between the 1D and 3D modellings for the power ramps. The future analysis of the available profilometries, with a particular emphasis on the cladding diameter increase at Mid-Pellet and Inter-Pellet planes and the evolution of the heights of the primary and secondary ridges will allow a better adjustment of the models used in ALCYONE and thus will improve the robustness and the accuracy of the code.

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A model of irradiation-induced densification of oxide nuclear fuel

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Extended Abstract

During the first 10^2 - 10^3 hours of fuel irradiation in the reactor core, a decrease in the geometrical sizes of UO_2 fuel pellet and fuel column takes place [1-3]. This phenomenon is called the “irradiation-induced densification” because the decreasing of the pellet volume without mass loss is accompanied by density alteration. The maximum value of densification is equal to 0.1-1.5% and depends not only on irradiation condition but on structure of fuel pellet [4,5]. Maximum densification occurs at not very high burnup ~ 0.2 – 2.0 MW.day/kgU ($\sim 10^{19}$ - 10^{20} fission/cm³). At further burn up an intense swelling of uranium dioxide suppress the process of densification. The structure studies of irradiated samples show that the cause of irradiation-induced densification is the closing of pores in fuel [1]. Density of fuel pellet is about 94.9-97.6% of theoretical density. The rest 3-5% of volume corresponds to the pores. Pores appear during the pellet creation process with following sintering or they are specially being created in pellet by addition of pore-forming component to the press-powder.

It is experimental fact that during the process of pellet irradiation, the closing of submicron pores takes place [1]. Wherein there is the decreasing of submicron pores fraction in the pore size distribution. The fraction of coarse pores and their characteristic size, practically, are not changed under irradiation of the fuel pellet.

During experimental research it was established [1-5] that the maximum in-pile change of density had occurred in fuels that:

1. have lesser initial density;
2. have the main fraction of pores belonging to the submicron range of sizes;
3. have been irradiated at high temperature (fission rate per unit volume).

The goal of this work is to develop the model of irradiation-induced densification of oxide nuclear fuel and to highlight the mechanism of fuel densification.

During nuclear fission of uranium, the high-energy fission fragments with mass number $A \sim 100$ and energy 10^2 MeV are created. So, for example, the main nuclear yield in ^{235}U fission reaction has Xenon. While passing of such fission fragment through the substance the track is created. The main part of initial energy (~ 98 - 99%) of fission fragment is spent on excitation of electrons of medium along the track [9]. So, for Xe^+ ion having initial energy $E_0 = 100$ MeV the electronic stopping loss $(dE/dx)_e = 25 \cdot 10^2$ eV/Å that is 100 times higher than the nuclear stopping loss $(dE/dx)_n = 24.5$ eV/Å [9]. The path length of fission fragment at energy E_0 is equal to $L_{\text{Xe}} = 5.4$ μm. Therefore, the number of excited electrons per track length is $N_e/L_{\text{Xe}} \sim |dE/dx|_e/I = 4.6 \cdot 10^{10}$ cm⁻¹ where $I = 5.5$ eV is the ionisation potential of uranium dioxide. The maximum energy obtained by electron during collision with Xe-ion is not too large $\epsilon_e \sim (4m_e/M_{\text{Xe}})E_0 \sim 4$ keV. The path length of such electron is about $L_e \sim 10$ nm.

Therefore, the mean concentration of electrons of “first generation” in the track volume is close to Loschmidts constant $N_e/L_{Xe\pi}(L_e) \sim 2.5 \cdot 10^{19} \text{ cm}^{-3}$. In turn, the electron having energy $\varepsilon \sim 4 \text{ keV}$ can excite about 80 electrons of “second generation”. The path length of the electrons of «second generation» is defined by the process of its scattering on the lattice vibrations (phonons) and its path length is equal to several lattice parameter. Therefore, the energy relaxation mechanism of electrons of “second generation” is electron-phonon interaction.

Thus, the total concentration of excited electrons in tracks volume is about 10^{21} cm^{-3} . Whereas even at melting temperature the equilibrium temperature concentration of electrons in the conduction band of uranium dioxide is $\sim 10^{18} \text{ cm}^{-3}$. The temperature $\sim 10^4 \text{ K}$ formally corresponds to such concentration of electrons in the conduction band. That is why this energy transmitted by fission fragment to the electron subsystem will go to the heating of lattice.

The fission fragment can heat the ion subsystem up to the excess temperature $\Delta T_i \sim |dE/dx|_e / \lambda \tau \sim 80 \text{ K}$ that defined by the nuclear energy loss and the value of thermal conductivity $\lambda \sim 2 \text{ W/m}\cdot\text{K}$ of UO_2 : where $\tau \sim 10^{-10} \text{ s}$ is the characteristic time of thermal conduction.

On the other hand, the electron subsystem heats the lattice up to excess temperature that can be estimated from $C_v L_{Xe\pi}(L_e) 2\Delta T_e \sim E_0$, where C_v is the molar specific heat at constant volume of uranium dioxide. As result the temperature jump is equal to $\Delta T_e \sim 300 \text{ K}$. Thus, the total heating of lattice in tracks volume exceeds the melting temperature ($T_m = 3120 \text{ K}$) of uranium dioxide $\Delta T_e + \Delta T_i > T_m$. Therefore, the substance melts.

Due to difference of specific volumes of melt and solid phase near the track boundary ($\delta V/V = 5.9\%$) the compressive stresses appear $\sigma = K(\delta V/V) \sim 1.6 \text{ GPa}$ (K - compression modulus) is higher than yield strength σ_T of uranium dioxide. Zone of plastic yield appears around melt substance in track with characteristic size $r_p = L_{e\pi} \exp(\sigma/2\sigma_T - 1/2) \sim 1 \text{ }\mu\text{m}$ [10].

At such high fission rate per unit volume as $F = 10^{11} - 10^{12} \text{ fiss}/(\text{cm}^3 \cdot \text{s})$ the time interval required to cover the arbitrary volume of fuel pellet by nonintersecting tracks is equal to $\Delta t = 1/2\pi \cdot (r_p)^2 L_{Xe} F \sim 1.5 - 15 \text{ s}$. That is considerably lower than the duration of irradiation-induced densification process at whole. Therefore, one could suppose that the substance in vicinity of pores is in plastic state permanently.

In plastic (viscous) medium the pores decrease in size under influence of compressive stresses in tracks and under influence of capillarity forces. The process of the closing of single pore is described by the system of equation which represents the equation for energy dissipation, the Navier-Stokes equation for viscous, incompressible “liquid” and the number of particle conservation law.

$$\begin{cases} \sigma \frac{dV}{dt} + \gamma \frac{d\Sigma}{dt} = - \int dV' \frac{\sigma_{ik}^2}{2\eta}, \\ \Delta \vec{v} = 0, \\ \int_{\Sigma} d\vec{S} \vec{v} = - \frac{dV}{dt}. \end{cases} \quad (1)$$

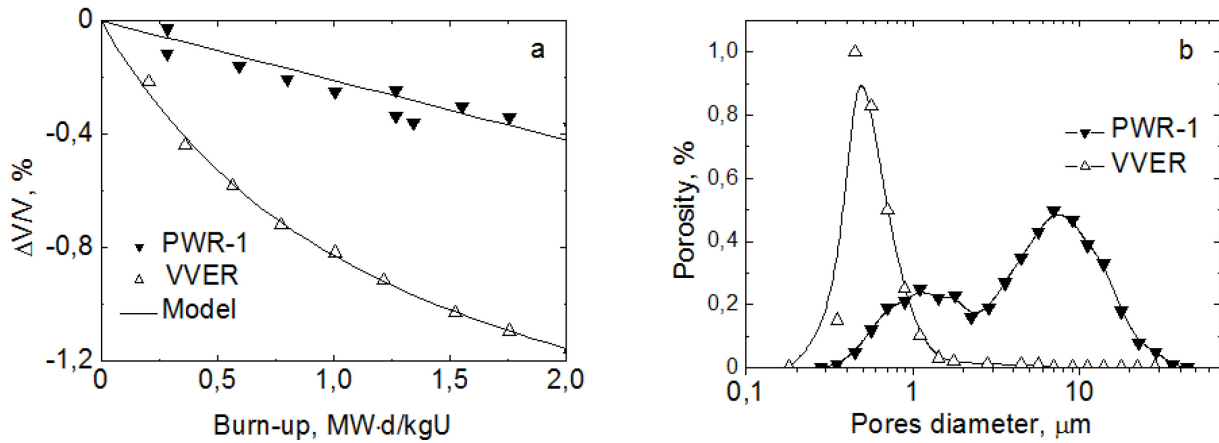
Here γ is surface energy; $\vec{v}$ is velocity of mass flow to the pore; V' is the volume of medium without pore's volume V , Σ is pore's surface; σ_{ik} is the tensor of yield strain; η is viscosity factor of uranium dioxide.

In steady flow approximation the solution of this system leads to exponential law of closing of pore with time:

$$R(R_0; t) = R_0 \exp \left\{ -\frac{\sigma}{4\eta} (t - t_0) \right\}, \quad (2)$$

where R_0 is the initial pore's radius.

Figure D.13. The burnup dependence of irradiation-induced densification of experimental samples of oxide nuclear fuel (a) having different types of pore size distribution functions (b) [4,5]



The size of submicron pores is equal to the radius of yield zone therefore the process of its closing occurs exponentially fast. Vice versa to complete closing of large pore it is required many tracks and considerably longer period of time. If the initial pore size distribution function in pellet $f_0(R_0)$ is known then the value of densification is calculated using this formula:

$$\frac{\Delta V}{V_0} = \frac{\int_0^\infty dR_0 (R^3(R_0; t) - R_0^3) f_0(R_0)}{\int_0^\infty dR_0 R_0^3 f_0(R_0)} \quad (3)$$

In the Figure D.13a it is shown the comparison of experimental data on densification of 2 types of the experimental samples with calculations by means of proposed model. The samples have different pore size distribution functions (see Figure D.13b). It is seen that the calculation by means of the developed model is consistent with experiment.

Thus, the irradiation-induced densification of uranium oxide nuclear fuel is consequence of closing of pores as result of plastic flow under influence of stresses appearing in the fission fragment tracks in UO_2 .

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