# ANNUAL REPORT 2023

**Swedish Centre for Nuclear Technology**
**Svenskt Kärntekniskt Centrum**

**March 2024**

KTH – Royal Institute of Technology
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**This is SKC**

The Swedish Center for Nuclear Technology (Svenskt Kärntekniskt Centrum, SKC) secures the availability of competence and helps to solve complex problems by investing in nuclear research and education in Sweden. These are critical tasks for safe and sustainable operation of the nuclear power industry.

SKC connects the Swedish nuclear power industry, the regulator and the three Swedish universities that provide the majority of education and research opportunities within disciplines of nuclear technology by funding education and research in a way that benefits all parts.

The SKC collaboration is planned in cycles and the current annual report mainly covers the contract period 2020-2023. However, some of the preparations for the next contract period 2024-2027 are also described.

**Organisation**

Chalmers University of Technology
KTH – Royal Institute of Technology
Uppsala University
Swedish Radiation Safety Authority
Forsmarks Kraftgrupp AB
Oskarshamn Kraftgrupp AB
Ringhals AB
Westinghouse Electric

SKC
Swedish Centre for Nuclear Technology

# Director's message

The growing awareness of the importance of a reliable, affordable and fossil free energy production has resulted in a rapidly increased interest in nuclear energy. Several different options for new nuclear are being investigated and the operating plants are looking at life time extensions up to 80 years of operation. As a result the need for competence and knowledge development within the nuclear area is greater than ever.

Here the Swedish Center for Nuclear Technology (Svenskt Kärntekniskt Centrum, SKC) has an important role to play. SKC has provided support to academic education and research in the nuclear area for more than 30 years which has made it possible to retain the competence at the three SKC partner universities that is necessary to develop the excellence that is required for the current nuclear development to be successful.

As SKC is entering a new program period in 2024 a call for new research projects was made during 2023 and eight very interesting projects have been selected to receive funding by the technical advisory council. It has also been decided to start a new advisory council for competence related questions to focus on and improve activities to attract new students to the nuclear power sector. I hope that this will further increase the usefulness of SKC to all the exiting initiatives that are planned for nuclear energy in Sweden.

Göteborg, March 1st 2024

Cilla Andersson

Director, SKC

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# Swedish Centre for Nuclear Technology

# SKC

The Swedish Centre for Nuclear Technology (Svenskt Kärntekniskt Centrum, SKC) was originally founded in 1992 at KTH Royal Institute of Technology. Later, the centre was expanded to include Uppsala University and Chalmers University of Technology. Today the centre is a collaboration administrated at the School of engineering sciences at KTH.

The main mission of SKC is to secure the availability of high-skill competence needed in the nuclear industry and to preserve high quality nuclear research and education in Sweden.

SKC connects the Swedish nuclear power industry, the regulator and the three Swedish universities that provide the majority of education and research opportunities within disciplines of nuclear technology by funding education and research in a way that benefits all parts. The majority of the funding that SKC directs to the universities enables hiring new doctoral and post-doctoral researchers as well as retaining senior researchers and technical staff but efforts are also made to make new students aware of this area of work and research.

# Organisation

## Board

The SKC's Board has a decision mandate over the operations of SKC and serves the shared interests of all partner-organisations. For that reason the Board consists of a chairman and one representative from each partner-organization.

The Board members during 2023 are listed below.

**Karl Bergman**
Chairman of the board
Head of R&D, Vattenfall AB

**Johan Börjesson**
Deputy Managing Director
Forsmark Kraftgrupp AB

**Monika Adsten**
Head of R&D
Ringhals AB & Forsmark Kraftgrupp AB

**Jan Karjalainen**
Head of Engineering
Oskarshamns Kraftgrupp AB

**Lena Oliver**
Consulting Engineer
Westinghouse Electric Sweden AB

**Per Seltborg**
Head of R&D
Swedish Radiation Safety Authority

**Thomas Nilsson**
Head of department
Chalmers University of Technology

**Oscar Tjernberg**
Deputy head of school
KTH Royal Institute of Technology

**Jonas Fransson**
Professor
Uppsala University

## Operations

A director that answers to the Board, is responsible for the operations. Since the beginning of 2023 this position is held by **Cilla Andersson**.

## Advisory Council

The Advisory Council serves as a reference group in which discussions on strategy and funding take place. The members are selected to give the advisory council a collective competence profile that is relevant for ongoing and future SKC activities. The council advises the SKC board and director but takes no decisions.

The members of the Advisory Council during 2023 are listed below.

**Michael Knochenhauer** (January-May)/
**Ingemar Jansson** (June-December)
Chairman of the Advisory Council

**Mattias Olsson**
Radiochemistry expert
Forsmarks Kraftgrupp AB

**Georg Lagerström**
Reactor safety engineer,
Oskarshamns Kraftgrupp AB

**Björn Forssgren**
Senior Specialist
Ringhals AB

**Anna Alvestav**
Reactor technology analyst
the Swedish Radiation Safety Authority

**Carl Adamsson**
Principal Engineer
Westinghouse Electric Sweden AB

**Henrik Sjöstrand**
Associate Professor at Department of Physics and Astronomy,
Applied Nuclear Physics
Representative of KTH, Uppsala University & Chalmers

# The Contract period 2020-2023

On the first of January 2020 the SKC collaboration entered into a four-year contract period between eight partners. According to the agreement the five financiers the Swedish Radiation Safety Authority, Westinghouse Electric Sweden, Forsmarks Kraftgrupp AB, Ringhals AB and Oskarshamns Kraftgrupp AB have contributed with 52 million SEK that SKC has used to fund education and research that benefits all parts.

The main part of the funding has been used to fund specific research projects at the three partner universities Chalmers University of Technology, KTH Royal Institute of Technology and Uppsala University. The motivation for and progress of these projects are described in the last part of this report. Funding has also been used to provide base support for the continuation or development of education within the disciplines of nuclear technology which is further described in the third part of this report. Finally SKC has organized events for students, held annual symposiums and recognized young talents by annual awarding the Sigvard Eklund´s prize. The activities during 2023 are described in the second part of this report.

# The next Contract period 2024-2027

During 2023 SKC started to prepare for a new four-year contract period starting 2024 and continuing to the end of 2027. In line with the original principles and intentions of SKC the following overall goals have been formulated for SKC:

- Attractive nuclear technology education should be provided in Sweden.

- The contracting parties' recruiting needs of highly skilled staff and academicians should be satisfied by relevant bachelor's and master's programmes and doctoral- and post-doctoral research projects.

- Internationally recognized research groups within disciplines that are vital for the safe and sustainable nuclear operation should exist in Sweden.

- Research and education that is of value to the contracting parties should be conducted.

Education and research that receive priority funding from SKC belong to the following disciplines:

- Reactor Physics
- Detector technology
- Nuclear chemistry
- Thermal hydraulics
- Nuclear fuel technology
- Material science, with an emphasis on ageing
- Severe accident analysis

A call for new research projects was made September 1st 2023 and eight very interesting projects have been selected to receive funding based on recommendations from the technical advisory council.

# Results and Activities during 2023

# Financial Results 2023

Below the payments from the five financiers and the SKC expenditures during 2023 are summarized.

Project support has been used to fund the projects that are described in the final section of the annual report. Since most projects started after January 2020 the payments to these research projects will continue after 2023.

Base funding has been used according to the next section of the annual report.

The SKC central organization cover costs associated to administration, the advisory council, activities for students, the Sigvard Eklund's prize and the annual symposium which are description in this section of the annual report.

| Payments to SKC from financiers | |
|---|---|
| Swedish Radiation Authority | 4 000 000 |
| Forsmarks Kraftgrupp AB | 2 829 904 |
| Oskarshamns Kraftgrupp AB | 1 581 014 |
| Ringhals AB | 2 089 082 |
| Westinghouse Electric Sweden AB | 1 500 000 |
| **Total payments 2023** | **12 000 000** |

| Expenditures by SKC | |
|---|---|
| Project Support | -6 000 000 |
| Base Funding | -3 999 666 |
| SKC central organisation | -1 218 213 |
| **Total expenditures 2022** | **-12 291 601** |

| Balance | |
|---|---|
| Reserves for project support | 3 500 000 |
| Resources at the start of 2023 | 5 030 002 |
| Unallocated resources | 2 563 209[1] |
| **Balance 2023/2024** | **5 813 209** |

[1] Payments to the reviewers of the nominations for Sigvard Eklunds prize 2023, student support for YG participation 2023, work of the SKC director during December and part of the base funding for KTH was not paid during 2023.

# Symposium 2023

Each year SKC organizes a symposium where academia, the regulator and the industry can meet and discuss research, education and future opportunities in nuclear engineering and technology.

*Participants at the SKC annual Symposium 2023*

More than 80 registered participants joined the 2023 symposium which was organized October 16-17 at Albanova University Centre. The program, which is available on the next page, included presentations of research projects funded by SKC, updates about ongoing research at the three SKC partner universities, an announcement of the winners of the Sigvard Eklund´s prize, presentations of the current situation and future expectations for nuclear power in Sweden, updates from the partner Universities and a panel discussion about important activities to secure competence for future nuclear power in Sweden.

*Program during the SKC annual Symposium 2023*

**October 16th**

| | |
|---|---|
| 09:30-10:00 | Assembly |
| 10:00-10:15 | Introduction<br>Cilla Andersson, SKC |
| 10:15-10:40 | *Future electricity production in Sweden*<br>Kristian Gustafsson, Vattenfall |
| 10:40-11:30 | Research project presentations<br>Kristoffer Tofveson Pedersen, CTH<br>Shuyue Wang, KTH |
| 11:30-12:00 | Coffee break |
| 12:00-12:50 | Research project presentations<br>Mustafa Subasic, KTH<br>Ibrahim Batayneh, KTH |
| 12:50-13:50 | Lunch |
| 13:50-15:45 | Research project presentations<br>Gustav Robertsson, UU<br>Yi Meng Chan, KTH<br>Luca Gagliani, KTH<br>Michal Sedlak Mosesson, KTH |
| 15:45-16:15 | Coffee break |
| 16:15-16:40 | Research project presentation<br>David Mayweg, CTH |
| 16:40-16:50 | KTH Master's program<br>Jan Dufek, KTH |
| 16:50-17:20 | *Politics and plans for energy and nuclear power I*<br>Maja Lundbäck, Regeringskansliet |
| 18:00 | Dinner |

**October 17th**

| | |
|---|---|
| 08:30-09:00 | Assembly |
| 09:00-09:15 | *Politics and plans for energy and nuclear power II*<br>Daniel Westlén, Regeringskansliet |
| 09:15-10:15 | Ongoing nuclear research<br>- CTH<br>- UU<br>- KTH |
| 10:15-10:30 | Quick break |
| 10:30-11:30 | Sigvard Eklunds prize<br>- Announcement of the winners<br>- Presentation of theses |
| 11:30-11:50 | Coffee break |
| 11:50-12:20 | YG, SAINT, SKS, ANItA |
| 12:20-12:50 | Panel discussion: *Important activities to secure competence for future Nuclear power in Sweden*<br>Johan Börjesson, FKA/SKC<br>Per Seltborg, SSM/SKC<br>Lovisa Lundholm, SU/SAINT<br>Balder Hagert, AFRY/SKS<br>Ane Håkansson, UU/ANItA |
| 12:50-13:00 | Summary and closure of the Symposium<br>Cilla Andersson, SKC |
| 13:00-14:00 | Lunch |

# Sigvard Eklund's Prize

Dr Sigvard Eklund played a key role in establishing the Swedish nuclear power industry through his various roles and assignments and during the period of 1961 and 1981 he was the Director General of IAEA. The foundation for his lifelong contributions to the research, development and application of nuclear technology originates back to both Uppsala University where he obtained his academic degrees and to KTH Royal Institute of Technology where he became a docent.

Sigvard Eklund's prize has been established by SKC to recognize outstanding academic work by bachelor students, master students and doctoral students and has been rewarded annually since 2004 according to the table below.

| Year | Doctoral thesis | Master's thesis | Bachelor's thesis |
|---|---|---|---|
| 2004 | Christophe Demazière, CTH | Dereje Shiferaw, KTH | |
| 2005 | Staffan Jacobsson Svärd, UU | Henrik Lindgren, KTH | |
| 2006 | Marcus Eriksson, KTH | Simon Walve, KTH | |
| 2007 | Carl Sunde, CTH | | |
| 2008 | Olivia Roth, KTH | Andreas Carlson, KTH | |
| 2009 | Åsa Henning, LU | Petty Bernitt Cartemo, CTH | |
| 2010 | Andreas Enqvist, CTH | Paul Bramson, KTH | |
| 2011 | Chi Thanh Tran, KTH | Martin Lundgren, Chalmers | Katja Göller, UU |
| 2012 | Anders Puranen, KTH | Antoine Claisse, KTH | Azur Bajramovic, UU |
| 2013 | Cláudio Miguel Lousada Patrício, KTH | Claudio Torregrosa Martin, KTH | Johan Erlandsson, UU Patrik Berg, UU |
| 2014 | Victor Dykin, CTH | Kaur Tuttelberg, KTH | |
| 2015 | Cheuk Wah Lau, CTH; Klara Insulander Björk, CTH | Giulio Imbalzano, KTH | Johan Larsson, UU |
| 2016 | Luca Messina, KTH | Alicia Marie Raftery, KTH | Fredrik Höök UU Adam Bruce, UU |
| 2017 | Zsolt Elter, CTH | Mimmi Bäck, KTH | |
| 2018 | Klas Jareteg, CTH | Anna Benarosch, KTH | Daniel Karlsson, KTH Amanda Rasmussen, KTH |
| 2019 | Mattia Bergagio, KTH | | Daniel Fransén, KTH |
| 2020 | Kristina Lindgren, CTH | Govatsa Acharya, KTH Fredrik Dehlin, KTH | |
| 2021 | Magnus Boåsen, KTH | Emma Ekberg Berry, UU | |
| 2022 | Lojos Nagy, CTH | Georgios Zagoraios, KTH | |

| | | | |
|---|---|---|---|
| 2023 | Diogo Ribeiro Costa, KTH | Gabriela Lapinska, KTH | Wenhan Zhou, UU |

Aside from receiving recognition for outstanding research, the 2023 prize entailed a monetary reward of 75,000 SEK for the best PhD thesis, 40,000 SEK for the best Master's thesis and 30,000 SEK for the best Bachelor's thesis.

## Winners 2023

Diogo Ribeiro Costa was awarded the prize for best Doctoral thesis for his work Development of Encapsulated UN-UO2 Accident Tolerant Fuel.

The thesis was written at KTH with Pär Olsson as supervisor and the evaluation committee motivated their decision as follows:

*The thesis addresses the development of accident tolerant fuel in a very targeted and efficient way with a large output of journal papers describing a new fuel concept consisting of UN microspheres embedded in a UO2 fuel matrix* and also *that the candidate has shown great experimental skills to fabricate, characterize and investigate these new concepts and has shown to be able to efficiently collaborate with other researchers to efficiently generate results.*

The prize for the best MSc thesis was awarded to Gabriela Lapinska at KTH for her thesis Effect of Proton Irradiation on the Mechanical Properties of Fe-10Cr-4Al in Liquid Lead and the prize for the best BSc thesis was awarded to Wenhan Zhou at Uppsala University for his thesis Deep Neural Networks as Surrogate Models for Fuel Performance Codes.


*To the left: The SKC Director and the three winners. To the right: Diogo Costa, winner of the prize for best PhD Thesis*

# Student events during the year

## Seminar together with Westinghouse

On April $17^{th}$ SKC organized a seminar for students at KTH together with Westinghouse.

## Participation in career fairs at the Universities

SKC participated at the career fair CHARM at Chalmers on February $7\text{-}8^{th}$ and at UTNARM at Uppsala University on November $9^{th}$. The interest from the students to hear more about the nuclear industry was high and many visitors tried their knowledge in the area by answering the SKC quiz about nuclear energy in Sweden.  In Uppsala staff from Applied Nuclear Physics also participated in the SKC booth and talked about the courses and programs they offer.


*SKC at UTNARM together with staff from Applied Nuclear Physics at Uppsala University*

## Nuclear Thesis Speed dating

Nuclear Thesis Speed Dating events were arranged at KTH and Uppsala University during the autumn. The aim was to bring students and industry representatives together to discuss opportunities for thesis writing. All companies that provide working opportunities within the nuclear industry were invited to participate.

Each event started with short presentations by the participating companies which were followed by an opportunity for the students to walk around and talk to the industry representatives individually.

Most participants assessed the events as useful and hence similar events will be scheduled next year.

*Students talking to industry representatives at the Nuclear Thesis Speed Dating event at Uppsala University*

## Funding for student participation in Young Generation

Young Generation (YG) is a network for young professionals in the nuclear power industry which was launched in 1994 by the CEO of ABB Atom (today Westinghouse Electric Sweden). The initiative has continued ever since and also become global.

YG Sweden is open for professionals employed by the nuclear power industry who are up to 35 years but during 2023 YG also admitted two students, Erik Backlund and Matilda Dickman Ekvall, who received scholarships for their participations from SKC. Participation in YG Sweden consists joining a one-year-long programme consisting of three 2-day seminars and two themed study visits to nuclear facilities, employers or conferences.


*The two KTH students Erik Backlund and Matilda Dickman Ekvall who received scholarships from SKC for participation in YG 2023*

# Board Meetings and discussions

The board of SKC have had five meetings during the year to discuss ongoing and planned work. In connection to the meeting in May the Board also had an extended strategy discussion to prepare for the next program period.

# Advisory Councils

## Advisory Council for technicl questions

The SKC advisory council had four meeting during 2023. The main focus was to prepare for the next program period, to formulate a call for new research projects and to evaluate the received applications but the council also discussed the agenda for the Symposium, participation in YG, use of the base funding and other SKC issues.

*The SKC Advisory Council and the SKC Director at a meeting at Albanova University Center in June*

## Advisory Counsil for competence related questions

The main mission of SKC is to secure the availability of high-skill competence needed in the nuclear industry and to preserve high quality nuclear research and education in Sweden.

The current SKC advisory council was formed in 2011 to assist the SKC director and board in the planning and evaluation of technical activities. The council assists SKC in the effort to to preserve high quality nuclear research and education in Sweden. To get additional support with the other part of the SKC mission, i.e. to secure the availability of high-skill competence needed in the nuclear industry, SKC has initiated the formation of an additional advisory council focusing on competence related questions. Two initial meetings were held during 2023 and the decision was taken to include the new council in the work of SKC during the next program period.

# Call for new research projects

A call for new research projects was made September 1st and more than 20 applications were received and evaluated by the advisory council. The result was a recommendation to the SKC board to support eight new projects during the next program period.

# Participation in the SSM National radiation safety and research days

Competence supply was an important theme during the National radiation safety and research days that were organized by SSM on October 26-27th. SKC was mentioned several times as an important part in the work to secure future competence to the nuclear industry and the chairman of the SKC board Karl Bergman presented the work of SKC and the plans for the next program period.


*Karl Bergman presenting SKC at the National radiation safety and research days organized by SSM*

# Use of the Base Funding

# Distribution and use of the Base Funding

During 2023 the SKC base funding of 4 MSEK was distributed evenly among the three partner universities. In the next sections they describe how it has been used to promote research and education.

# Chalmers University of Technology

## General Information

Research and education in nuclear science and technology is carried out at Chalmers University of Technology by three entities:

- The Division of Subatomic, High Energy, and Plasma Physics (Department of Physics).
- The Division of Microstructure Physics (Department of Physics).
- The Nuclear Chemistry group, Division of Energy and Materials (Department of Chemistry and Chemical Engineering).

At the **Division of Subatomic, High Energy, and Plasma Physics**, activities in reactor physics, modelling and safety are pursued along two main tracks: computational nuclear reactor physics, and safeguard and core diagnostics, with applications to commercial reactors.

At the **Division of Microstructure Physics**, structural nuclear materials are characterized using electron microscopy and atom probe tomography. The main focus areas are fuel cladding and reactor pressure vessel steel.

At the **Nuclear Chemistry group**, the properties of atom nuclei using chemical methods and chemical processes are studied. A particular focus is on topics relevant to the entire fuel cycle: innovative fuel cycles, partitioning and transmutation, new types of nuclear fuel, pollution prevention in severe accidents, reactor water chemistry, and chemistry of the disposal of nuclear waste. Research is also pursued in the production of radiopharmaceuticals for cancer treatment and radio analytical chemistry for the measurement of radioactive substances in the environment.

Chalmers is also a member of SAINT (Swedish Academic Initiative for Nuclear Technology).

## Overview of base funding utilisation in 2023

The SKC base funding amounted to 1.33 MSEK for 2023 and was distributed as follows at Chalmers University of Technology:

- 0.538 MSEK to the Division of Subatomic, High Energy, and Plasma Physics.
- 0.304 MSEK to the Division of Microstructure Physics.
- 0.491 MSEK to the Nuclear Chemistry Group.

The use of the base funding at each group is described in the following sections.

### Division of Subatomic, High Energy, and Plasma Physics

The SKC base funding was mostly used to cover parts of the salary of Prof. Christophe Demazière and Assoc. Prof. Paolo Vinai.

3 PhD students, supervised by Prof. Demazière and Assoc. Prof. Vinai, worked in areas of direct interest to SKC:

- PhD student Kristoffer Tofveson Pedersen (SKC-sponsored XEROM project on Reduced Order Modelling of xenon instabilities).
- PhD student Hirepan Palomares Chavez (VR-sponsored HYBRID project on hybrid neutron transport methods applied to fast reactors).
- PhD student Salma Hussein (ANitA-sponsored project on core monitoring and diagnostics in SMRs using neutron noise and machine learning).

1 MSc thesis project was supervised by Prof. Christophe Demazière. The project was carried out by Fredrik Öhrlund and was titled "Non-linear time-dependent modelling of heterogeneous nuclear reactors – Applications to Xenon oscillations in pressurized water reactors".

Moreover, Yi Meng Chan, PhD student at KTH working on the use of artificial neural networks in reactor physics calculations, is co-supervised by Prof. Demazière (the main supervisor being Assoc. Prof. Jan Dufek at KTH).

In the area of education, the Division has been developing innovative pedagogical methods, combining flipped classroom and active learning methods, and offered in a hybrid learning environment. Such an environment allows offering courses to both on-site and off-site students and is thus suited to distant education and life-long learning. As a result of its expertise and following the same pedagogical principles, the Division has been coordinating the Horizon 2020 project GRE@T-PIONEeR project since 2020. The project aims at developing a specialized education in reactor physics and nuclear reactor safety for PhD and postdoc students, for nuclear engineers, and taken as advanced courses for MSc students. The education encompasses both theory and hands-on training exercises, the latter heavily relying on the use of research/training reactors and of computer-based modelling environments. The aim is for the students to be able to perform nuclear reactor safety simulations understanding all the approximations on which such simulations rely. The use of pre-recorded lectures and electronic teaching resources allows students to learn at their own pace and get prepared for the hands-on training sessions. Those sessions, offered both on-site and remotely, use active learning methods under the close supervision and support of the teachers, thus promoting student learning. Nine GRE@T-PIONEeR courses were offered in 2023. Chalmers was heavily involved in the teaching of four of those courses.

As part of the ENEN2+ Horizon 2020 project, a course on the "Deterministic modelling of nuclear reactor Multiphysics" was organized in late 2023, following the same pedagogical principles as for the GRE@T-PIONEeR project. 83 persons applied for the course (53 were accepted and enrolled in the course).

Despite the absence of a master program in nuclear engineering at Chalmers, the Division is involved in parts of a master course in Computational Continuum Physics, in which the practical exercises are all based on nuclear reactor simulation examples, thus increasing the visibility of this area to the Physics master students and possibly attracting them to MSc thesis projects in this area.

The members of the Division also act as guest lecturers in various courses at the Bachelor and Master level at Chalmers presenting nuclear power.

A new multi-disciplinary course in Chalmers titled "Modern Energy Technologies and Systems" was developed as a result of a collaboration between seven teachers in Chalmers led by Prof. Demazière, who is one of the teachers and also the examiner of the course. Such multi-disciplinary courses are referred to as a TRACKS courses in Chalmers. TRACKS courses offer much more flexibility (collaboration between different teachers from different departments, format, set-up, and courses offered typically to all Chalmers students, Chalmers Alumni, Chalmers employees, and professionals active in Sweden). The present course describes various carbon-neutral energy technologies to tackle climate change, their advantages/disadvantages and their interdependencies. By following the course, the students are able to understand how those technologies work and how they contribute to some of the United Nations Sustainable Development Goals. The course was first offered in the academic year 2023/2024 and had 35 applicants.

Applications for two additional TRACKS courses were prepared in 2023 and approved. A course titled "Nuclear reactor technology – past, present and future" and a course titled "Nuclear power safety" will be first offered during the academic year 2024/2025. Preparations are already on-going. The first course focuses on the development of nuclear reactor technology from its early days, how it works, its advantages, disadvantages, limitations, and how it contributes to some of the United Nations' Sustainable Development Goals. The second course details the principles of nuclear safety, the assessment of the risk associated with nuclear energy, and the implementation of safety in nuclear reactors.

Finally, following the Open Educational Resources (OER) initiative, three self-paced open course modules in nuclear engineering at an introductory level were developed:

- Nuclear power, an old story, presenting the history of nuclear power development.
- Nuclear reactor technology, presenting the technology and physics of nuclear reactors.

- Nuclear power, saving the world?, discussing how nuclear reactor technology could be used for climate mitigation.

The Division is actively involved in various networks in Sweden (SKC, SSM, SAINT, and a collaboration with KTH), as well as internationally (IAEA, ANS, ENEN and SNETP), and has been a contact point with SSM for discussing knowledge preservation in nuclear and radiation science.

In 2023, many applications for funding were prepared to various funding agencies (SSM, SKC, Energimyndigheten, Euratom).

#### Division of Microstructure Physics

The funding has mainly been used for the salaries of Assoc. Prof. Mattias Thuvander and Senior Professor Hans-Olof Andrén. Thuvander has been supervisor for one PhD student:

- Andrea Fazi (funded by SSF). Fazi defended his thesis "Development and performance evaluation of accident-tolerant coated fuel claddings for light water reactors" in February 2023. He is now employed at the division and works with an NKS-funded project on dissimilar welds, in cooperation with KTH and VTT.

Thuvander was furthermore supervisor of one post-docs:

- Dr David Mayweg. Mayweg has been doing research on irradiated zirconium cladding tubes, funded by SKC, and has participated in the EU-funded project ENTENTE on reactor pressure vessel steel.

Thuvander is leading an SSF project on ATF, involving Chalmers, KTH and UU. This project deals with coated claddings, alloying of UN and development of gamma emission tomography for fuel inspection. The SSF project ends in early 2024. Thuvander and Mayweg have carried out commissionary work for Studsvik Nuclear.

Regarding teaching, some nuclear materials issues are included in the master course "Physics of Materials".

During 2023, a new instrument for atom probe tomography has been commissioned at Chalmers, following a 32 MSEK grant from the Swedish Research council (VR). This tool is of importance for studying irradiation effects in claddings and RPV steel. This technique has been used in projects together with Studsvik Nuclear, and projects are planned for 2024.

Thuvander is taking part in the ANItA project on SMRs, funded by the Swedish Energy Agency, where a post-doc (Jennika Greer) will soon start. She will work on ion-irradiation of materials. A cooperation with NOMATEN, Poland, has been initiated concerning studies of ion-irradiated steels and high entropy alloys. Andrén is taking part in the on-going projects on cladding tubes at the division, and he is a member of the advisory board of the MIDAS project in the UK. The division takes part in mostly Swedish networks (SAINT and SKC) and Thuvander is member of SSM's "forskningsnämnd". An important activity during 2023 was to participate in writing research proposals to calls by SSM and the Energy Agency.

**Nuclear Chemistry group**

Nuclear Chemistry has several active courses (Nuclear Chemistry I and II, Solvent Extraction, Radiopharmacy) at Chalmers University at the MSc and PhD levels.

The group comprises currently 8 PhD students and 5 senior researchers in Nuclear Chemistry and recruitments are ongoing for two more students. 1 PhD student defended his work during 2023 within the areas of accident tolerant nuclear fuels.

### Senior staff

Professor Christian Ekberg, Professor Teodora Retegan-Vollmer, Dr Marcus Hedberg, Dr Stefan Allard and Dr Stellan Holgersson.

### Active PhD students

Fredrik Börjesson Sanden , Severe nuclear accidents, tellurium chemistry

Esraa Darwish, Separations for Gen IV systems

Georgios Zagoraios, 3d-printing of nitride fuels from recycled materials

Luca Gagliani, Corrosion of nuclear materials

Pawan Kumar, Sorption of radionuclides on minerals

Mustapha Saleh, Co-precipitation and leaching of U+Pu material

Dogac Tari, Fuel, cladding coolant interaction for lead bismuth coolants

Marvin Shobel, corrosion of metallic thorium

### Diploma workers

Isak Lundell and Sven Ekman in collaboration with UU, "Tillverkning av kalibrerstandard för ämnesbestämning i kärnbränslen"

During 2024, PhD students will be active in, e.g., corrosion studies of nuclear materials under irradiations, advanced manufacturing of nitride fuels, severe nuclear reactor accidents and their mitigation, separations for Gen IV, sorption of radionuclides from a final repository and fuel-coolant-cladding interactions.

The group is conducting research in several areas of the nuclear field, like safety of nuclear reactors, severe nuclear accident scenarios and advanced safety through research in Accident Tolerant Fuels as well as is involved in several EU projects (EURATOM). During 2023, 3 different proposals have been sent in. There are mainly in the field of nuclear fuel research but also regarding final repositories.

It is worth noting that the nuclear chemistry group is the only group dealing with radioactive material in amounts relevant to some industrial and research uses. We are also a nuclear installation. This means that there is a significant effort spent in practical radiation protection as well as on a more theoretical level in relation to all the requirements from the radiation protection authority. Thus, our personnel and students will be amply familiar with all these procedures as the only university facility in Sweden.

The SKC funding was used to cover the activities of Professor Christian Ekberg, Professor Teodora Retegan Vollmer, Dr. Stefan Allard, Dr Marcus Hedberg and Dr. Stellan Holgersson which are actively involved in teaching and research including radiation protection. During 2023 Professor Teodora Retegan Vollmer has been on parental leave the majority of the year. Special emphasis was put on supporting the coordination of a large-scale EU project in fuel cycle research as well as the national project ANITA coordinated by Uppsala University. Support has also been given in nuclear fuel manufacturing to, e.g., the KTH group and Westinghouse.

Both Prof. Ekberg and Prof. Retegan Vollmer are guest lecturers in various courses at the Bachelor and Master level, at Chalmers and also abroad.

Professor Ekberg is since 2022 coordinator of the EU project FREDMANS dealing with the recyclability of nuclear fuels with special emphasis on nitrides.

Prof. Retegan Vollmer is active in the 4th round of CINCH Project (currently called A-CINCH) standing for Cooperation in Education in Nuclear Chemistry in Europe, under EURATOM Horizon2020 program. The educational projects series have started in 2010 and aims at unifying the European curricula and teaching methodology at European level, by means of modern tools, including on-line teaching, learning and evaluation. We do have a close contact with our colleagues on physics from GRE@T-PIONEeR. She is also the Chalmers representative in ENEN+.

As our colleagues, we are active in various networks in Sweden (SKC, SAINT, and a collaboration with KTH) as well as international (ENEN, ANS, SNETP) as well as international collaborations on several EURATOM projects relevant for SKC.

During 2023, Chalmers hosted the international SNETP annual meeting during the Swedish chairmanship of the EU. This was organised by Prof. Teodora Retegan Vollmer and Prof. Christian Ekberg but due to prof Retegan Vollmers parental leave only Ekberg was on site for the event.

#### MSc and PhD theses completed in 2023

Andrea Fazi, "Development and performance evaluation of accident-tolerant coated fuel claddings for light water reactors", PhD thesis.

Luis Gonzales, "Fabrication and testing of doped uranium nitride as accident tolerant fuel alternative", PhD thesis.

Fredrik Öhrlund, "Non-linear time-dependent modelling of heterogeneous nuclear reactors – Applications to Xenon oscillations in pressurized water reactors", MSc thesis.

# KTH Royal Institute of Technology

## General Information

The following divisions and departments are engaged in nuclear education and research at KTH:

- Division of Nuclear Engineering / Department of Physics
- Division of Nuclear Power Safety / Department of Physics
- Division of Nuclear Physics / Department of Physics
- Group of Nuclear Chemistry / Department of Chemistry
- Division of Solid Mechanics / Department of Engineering Mechanics

The Centre for Nuclear Engineering at KTH (CEKERT) is the platform to coordinate nuclear education and research at KTH, with the involvement of 13 faculty members (7 professors and 6 associate professors) in 2023.

The Master's Programme run by KTH is among one of the largest Master's Programmes for nuclear technology education in the world in terms of the number of students and courses. So far more than 250 students have been admitted to the Programme. In 2023, totally 47 students are enrolled within the Master's Programme and the associated double-degree programmes (e.g.  EMINE).

## Overview of base funding utilisation in 2023

The SKC base funding to KTH has been a vital component in keeping the critical activities of Nuclear Engineering education alive at KTH, since the actives are not fully supported by KTH alone.

The SKC base funding to KTH in 2023 was 1,333,000 SEK, among which 650 000 SEK was used to pay the partial salaries of the 13 faculty members (50 000 SEK per member), who were involved in the general education of BSc, MSc and PhD students. The remaining SKC base funding to KTH was used to pay partial salaries of the director and the deputy of the Master's Programme in Nuclear Energy Engineering for their management of the programme, and partial salaries of teachers who taught courses in the programme.

The usage of the SKC base funding is summarized as in the following table.

| Areas of support | Items | Cost calculations | Costs (SEK) |
|---|---|---|---|
| Faculty members | – 7 professors<br>– 6 associate professors | 50 hours per faculty member spent on preparation of teaching materials and supervision of postgraduate students (hourly rate of 1000 SEK) | 650,000 |
| Master's programme management | – Programme director and deputy | 208 hours of work for Assoc Prof Jan Dufek and Dr Vasily Arzhanov | 285,000 |
| Lab exercises on the VR-1 training reactor (covering a partial cost) | – VR-1 training fee<br>– Hotel<br>– Flights | 29 students * 10000 SEK/person | 290,000 |
| Courses | – Fees for external lecturers* in the course SH2610<br>– License fee for the APROS code in the course SH2705 | – 50,000 SEK for the invited lecturers<br>– 38,000 SEK for the license fee of the APROS code | 88,000 |
| Misc | – CEKERT:s kansli | – 20,000 | 20,000 |
| **Total** | | | **1,333,000** |

* Kerstin Dahlgren, Lennart Carlsson, Anders Jörle, Tord Sterner, Per Lindell, Lars Axelsson, Martin Luthander

The faculty members that have benefitted from the SKC funding and their contributions to teaching and supervision are summarized in the following table.

| Faculty member | Courses offered in 2023 | Postgraduate students supervised in 2023 |
|---|---|---|
| Prof. Olsson / Pär | SH2605: Radiation damage in materials<br>SH2774: Numerical methods in nuclear engineering<br>SH3141: Multi-scale modelling of nuclear materials | Ebrahim Mansouri (PhD)<br>Elina Charatsidou (PhD)<br>Maria Giamouridou (PhD)<br>Qiuguo Yang (PhD)<br>Franck Louba Nadji (PhD)<br>Kaitlyn Bullock (MSc)<br>Aurora Jahan (MSc)<br>Luis Guerra (MSc)<br>Kamila Oppelova (MSc)<br>Matilda Dickman Ekvall (MSc) |
| Prof. Wallenius/ Janne | SH2613: Generation-IV reactors<br>SH2615: Neutron transport theory<br>SH2611: Small modular reactors<br>SH2772: Chemistry and physics of nuclear fuels | |

| | | |
|---|---|---|
| | SH2614: The nuclear fuel cycle<br><br>SH3500: Non-proliferation of nuclear materials | |
| Assoc. Prof. Kudinov / Pavel | SH2702: Nuclear reactor technology | |
| Assoc. Prof. Dufek / Jan | SH2600/ SH2601: Reactor physics<br><br>SH2704: Monte Carlo methods and simulations in nuclear technology<br><br>SH2009: Project work in physics, smaller course | Yi Meng Chan (PhD)<br>Lei Shi (MSc) |
| Prof. Bechta / Sevostian | SH2610: Leadership for safe nuclear power industry | Lu Zhao (PhD)<br>Liang Chen (PhD)<br>Graeme Trundle (PhD)<br>Xiangyu Li (PhD) |
| Assoc. Prof. Ma / Weimin | SH2612/FSH3773: Nuclear power safety<br><br>SH2705: Compact reactor simulator<br>SH2706: Sustainable energy transformation technologies<br><br>SH2701: Thermal hydraulics in nuclear energy engineering | Yan Xiang (PhD)<br>Yucheng Deng (PhD)<br>Wanhong Wang (PhD)<br>Di Fang (PhD)<br>Disen Liang (PhD)<br>Björn Engström (PhD)<br>Karl-Edvin Strand (MSc)<br>G. Delesalle (MSc) |
| Prof. Cederwall / Bo | SH2302: Nuclear physics<br><br>SH3301: Experimental nuclear physics<br>SH2306/FSH3306: Experimental techniques for nuclear and particle physics | Jana Vasiljevic (PhD)<br>Vivian Peters (PhD) |
| Prof. Nyberg / Ayse | SH2306: Experimental techniques for nuclear and particle physics<br><br>SH2101/SH2102: Subatomic physics | |
| Assoc. Prof. Bäck / Torbjörn | SH2603: Radiation, protection, dosimetry and detectors<br><br>SH2007: Research methodology in physics | Linda Eliasson (PhD)<br>Ebba Cederlöf (PhD).<br>Nicolas Cortonne (MSc)<br>Jarl Wallheden (MSc) |
| Assoc. Prof. Qi / Chong | SH2011: Theoretical nuclear physics<br><br>SH3311: Theoretical nuclear physics<br><br>SH3312: Symmetries in physical systems<br><br>SH3313: Quantum many body physics | Daniel Karlsson (PhD)<br>Mateo Bellouard (MSc) |
| Prof. Jonsson / Mats | CE2010: Nuclear chemistry<br><br>KD2370: Photo, radiation and radical chemistry | Yi Yang (PhD)<br>Junyi Li (PhD)<br>Daniel Olsson (PhD)<br>Felicia Karlahag (PhD)<br><br>Luca Gagliani (PhD)<br><br>Fredrik Petersson (MSc-PhD) |
| Adj. Prof. Efsing / Pål | SE2137: Fatigue | Mustafa Subasic (PhD)<br>Michal Sedlak (Post/Dr)<br>Peter Enblom (MSc)<br>Aaron Ireland (MSc) |
| Prof. Faleskog / Jonas | SE2139: Fracture mechanics<br><br>SE2860: FEM modelling | Shuyue Wang (PhD)<br>Daniela Klein (PhD) |

# Uppsala University

## General Information

Research and education within nuclear science and technology at the division of applied nuclear physics at Uppsala University span a wide range of topics. Current research and development are being conducted within the following areas:

- nuclear waste management, including spent fuel,
- nuclear data, including uncertainty propagation in nuclear systems,
- nuclear safeguards and non-proliferation,
- fuel performance modelling and experiments,
- design of instrumentation for studies of nuclear fuel behaviour,
- detector development for radioactivity monitoring

SKC provides an important contribution to the research listed above in the form of base funding and/or specific project funding. This funding complements faculty funding and external funding from, for example, the Swedish Research Council (VR) and the Swedish Foundation for Strategic Research (SSF). The research is performed in close collaboration with both national and international partners. International partners include IAEA, LANL, INL, SCK CEN, NEA, GANIL, JRC, Jyväskylä University, HRP, ESARDA and others.

Uppsala University provides education in nuclear science and technology on all levels, which includes teaching and supervision of students. Additionally, a substantial volume of contract education directed towards industry and authorities is provided and is available through Uppsala University's portal "Nordic Academy for Nuclear Safety and Security, NANSS".

## Overview of base funding utilisation in 2023

SKC's base funding is used for supporting efforts in research, teaching courses that are in line with SKC's goals and supporting extensive outreach. For example, UU can support initiatives that are outside regular activities aiming at finding opportunities for new research projects. An overall report of the use of funds for 2023 is provided below.

## Staff

During 2023 the salaries for the following individuals have to a various degree been supported by the SKC base funding.

**Prof. Ane Håkansson** has been devoted to outreach and supervision in parallel to the work as director of the national competence centre ANItA (Academic-industrial Nuclear technology Initiative to Achieve a sustainable energy future). ANItA's mission is, among other things, to provide society with adequate knowledge to implement small modular light-water reactors in Sweden.

Part of this outreach, which certainly is of value also for SKC, is to take advantage of every opportunity to spread the message about what nuclear power is and what values nuclear power has given and may bring to society in the future. There has been a great deal of interest from various associations, not least political associations, to take part in this message. This has meant appearances on more than ten occasions in 2023 with typically between twenty and fifty participants on each occasion.

**Dr. Peter Andersson** performed work in the development of novel approaches for post-irradiation examination within the framework of his starting grant from the Swedish Research Council. This work entails detector and instrument development for improved spatial resolution in gamma emission tomography of irradiated nuclear fuel and also gamma-ray micro-densitometry of irradiated nuclear fuel, in order to obtain the radial swelling profile. The latter work was performed in collaboration with Studsvik Nuclear, where a transmission densitometer for nuclear fuel was assembled and successfully tested on an ADOPT pellet. TBq sources of Co-60 are used to interrogate the fuel density. Two students under Peter's supervision defended their PhD dissertations in June 2023. Lorenzo Senis and Vikram Rathore.

**Assoc. Prof. Henrik Sjöstrand and Dr. Erik Andersson Sundén** have continued to work with the development of nuclear data evaluation methods for structural materials such as iron and chromium. In addition, Henrik has done some preliminary work on project B1 within ANItA: "Fuel assembly and core design optimization for SMRs".

**Dr. Diego Tarrío** has been working on new experiments to study neutron-induced reactions at the new neutron facility NFS at GANIL, France. In particular, in the study of differential cross-sections of light-ion emission on different materials when irradiated with neutrons. Some experimental campaigns have been done in the recent years to develop the Medley setup and to make it suitable for use in a pulsed neutron beam with a white spectrum, like the one available at NFS, which covers from 1 up to 40 MeV in neutron energy. During 2023, a new experimental campaign took place, in which iron and chromium were the studied materials. The experiments had been led by the Uppsala group, in close collaboration with the local team from GANIL. A new Ph.D. student (Lucas de Arruda) is working on the project, by doing a joint Ph.D. between UU and the University of Caen-Normandy (France). The student is analyzing the data collected in the different experiments done with Medley, and has presented the status of the analysis in some scientific meetings. Dr. Tarrío and Prof. Stephan Pomp, from UU, and Dr. Xavier Ledoux from GANIL are supervising this Ph.D. project.

Moreover, Dr. Tarrío is also working in experiments at the neutron time-of-flight facility n_TOF at CERN. Together with colleagues from the University of Santiago (Spain), and the local team at CERN-n_TOF, he is preparing a new experiment to deep into fundamental aspects of the fission process induced by high-energy neutrons.

**Dr. Mattias Lantz** has during 2023, together with Assoc. Prof. Cecilia Gustavsson and Dr. Erik Andersson-Sundén, used the UGGLA facility in a number of different projects. Dr. Lantz has supervised the following student projects. Arvid Sandström performed his BSc diploma work by using UGGLA and another HPGe detector for gamma-spectroscopic background measurements at different locations at Ångströmlaboratoriet. The measured data were compared with measurements at the Forsmark nuclear power plant. Part of the M.Sc. Diploma work of Etienne Varenne-Paquet was focused on investigating the background contributions of the UGGLA facility, and suggesting actions for how to reduce them. Lisa Hessentaler performed a student project where she compared the levels of potassium-40 in different vegetables. Elias St. Onge Arnqvist performed a student project where metal foils irradiated at the NESSA2.5 neutron source were measured with the UGGLA facility in order to identify activation products and deduce the neutron field from NESSA2.5. Elias St. Onge Arnqvist also performed a project where he systematically tested and calibrated nine NaI scintillator detectors. In August 2023 Dr. Lantz arranged a summer school on nuclear power for 22 European students through the BEST network. The UGGLA facility was used during the summer school in a laboratory exercise.

**Assoc. Prof. Andreas Solders** has, together with his Ph.D. student Zhihao Gao, continued the research on fission yields in collaboration with the University of Jyväskylä, a project that is partly funded from the Swedish Research Council. In december 2023, Gao defended his doctoral thesis. The thesis contain five published papers, describing the progress of the design of a new ion guide for neutron induced fission, a new method to analyze the data using machine learning and improved decay corrections, and the result of the measurement of 19 isomeric yield ratios in proton induced fission. It also contains an unpublished manuscript on how to derive angular momentum distributions of the fission fragments from the experimentally determined isomeric yield ratios, to be published in 2024.

**Dr. Ali Al-Adili** has continued to analyse fission-neutron data obtained from a fast-fission experiment on U-235. This experiment builds upon previous thermal measurements and required six weeks of beam time at the MONNET Tandem facility at JRC in Geel, Belgium. With financial support from the Swedish Research Council, Al-Adili and Ph.D. student Ana Maria Gomez Londoño have been developing the VERDI (Velocity for Direct Particle Identification) spectrometer for fission- yield and neutron studies. Their primary focus has been on characterising PIPS detectors and Micro Channel Plates (MCP) for detecting fission fragments, both at the LOHENGRIN facility located at the ILL high-flux reactor in Grenoble, France and at the JRC. Recently Gomez defended her Licentiate thesis successfully and a full journal paper from the LOHENGIN campaign is in preparation for submission. The team recently secured funding from Carl Tryggers foundation to purchase new MCPs for VERDI. The new detectors were successfully installed and tested. In addition, Dr. Al-Adili has collaborated with colleagues from the IAEA's nuclear data section on theoretical fission modelling, resulting in a publication and has supervised the Master theses of Peter Karlsson and Steven Bjil. Finally, a new supervision project is starting in partnership with SCK CEN, featuring Elias Arnqvist's work to analyse the neutron response function of a novel scintillator detector.

### Staff changes

During the year, we have unfortunately lost several employees who have gone to other activities outside academia. This has created an increased workload for the division as a whole and have forced us to distribute funds in a different way than planned. However, we can state that through this procedure we have been able to maintain the volume of our teaching and research activities.

### Infrastructure

The above-mentioned SKC-funded activities in the division of applied nuclear physics are heavily dependent on the availability of adequate experimental infrastructure. Besides laboratories abroad and, to some extent, Clab in Oskarshamn, significant efforts have been made to establish experimental infrastructure on-site in Uppsala. Funding for personnel working on infrastructure development comes to a small degree from SKC, and largely relies on other funding sources.

#### NESSA

Late 2022 we were forced to terminate the contract with the vendor of the neutron generator, since it became clear that they are not capable of delivering the generator according to specifications in the contract. During spring 2023, we eventually agreed on a settlement with the vendor and are now planning for a new procurement process. To that end, SKC approved during autumn 2023 to fund a postdoctoral position. In 2024, we will thus be able to hire a candidate and can give the facility development the needed restart.

#### BETTAN

The BETTAN facility is an experimental platform for developing measuring strategies and algorithms for tomographic applications including nuclear fuel. A unique feature of BETTAN is that irradiated fuel assemblies are simulated with pipes filled with a radioactive substance that can be robotically arranged into various fuel geometries. During 2023 the BETTAN platform was successfully returned to operating status after many years of inoperation. Experimental activities using BETTAN were carried out during 2023 and the results thereof are parts of the Ph.D. theses defended by Vikram Ratore and Lorenzo Senis. Further utilization of BETTAN is planned in 2024 in collaboration with Helsinki Institute of Physics.

#### UGGLA

The Uppsala Generic Gamma Laboratory (UGGLA) has been used for data taking from environmental samples during 2023. Measurements have also been performed on samples irradiated by neutrons in order to characterise the so-called NESSA2.5 neutron irradiation facility. The analysis methods have been significantly improved compared with earlier projects, which will be very useful for future projects with the planned NESSA facility. Several studies of the UGGLA facility has been performed in order to investigate the background contribution, and the sensitivity of the detector setup with respect to geometrical aspects of the measured samples.

## Supported teaching

The teaching supported by SKC included the following courses.

| | | |
|---|---|---|
| Civ ES4, STS5 | Kärnkraft - teknik och system | 1FA410 |
| Civ F4, Master | Energifysik II med kärnkraft | 1FA403 |
| Civ F4, Fk3, Master, GyL | Energifysik I | 1FA402 |
| Civ F4, Master | Energifysik II med kärnkraft | 1FA403 |
| ES4 | Säkerhetsanalyser inom energisektorn 33%, Dagtid, Normal, Sv | 1FA594 |
| Civ STS | Komplexa system i teknik och samhälle - teknik | 1FA455 |
| Master | Modellering och simulering av partikeltransport | 1FA451 |
| fristående | Introduktion till kärnkraft | 1FA400 |
| Civ STS3 | Energisystemfysik | 1FA401 |
| Civ ES4, STS5 | Kärnkraft - teknik och system | 1FA410 |
| fristående | Introduktion till kärnkraft | 1FA400 |
| Civ ES4 | Framtida nukleära energisystem - analyser och simuleringar | 1FA412 |

## Finished Diploma work

Dimitrios Zisis, master, *Design of a New Penning Trap for SPECTRAP*

Sigfrid Stjärnholm, master, *Propagation of Nuclear Data Uncertainties for Reactor Physics Parameters in Fluorine-19-based Molten Salt Reactors*

Steven Henrik Bijl, master, *Machine Learning for Pulse Shape Analysis of Heavy Ions*

Gustav Södergren, ES, *District heating with small modular reactors utilising an adaptive a-value*

Waldermar Andersson, ES, *Non-proliferation and safeguards aspects of SMR's in Sweden: A study on the future electricity demand in Sweden and the implications on nuclear safeguards from the deployment of SMRs in Sweden*

Jonathan Eriksson, ES, *Monte Carlo analysis of BWR transients: A study on the Best Estimate Plus Uncertainty methodology within safety analyses at Forsmark 3*

Erik Backlund, ES, *Modellering, simulering och analys av kärnreaktorn BWRX-300*

Matilda Tiberg, F, *Simulation of IB-LOCA in TRACE: A semi-blind study of numerical simulations compared to the PKL test facility*

Peter Karlsson, F, *Total Monte Carlo of the fission model in GEF and its influence on the nuclear evaporation in TALYS*

André Pousette, KandFy, *Simulations of energy losses of fission fragments in Mylar foils at LOHENGRIN*

Johan Uggla, Willy Ohlsson, KKI, *Datorbaserad reaktorsimulator för utbildningssyfte*

Theodor Gunnberg Querat, Gustaf Krottler, KKI, *Modell för digitalisering av kurs: Reaktorfysik grund KSU*

Hanna Damsgard Falck, Julia Ibstedt, CIV F, *Machine learning analysis of Finnish spent nuclear fuel measurements*

Isak Hedberg, Axel Hallander, Stina Fredriksson, Civ F, kand, *Assessment of How Design and Operational Parameters Affect Plutonium Production for Pressurized Heavy Water Reactors: A Study of the Ågesta, NRX and CANDU Reactors*

# Research Projects funded by SKC

# Introduction

Project funding decisions for the program period 2020-2023 were made in 2020. The projects were started during 2020 and 2021 and are described below.

# Study of core stability during load follow with ROM methods (2019-1)

Research host:
Chalmers University of Technology
Department of Physics

Doctoral Student:
Kristoffer Tofveson Pedersen

Formal project start:
2020-09-01

Expected completion time:
2025-08-31

Main Supervisor:
Prof. Christophe Demazière

Co-supervisor:
Assoc. Prof. Paolo Vinai

## Motivation

With the decreasing share of electricity produced by nuclear power in Sweden in the years to come and the corresponding increasing share of electricity produced by wind and solar power systems, an increasing reliance on intermittent energy sources in the Swedish grid is expected. As a result of this, the Swedish nuclear fleet will have to shift from a base load production mode to a load-follow production mode.

Adjusting the reactor power to follow the demand on the grid might nevertheless result in instabilities in the neutron flux under unfavourable core conditions, caused by the production/consumption of the xenon fission product. Such oscillations have a period of ca. 15-30 hours. Because of their relatively long period, the oscillations might remain unnoticed before they develop significantly, then requiring operator action in form of partial control rod insertion. In addition to detecting these oscillations when they develop, it is of utmost importance to determine whether a core configuration is stable or unstable with concerning xenon oscillations.

In this PhD project, Reduced-Order Model (ROM) techniques are used to study the stability properties of nuclear reactors during load follow conditions. In a ROM, the balance equations describing the time- and space-dependence of the neutron flux are projected onto a few properly chosen basis functions of space only. The main advantage of a ROM is to replace the complexity of the modelling of a nuclear reactor with a set of reduced balance equations, which adequately describe the physical phenomena being considered.

The main objective of the work is to be able to understand the parameters involved when studying the stability of a nuclear reactor concerning load-follow conditions and to be able to assess whether a core loading is stable or unstable directly from the ROM, without turning to lengthy and complex high-fidelity simulations.

## Progress

The PhD project started on September 1st, 2020. Since then, a three-dimensional heterogeneous PWR core model was considered and used as a basis to construct an equivalent three-dimensional homogeneous core model. From this, the governing equations could be derived in a simple linear one-energy group form to maximise the transparency of the underlying physics. A "physics"-based ROM was developed. The spatial basis functions, on which the spatial dependence of the neutron flux is projected, were chosen as the eigenmodes of the neutron diffusion operator. From this expansion, the time dependence of each mode was derived analytically, as well as computed numerically. Both approaches led to identical results when using the same assumptions. The main advantage of the numerical approach lies in the capability to resolve the true interdependency between the modes. The analytical approach, on the other hand, allows for identifying which modes are driving any oscillatory or diverging behaviour. These results were an offset to creating a similar 3-dimensional heterogeneous model with two energy groups. The model was compared to the one-group homogeneous model to analyse the effects of increasing the spatial and energy resolution of the ROM. The two-group heterogeneous model predicted a significantly more unstable system than its simpler counterpart. The terms of the underlying equations responsible for the difference were identified. The coupling between modes was dependent on inner products between the adjoint and forward modes as well as either the equilibrium flux or the equilibrium xenon distribution. The normalised axial shape of two of these functions is shown in the figure below.

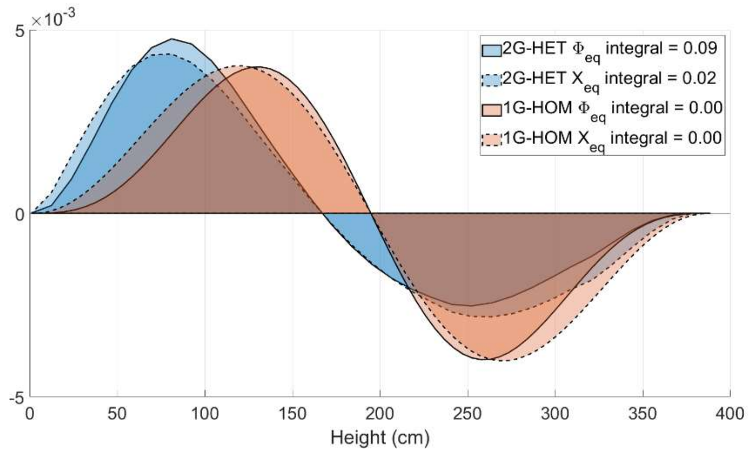


*Figure 1 Comparison of the axial shape of two integrands between each of the two models along with the value of integration.*

The discrepancy could be caused by an inconsistent feedback term between the different models. Consequently, work has been done to correct this. The results of this work will soon be ready for publication.

A significant amount of collaborative work has been undertaken with the Ringhals AB nuclear core analysis group to simulate high-fidelity reference data based on real data from R3 and R4 at Ringhals utilizing SIMULATE 5. This dataset will be used to validate the reduced order model across various core configurations. A total of 13 different cases were simulated encompassing different cycles, core ages and reactors.

As part of a master project, a nodal non-linear time-dependent solver to model xenon oscillations was developed by Fredrik Öhrlund. This code could potentially serve to further validate the reduced order model and might be used internally on sets of three-dimensional macroscopic cross-section data to model the xenon-iodine dynamics of a reactor core.

Once the model has been compared to the high-fidelity simulation data and thoroughly analysed, another publication will be made of the findings.

## Method

The physics-based intrusive ROM is developed using a linear approximation of the diffusion equations. As such the model is only valid for small perturbations of neutron flux and xenon and iodine concentrations, which should still be sufficient to derive the system stability regarding xenon oscillations. To reduce the high number of degrees of freedom in a three-dimensional full-core analysis, this model uses modal methods to project the behaviour of the core onto a few eigenmodes of the equilibrium flux. The reduced order model enables the calculation of xenon-iodine dynamics throughout tens of hours in less than a minute, a task that would typically require much more time using conventional methods. Furthermore, the projection of the solution onto the eigenmodes of the system enhances the interpretability of the results compared to conventional methods.

Reference simulations are conducted using Studsvik Scandpower's code SIMULATE 5 and performed by the nuclear core analysis group at Ringhals. For this real reactor, data such as macroscopic cross sections, neutron flux and xenon and iodine concentrations serve as starting points for the simulation. A simulated perturbation is introduced, followed by the simulation of free xenon oscillations without control from boron injection or control rods for a duration of 75 hours.

## Communications

The project was presented at the SKC annual symposium at KTH on October 16$^{th}$ -17$^{th}$, 2023. A conference paper on the two-group heterogeneous model was accepted and presented at the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C), held on August 13$^{th}$-17$^{th}$ 2023 in Niagara Falls, Canada. A scientific poster of the project was presented at the SSM event "Nationella strålsäkerhets- och forskningsdagar" on October 26$^{th}$-27$^{th}$, 2023 as well as at the Annual meeting of the Danish Physical Society on November 13$^{th}$ – 14$^{th}$, 2023. The Licentiate thesis was successfully defended on September 19$^{th}$, 2023.

# Influence of ageing and radiation on ductile fracture in the DBT temperature region (2019-2)

Research host:
KTH Royal Institute of Technology
Department of Engineering Mechanics

Doctoral Student:
Shuyue Wang

Formal project start:
2020-08-17

Expected completion time:
2025-06-25

Main Supervisor:
Jonas Faleskog

## Motivation

Ductile fracture involves a significant amount of plastic dissipation which increases the resistance of a material to withstand the growth of existing defects to failure. However, long-term operation at elevated temperatures may lead to a degradation of this resistance and consequently a less ductile material. If the material also is subjected to a hostile environment as found in nuclear power plants, this degradation can be accelerated.

The objective of the proposed study is to understand the influence of time-dependent ageing and degradation mechanisms on the ductile behaviour of low alloy steels at temperatures above the Ductile to Brittle transition temperature, DBTT. Specifically, the possible influence of microstructural entities and defects on the scale ranging from about ten nanometers to one millimeter combined with an overall change in plastic flow properties on ductile fracture will be investigated. The work involves the development of theory, numerical methods, and experiments. The study aims to develop a numerical tool to analyse and predict how ductile failure can be affected by aging and radiation in elevated temperatures above DBT.

## Progress

The project started in August 2020 and has since focused on developing the constitutive model capable to capture crack initiation and propagation in a structure. The classical damage continuum mechanics material model is not sufficient to describe crack initiation and propagation where the numerical problem arises with strain softening and localization. To solve strain localization, a non-local constitutive model using two length scales associated with two different failure mechanisms – shear failure by void sheet formulation, and flat dimple rapture – has been developed and implemented into a Finite Element Method program. Numerical models for different test geometries have been developed to capture possible modes of failure in the material during degradation. Tensile geometries prone to flat dimple rupture, shear-type of geometries prone to shear failure, and a fracture test geometry with sharp crack have been investigated. Careful numerical studies have been carried out and the modelling concept has proven capable of capturing the relevant modes of failure occurring at different length scales as observed in experiments. Possible failure modes of a uniaxial tensile test are shown as an example in Figure 1.

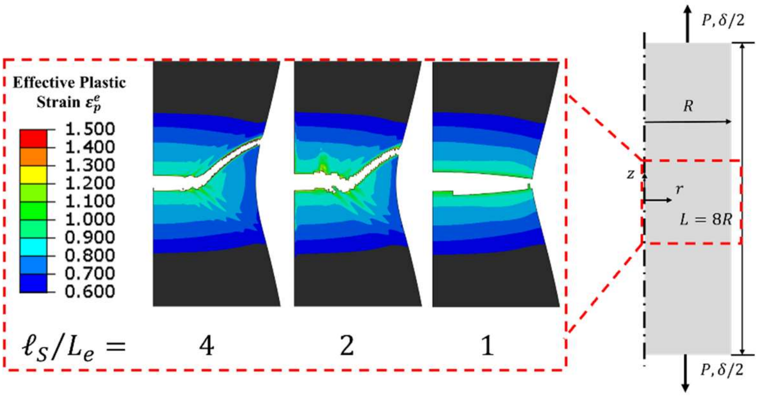


*Figure 1. Possible failure modes in a uniaxial tensile test captured by the numerical analysis.*

Experiments have been carried out on low alloy steel A508 with similar ductile properties and corresponds to a forged version of A533B. The experimental data sets are used to calibrate and validate the numerical modelling framework. The framework will be further applied to experiments to be conducted on the referential and aged weld material taken from the decommissioned pressurizer from Ringhals 2. The experimental results and numerical studies on the latter material is expected to clarify the influence of ageing and degradation mechanisms on ductile failure at elevated temperatures, and thus give a sound basis for the assessment of the structural integrity and improve nuclear safety. The calibration of the numerical model using experimental data sets from material A508 is in progress. Figure 2 presents the failure modes and the global responses of the fracture test with deep/shallow crack in black/red, respectively. The experiments based on material A533 have been planned and are on schedule.

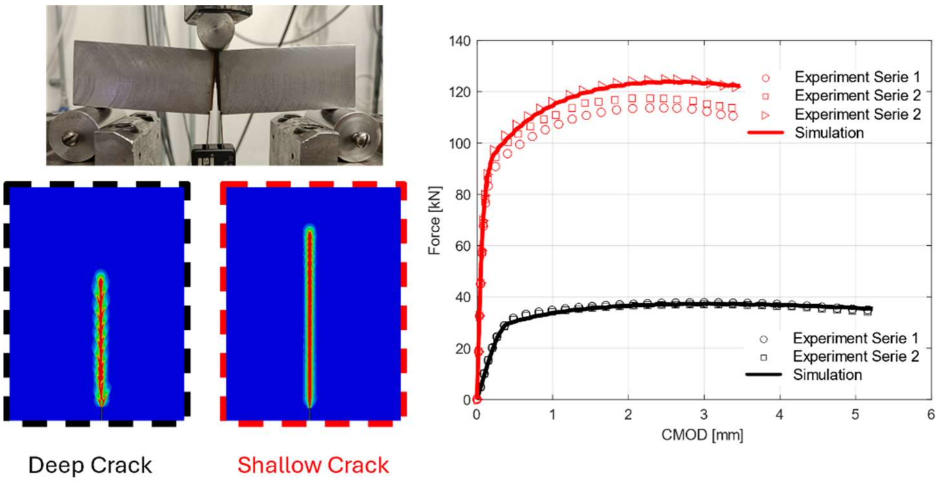


*Figure 2. The global response of fracture tests using material A508.*

It has been observed that failure modes in uniaxial tensile test is controlled by length scales. The need to effectively separate these scales for accurate characterization of cup cone failure is illuminated through extensive tests results. Furthermore, the role of specimen diameter in shaping failure mechanisms is showed. The failure mode shifts to cup-cup failure as the diameter decreases and aligns with length scales. Thus, a spin-off side project has been created and is in progress, focusing on how size effect of the uniaxial tensile specimen influences the failure modes. The purpose of this investigation is to increase the understanding of how specimen dimensions affect failure behaviour. Figure 3 presents the scanned fracture surface classical cup-cone failure observed in uniaxial tensile specimens with three deformed diameters, and Figure 4 shows the cup-cup failure captured by SEM.

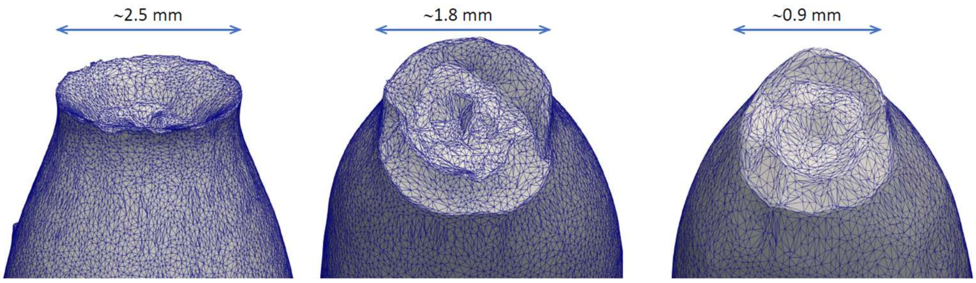


*Figure 3. Classic cup cone failure presented in uniaxial tensile specimens.*

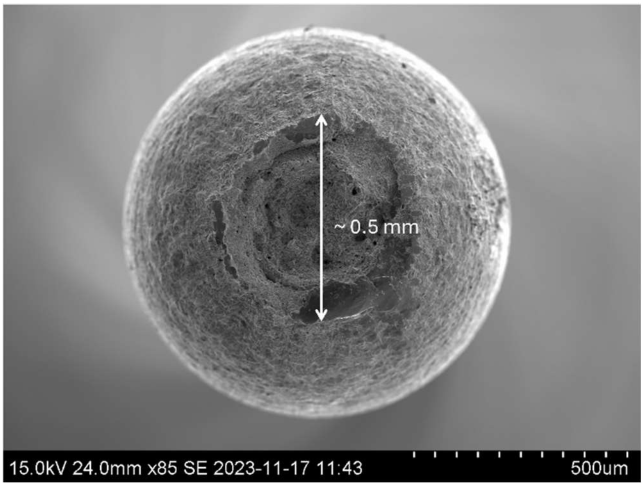


*Figure 4. Cup-cup failure presented in a uniaxial tensile specimen.*

## Methodology

The degradation of weld material used in nuclear power plants will be systematically investigated in the upper transition to the upper shelf region by experiments. The constitutive material model is based on the damage model known as the Gurson-Tvergaard-Needleman model (GTN model) modified for shear failure.

In the GTN model, damage evolution is described by a state variable $f$ corresponding to the void volume fraction in the material and the yield condition $\Phi$ is defined by

$$\Phi = \left(\frac{\sigma_\mathrm{e}}{\sigma_\mathrm{M}}\right)^2 + 2f^* q_1 \cosh\frac{3q_2\sigma_\mathrm{h}}{2\sigma_\mathrm{M}} - (1 + q_2 f^*)^2 = 0,$$

where $\sigma_\mathrm{e}$ is the effective stress, $\sigma_\mathrm{h}$ is the hydrostatic stress, $\sigma_\mathrm{M}$ is the flow stress of the matrix material, and $q_1$ and $q_2$ are two material constants. The model assumes that plastic localization and degradation of the material involves damage mechanisms that are active in two different length scales, a deviatoric $R_s$ and a dilatational $R_h$. The introduction of these length scales, rendering the constitutive description to be non-local, prevents a premature and non-physical strain localization and avoids a pathological mesh dependency. Here, an integral approach is used to for non-local treatment of evolution void volume fraction, $\dot{f}$. The non-local damage evolution can be either conducted in the referential or the spatial configuration. In the reference configuration with material volume $V_0$, the damage evolution at a material point $\mathbf{X}$ is obtained by

$$\dot{f} = \frac{1}{W_{\mathrm{h}}(\mathbf{X})}\int_{V_0} \dot{f}^{h}_{\mathrm{local}}(\tilde{\mathbf{X}})w\frac{\mathbf{X}-\tilde{\mathbf{X}}}{R_{\mathrm{h}}}d\tilde{V} + \frac{1}{W_{\mathrm{s}}(\mathbf{X})}\int_{V_0} \dot{f}^{\mathrm{s}}_{\mathrm{local}}(\tilde{\mathbf{X}})w\frac{\mathbf{X}-\tilde{\mathbf{X}}}{R_s}d\tilde{V},$$

where $W_{\mathrm{s}}$ and $W_{\mathrm{h}}$ are the deviatoric and dilatational volume integral of the weight function $w$, respectively.

## Communication

The project was presented and is planned to be presented at the following international and national conferences and seminars:

- EMMC18 - 18th European Mechanics of Materials Conference, Oxford, United Kingdom, April 2022;
- Seminar at Vattenfall, Solna, Sweden, May 2022;
- SMD Svenska Mekanikdagar 2022, Luleå, Sweden, June 2022;
- Seminar at Kiwa, Stockholm, Sweden, November 2022;
- ICF15 -15th International Conference on Fracture, Atlanta Georgia, United States, June 2023;
- COMPLAS 2023 - XVII International Conference on Computational Plasticity, Barcelona, Spain, September 2023.
- Workshop on ductile fracture, Paris, September 27-29, 2023.

Publication:

- Wang S., Faleskog J., 2023, *A non-local GTN model with two length scales – application to ductile failure in a wide range of stress triaxiality*, Eur. J. Mech. A Solids 105056.

Further publications are in preparation:

- Calibration and verification of the numerical modelling framework based on experimental data sets using A508 (planned submission).
- Investigation of size effect on the cup con failure of uniaxial tensile test (under progress).

# Corrosion fatigue in LWR environment at cyclic thermal and mechanical loads (2019-4)

Research host:
KTH Royal Institute of Technology
Department of Engineering Mechanics

Doctoral Student:
Mustafa Subasic

Formal project start:
2020-08-17

Expected completion time:
2025-08-31

Main Supervisor:
Pål Efsing

## Motivation

Corrosion fatigue is a well-known degradation phenomenon in structural materials that may develop as a consequence of long-time exposure of components to cyclic thermal or mechanical loads at the presence of an aggressive environment in many industrial applications. If left unattended it will result in failures of the affected components. One such application is the piping systems in nuclear power plants where the water introduces an increased environmental risk for fatigue initiation. The existing Swedish nuclear power plants rapidly approaches the originally assumed service life of 40 years. The remaining 6 nuclear power plants in Sweden all have programs for life extension from 40 to 60 years, called Long Term Operation, LTO. The overall research objective is to add knowledge about the degradation mechanism, which can be used by the plant operators and the regulatory body during assessment of the readiness for LTO of the Swedish nuclear power plants. The objective of the project is to develop an improved risk and life prediction method for corrosion fatigue in the pipe systems.

The project results will be distributed to the engineers working at the Swedish nuclear power plants for review and dissemination. The overall goal is that the results together with other available sources of data can lead to improved assessment tools and methods against corrosion fatigue at mixing points and systems with stagnant and/or turbulent flow. It will as part of the nuclear utilities on-going LTO-programs assist in the establishment of a solid basis for in-service inspection programs and give improved data for decision on repair or replenishment of pipe joints. The knowledge on corrosion fatigue risk at Swedish nuclear power plant conditions will supply SSM with better understanding for the risk of rupture and improved judgement of safety margins. Based on these improvements SSM will be able to enhance proactive safety work at the utilities.

## Progress

The project started in August 2020. During 2021, the design and manufacturing of the experimental set-up including the hollow pipe specimens was finalized. The fatigue behaviour of the suggested design, which is modified compared to the original version, have been simulated and, based on the simulations and results in the literature, it was decided that the design meets the requirements for testing the damage mode at Swedish nuclear power plant conditions. An experiment plan has been defined and discussed within the project group. Test material has been selected and acquired from the Oskarshamn nuclear power plant. The material is a vintage type 304 stainless steel plate that was recovered from the archives after construction of the Barsebäck nuclear power plant. In 2021 a fatigue design curve, i.e. a S-N curve relating the number of cycles to failure, was developed for the chosen material using standard type specimens. Cyclic tests at elevated temperature was also performed and the cyclic plasticity of the material was modelled with a combined nonlinear isotropic and kinematic hardening model in a radial return mapping algorithm. Pipe samples have been manufactured for correlation of the hollow tube samples to investigate the consistency in their behaviour at elevated temperature and pressure. In 2022, the corrosion fatigue tests with the hollow specimens commenced in the Studsvik laboratory. The tests are still running in simulated BWR water chemistry conditions. This work is sponsored by the Swedish Utilities Materials group, MG.

Parallel to the experimental program, a mechanical-electrochemical coupled crystal plasticity finite element model is being developed. The model consists of Voronoi cells representing polycrystals generated from EBSD data on the material by use of the software Neper. A user material (UMAT) subroutine is being developed to combine crystal plasticity with corrosion degradation in Abaqus. The FE model will be used to make predictions on crack initiation during the corrosion fatigue process.

## Methodology

The experimental work at the Studsvik laboratory will be the key for a successful project. The experimental work will be a collaboration between three parties, KTH where the set-up has been designed and manufactured, Studsvik where the experimental part in autoclave will be performed, and Chalmers Microstructure Physics where microscopy and damage characterization will be executed.

The ongoing simulation work for understanding and verification is running in parallel to the experimental series. It is planned for two different set-ups. One will be the multi-physical simulation of initial conditions with coupled mechanical loads and corrosion process. The second will be the crack initiation on favourable crystal planes.

## Communication

The project was presented at the SKC Symposium 2023.

A project reference group has been established and constituted. The reference group comprise participants from all three Swedish nuclear power plants, SSM and the project parties KTH, Studsvik and Chalmers. Adjunct professor Pål Efsing from Ringhals serves as industry advisor and main supervisor. Carl Dahlberg at KTH serves as co-supervisor. Dr Jean Smith from EPRI in Chicago USA is connected to the project as expert advisor and a communication link has been established to Dr Seiji Asada at Mitsubishi Heavy Industries for the experimental work.

In July 2022, the project was presented at the "Environmental Degradation of Materials in Nuclear Power Systems" conference in Aspen, Colorado, USA. In addition, a presentation was also held in the "International Conference on Multiaxial Fatigue and Fracture" conference in November 2022 in New Orleans, Louisiana, USA. The results were also presented in June 2023 at the "International Conference on Fracture" conference in Atlanta, Georgia, USA, and in the "Environmental Degradation of Materials in Nuclear Power Systems" conference in Sankt Johns, Canada, in August 2023.

During 2023, a paper "Mechanical Characterization of Fatigue and Cyclic Plasticity of 304L Stainless Steel at Elevated Temperature" was published in *Experimental Mechanics*.

## References

[1] Subasic M, et al. Mechanical Characterization of Fatigue and Cyclic Plasticity of 304L Stainless Steel at Elevated Temperature. Exp Mech 2023.

# SEMRA: Steam Explosion Modelling and Risk Analysis for light water reactors (2019-7)

Research host:
KTH Royal Institute of Technology
Department of Physics

Doctoral Student:
Ibrahim Batayneh

Formal project start:
2021-01-15

Expected completion time:
2025-01-15

Main Supervisor:
Dmitry Grishchenko

## Motivation

Steam Explosions (SE) are an inherent risk in light-water reactors (LWRs), posed by the very use of water as a coolant during accidents. There is a need to better understand these risks in currently operating and future NPPs, but state-of-the-art on steam explosions remains fragmented, with large spread in the prediction of explosion loads across modelling approaches and code users. The SEMRA project develops what is intended to be the most comprehensive modelling approach for the analysis of ex-vessel steam explosions in LWRs, and couples it with a risk analysis methodology to support decision making in modifying severe accident management (SAM) strategies. The deterministic model we develop will be applicable for any type of LWR, and any scenarios of melt release. It will be accompanied by an artificial neural network (ANN)-based surrogate model to enable fast calculations for risk assessment and uncertainty analysis.

With SEMRA's use of state-of-the-art numerical methods, comprehensive model validation, uncertainty quantification, and decision-oriented risk analysis, we will provide a flexible, generalized tool for analysing the risks of steam explosions and potentially resulting containment failure. The outcomes of this work will be relevant for the scientific community, industry, as well as regulatory/licensing bodies. The results can be directly incorporated into the current probabilistic safety analysis (PSA) used by the nuclear industry and bring the issue of steam explosion to a final resolution.

## Progress

The PhD project started in January 2021. Since then, to get familiar with the topic and to see what is lacking in old steam explosion codes, 'TEXAS-5' code was used to analysis of the effects of multiple jets release on the energetics of steam explosion loads in Nordic BWRs. A full model solutions database was built from which a fast surrogate model was developed to analyse the effects of multiple melt-jets and their potential implications on the risk of containment failure. This study concluded the importance of multiple melt-jets release and the need to include it in SEMRA SE code.

The next step of SEMRA project started with the analysis of the different numerical schemes available to model the physical phenomena of steam explosion, to select the appropriate one for SEMRA SE code. A new solver for SE shock wave pressure propagation was coded and validated. The solver incorporates WENO solver with AUSM+-up and Godunov flux schemes to model pressure propagation in a multi-phase domain. The results obtained from this in-house code are compared with the experimental results from KROTOS facility and the results from TEXAS-V code. Currently, jet break-up (fragmentation) and debris bed formation and agglomeration models are being developed. Different models are compared to choose the optimum one for steam explosion application, then the developed model is validated against known experiments on jet agglomeration (DEFOR-A) and against TEXAS-V steam explosion code.

## Methodology

The calculation of steam explosion with multiple jets was carried out by, first, computing the explosion impulse for a single jet with cell cross-section area set according to a considered jet configuration scenario; and second, the impulse resulting from a single jet calculation was multiplied by the number of jets to provide the final explosion load. A sensitivity analysis and a parametric study were carried out to confirm that the surrogate model provides physically sensible behaviour for the different input parameters.

As for SEMRA SE code, after selecting the appropriate numerical model, the code is built gradually, starting with simple pressure and temperature calculations (1D and 2D), to including different SE phenomena such as multiple melt-jets release. Results of the 1D single phase pressure propagation models simulating the trigger analysis of KROTOS facility are shown in the figure below.

Different machine learning methods are also being investigated and incorporated in the project to produce surrogate models that accurately predict SE loads for the risk analysis part.

## Communication

The project was presented at the SKC Symposiums 2021 & 2022, 2023. A conference paper about steam explosion in conditions of multiple jet releases was presented in the 19th international topical meeting on Nuclear Reactor Thermal Hydraulics (NURETH-19), March 2022. Two conference papers were presented in NURETH-20 in August 2023 and another one presented at SCOPE conference in Saudi Arabia. Several conference papers are planned for next year in NUTHOS 24, ICAPP and ICONE 2024 conference. The papers span over different topics covering the code development part, TEXAS-V SE analysis of time dependent melt release and SE in SMRs and new machine learning methods used in SE predictions.

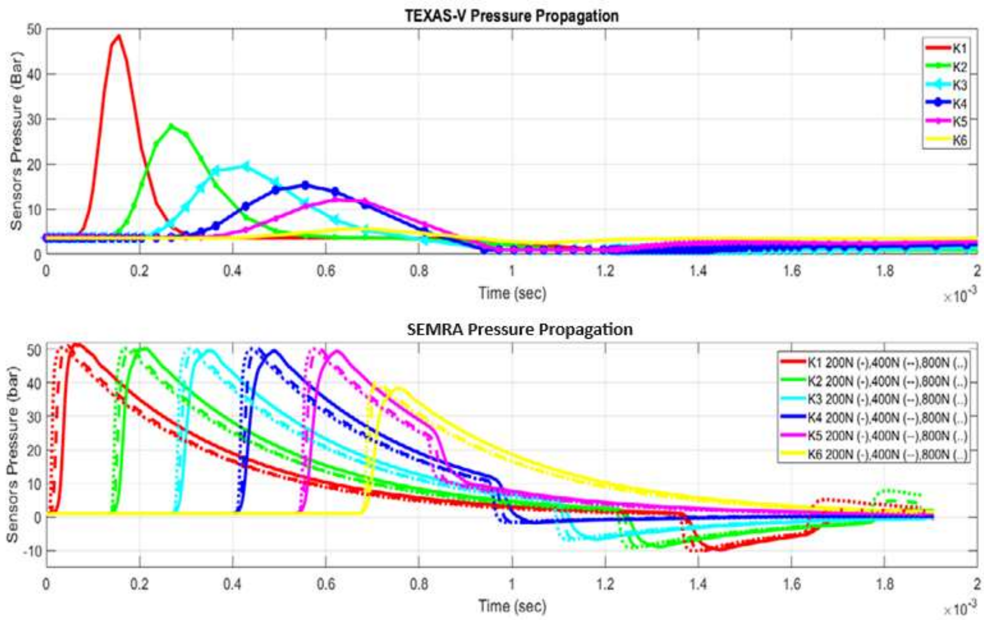


Figure 2: Trigger test pressure propagation of KROTOS facility in TEXAS-V (top) vs SEMRA (bottom).

# Calibration of fuel performance codes – treating model inadequacies, nuisance parameters, and unrecognized systematic uncertainties (2019-12)

Research host:
Uppsala University
Department of Physics and Astronomy

Doctoral Student:
Gustav Robertsson

Formal project start:
2020-09-01

Expected completion time:
2025-06-31

Main Supervisor:
Henrik Sjöstrand

## Motivation

The proposed project addresses challenges in the calibration of fuel performance codes. These codes include models that predict thermo-mechanical behaviour of the fuel and hence, the performance and safety functions of the fuel for regular reactor operation, anticipated operational occurrences, accidents, and back-end applications.

There are several challenges with acquiring calibrated predictive models with well-founded uncertainty estimates. These challenges include handling interlinked models; integral, biased, and sparse calibration data; various types of input uncertainties; computationally costly executions; and model inadequacies. Therefore, inverse uncertainty quantification (UQ) in fuel performance modelling is particularly challenging.

Specifically, the UQ within fuel performance simulations is crucial in establishing plant operation safety limits. This manifests as conservative estimates of operation limits or an evaluation showing that the fuel cladding barrier will not be breached for a given plant operation. In addition, the fuel rod behaviour plays a central role in accident analyses, for example, in the evaluation of loss-of-coolant accidents where the cladding embrittlement is a direct safety-related parameter. In this context, calibration plays a pivotal role as it defines the uncertainties utilized when providing the conservative estimate. Inaccuracy in calibration can lead to overstepping of established failure limits, which from a safety standpoint is not acceptable. Conversely, an overly cautious and conservative treatment causes less efficient operation and fuel utilization with both cost and increased waste disposal impacts.

One of the most demanding challenges in model calibration is caused by so-called model inadequacies. A model inadequacy is when the model cannot recreate the physical reality independent of the choice of model parameters and often has severe consequences if not accounted for properly. Figure 1 demonstrates a simple example where an inadequate model (blue line) is used to estimate a more complex reality (dashed line) from which measurements are taken (orange points). The figure demonstrates that the resulting blue uncertainty bands of the model do not reflect the model's error and are the calibration results that one would obtain without accounting for model inadequacy. Such a result would have significant safety implications if the model predicted a nuclear engineering safety parameter.

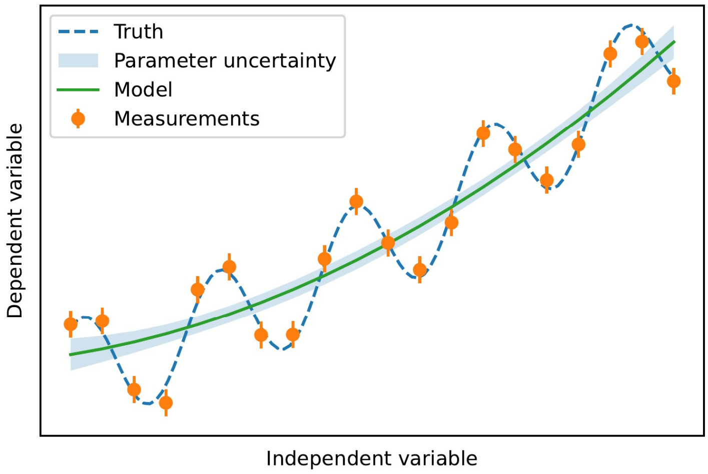


*Figure 1 - An example of an inadequate model with uncertainty bands in a standard calibration (blue).*

This project studies how model parameter uncertainties can be used to adapt the model prediction uncertainty to account for model inadequacies and other unknown sources of uncertainty. For this purpose, three main quantities have been studied: cladding oxidation, hydrogen pickup, and fission gas release. These phenomena, if not limited, can have a direct negative impact on fuel safety. For example, hydrogen uptake harms the mechanical properties of the zirconium alloy, cladding oxidation consumes the cladding, and the oxide is a much poorer heat conductor. In addition, the modeling of fission gas release is important since fission gases degrade the thermal conductivity of the gas inside the fuel rods and increase the internal pressure. Higher temperatures may also lead to negative thermal feedback since a depressed thermal conductivity will, in turn, enhance additional fission gas release.

To summarize, the project aims to ensure safety via reliable quantification of margins simultaneously as it enables efficient use of fuel and benefits all partners of SKC. The project is executed as a Ph.D. project in collaboration between Uppsala University (UU) and Westinghouse. Active within the project are Gustav Robertson (Ph.D. student, SKC-funded), Henrik Sjöstrand (Supervisor, UU, SKC-funded), Peter Andersson (Co-supervisor, UU, SKC-funded), Paul Blair (co-supervisor, Vattenfall Nuclear Fuel AB, in-kind contribution).

## Progress

In 2020, a method to address the problem related to model inadequacies in calibrating fuel performance models was developed and implemented. The method is designed to address model inadequacy by inflating the uncertainty of the calibration parameters to account for the discrepancies. Initially, the Ph.D. project lacked PIE data and a fuel performance code in contrast to previous studies, such as those presented in reference [1], which was performed at Westinghouse. Therefore, it was deemed meaningful at the beginning of the project to work with synthetic data since the performance of the tested methods can be more easily studied.

In 2021, the method has been further refined and completed. Quantitative metrics for the method's ability to compute well-founded uncertainties have been obtained, and it has been shown that the technique works well on validation data. I.e., with the new implementation, it is found that the obtained method can produce a successful joint calibration of both the oxidation and the hydrogen model where the uncertainties can explain the model error. The work has been presented at TopFuel2021 and published in the Annals of Nuclear Energy in August 2022 [2].

In 2021, publicly available fission gas ramp release data were collected to develop the proposed method further and demonstrate its applicability to more multivariate and more strongly interconnected problems using actual data and codes. For this purpose, the project has access to the fuel performance code Transuranus developed by the Joint Research Center (JRC) at the European in Karlsruhe, Germany. JRC has been supportive and supplied Transuranus input files for the public experiments studied. Based on the calibration methodology, a calibration framework to calibrate Tranuranus to those experiments has been implemented. A part of the framework has been to improve surrogate modeling to support the calibration methodology with derivative predictions. This work was conducted during 2022 and published at TopFuel 2022 [3]. The proposed calibration method and the improved surrogate models were presented as a licentiate thesis in April 2023 [4].

During 2022, additional development has been conducted on the calibration methodology to make it more robust by simplifying the relationship between model parameters and corresponding predictions by using transformations. In addition, commercial cladding oxidation data and corresponding input files were collected from Westinghouse to be used together with the abovementioned public fission gas ramp release data to evaluate the performance of the calibration methodology. Those applications - drafted during 2023 for publication in early 2024 [5] - demonstrate that the calibration methodology from ref. [2] is applicable for fairly linear problems such as cladding oxidation but needs more development for non-linear calibration problems such as fission gas release.

The methodology was improved during 2023 by using a Metropolis-within-Gibbs sampler to overcome the linearity assumption in the original method. This new method was successfully applied to calibrate the fission gas release model to the public fission gas ramp release data mentioned above, and this application was submitted to the BEPU2024 conference in 2023 [6]. During 2023, additional fission gas release measurements and corresponding input files were collected from Westinghouse to validate the new method's development further. The results confirm that the new method is successful in that it results in calibrated model parameters with uncertainties that, when propagated, explain the discrepancy between the model and the measurements. This application has been presented [7] and is intended for journal publication in 2024.

In 2022, a bachelor was proposed to improve the understanding of time-dependent surrogate models in calibration. This work started in 2023 and was based on a previous bachelor work conducted in the project in 2021, "Temporal Convolutional Networks In Lieu of Fuel Performance Codes" [8]. The new work [9] demonstrates that an ensemble between temporal convolutional networks and Fourier neural operators can be used to accurately predict time-dependent outputs of a fuel performance code, given a power-history input. This work - of which a derivative is drafted for a journal publication in 2024 - was awarded the Sigvard Eklunds Prize for best bachelor work in 2023.

Since 2023, Uppsala University has participated in an accelerated program to create supply security for Russian-designed VVER reactors operating in the EU (APIS project). The project is funded by the European Commission, coordinated by Westinghouse, and includes 12 partnering organizations. Gustav Robertson and Henrik Sjöstrand from Uppsala University will be active in the project and work with statistical development and news dissemination.

In 2022, Gustav Robertson supported a master's thesis work at Westinghouse [7], mainly with insight in applying Gaussian Processes to predict critical heat flux. The collaboration led to a conference paper, "Investigation of Machine Learning Regression Techniques to Predict Critical Heat Flux over a Large Parameter Space" that was published NURETH-2023 conference [10].

## Methodology

The project has been planned according to a staged approach to have an increasing complexity in physical models and statistical techniques over the project's duration. The idea is to move between artificial test beds and real code so that suitable methods can be first investigated in controlled environments and proved on real data. Therefore, the research initially began by developing and testing a calibration technique using synthetic data to address model inadequacy. Subsequently, recognizing the necessity for enhancing surrogate models, we made improvements accordingly. We then applied the combined methodology package to real-world data, specifically chosen to represent the intricate calibration requirements of a fuel performance code. Evaluating these results revealed the methodology's effectiveness for linear problems, albeit requiring refinement for non-linear problems such as fission gas release. Consequently, we directed efforts toward advancing the method beyond linear assumptions, and retesting yielded desirable outcomes.

## Communication during 2023

In April 2023, Gustav Robertson took a licentiate degree, and a thesis was presented [4].

The project and calibration results were presented at the Materials Modelling and Simulation for Nuclear Fuel (MMSNF) Workshop 2023 [7].

The project was presented at the Annual SKC Symposium.

The project was presented at the kick-off meeting for Work Package 6 in the APIS project.

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# Impact of radiation chemistry on surface processes in LWRs (2020-18)

Research host:
KTH Royal Institute of Technology
Department of Chemisrty

Doctoral Student:
Luca Gagliani

Formal project start:
2022-01-01

Expected completion time:
2026-02-01

Main Supervisor:
Mats Jonsson

## Motivation

Surface reactions such as metal corrosion, oxide deposition and oxide release/dissolution are processes that have a significant impact on the performance of and the occupational safety around nuclear reactors. These processes are largely governed by the fairly harsh conditions prevailing inside a nuclear reactor. These conditions include high temperatures, high pressures, intense neutron fluxes and intense gamma fluxes. The primary oxidative radiolysis products in gamma-irradiated water are hydrogen peroxide ($H_2O_2$), the hydroxyl radical (HO•) and to some extent also the hydroperoxyl radical (HOO•). Molecular oxygen ($O_2$) is subsequently formed project is to identify situations where the simplified approach can be sufficient and situations where this is not sufficient. The materials used in the experimental studies will include but not be restricted to cladding materials, grid spacer materials and oxide depositions.

## Progress

The project was started on February 2022 when the PhD-student was employed. In this first year of the project, Luca attended courses about corrosion, nuclear chemistry, and radiation chemistry, to get acquainted with the topic of the project and better understand the processes involved. Kick-off meetings with the reference group (Westinghouse, Vattenfall and OKG) were held in March and late April 2022 and a subsequent update meeting in October 2022. A second update meeting will be planned for late spring 2023. During 2022, the reference group provided some relevant cases on which further literature and experimental studies are now based. Also, significant test materials were provided and are now used for laboratory tests. Luca got first familiar with some experimental methods useful for the project's scope. Then he defined a reliable investigation procedure to monitor and determine $H_2O_2$ evolution and consumption under γ-irradiation conditions in heterogeneous systems involving water and the relevant alloys provided. In 2023 Luca's education was mainly centered on electrochemistry while the project enfolded the long-term irradiation of the selected materials and the development of procedures for the investigation of the effects of irradiation on the surface of the alloys. The focus was on the alteration of the surface scale and the dissolution of elements in the aqueous phase. In November 2023 the project's priorities for 2024 were outlined in a meeting with the reference group representatives in Västerås, at Westinghouse headquarters.

## Methodology

So far, the techniques most used for the present project are chemical dosimetry and titration, Ultraviolet-Visible (UV-VIS) spectroscopy and Induced Coupled Plasma Mass Spectroscopy (ICP-MS) to evaluate the extent of radiation-induced phenomena and products in the liquid phase. Other experimental methodologies such as Scanning Electron Microscopy (SEM), Energy-Dispersive X-ray (EDX) spectroscopy and electrochemical investigation techniques, such as Electrochemical Impedance Spectroscopy (EIS) have played a role in assessing the extent of radiation-induced phenomena on the surface of the solid, at the interface with the liquid. At this stage, X-ray Photoelectron Spectroscopy (XPS) is being used to integrate the data collected with EIS about the samples' surface conditions and to corroborate them.

## Communication

The project was presented for the first time at the SKC Symposium 2022, last October an update presentation was given at the SKC Symposium 2023 in Stockholm. A mid-PhD project seminar is planned for spring 2024 at KTH. The submission of two scientific articles dedicated to 1) the methodology of irradiation and experimental setup conditions and 2) the γ-assisted oxidation of alloys are also planned for 2024

# Application of artificial neural networks in reactor physics calculations (2020-19)

Research host:
KTH Royal Institute of Technology
Department of Physics

Doctoral Student:
Yi Meng Chan

Formal project start:
2021-08-16

Expected completion time:
2025-08-16

Main Supervisor:
Jan Dufek

## Motivation

Nodal diffusion codes, that are used in industry for reactor simulations require spatially homogenised and energy collapsed nodal data, such as group macroscopic cross sections, microscopic cross sections for selected nuclides, diffusion coefficients, discontinuity factors, etc. The nodal data depends on both instantaneous and historic state variables, such as fuel depletion, fuel temperature, moderator density, and others. Nodal data generation is carried out by computationally expensive neutron transport codes, and it is impractical to generate nodal data on demand from these codes, therefore, it is necessary to build simplified models of the nodal data based on its state dependencies.

These dependences are usually tabulated or approximated by multivariate functions (Dufek 2011), mostly polynomials. The general problem with the table models is that tables grow exponentially with the number of state variables. The amount of data stored in the tables and the number of lattice calculations needed to fill the tables can easily become impractically large for this reason. Therefore, the table models can consider only relatively few state variables.

In this PhD project, we propose the application of Artificial Neural Networks (ANNs) to represent nodal data. The advantage of Artificial Neural Networks is its capacity to represent highly complex and non-smooth functions, which we believe may lead to more accurate nodal data representation compared to the models in the current literature. This would allow for more flexible and accurate reactor simulations than possible with existing data models. This can translate into a better optimisation of fuel load patterns and an improved reactor economy.

## Progress

The PhD project started in August 2021. Since then, the project progresses according to the plan. The following points are completed or nearly completed:

- A proposed model combining Principal Component Analysis (PCA) with a Deep Neural Network (DNN) to perform multi-group self-shielded cross section reconstruction

- The model is able to handle a large number of nuclide concentration dependencies and instantaneous state parameters.

- The model showed high accuracy in generating generating multi-group cross-section libraries for the fuel pellet and subsequent lattice calculations showed a multiplication factor error of less than 1% compared to reference values."

- Work is ongoing to improve model performance and to expand the capability of the model to generate cross-section libraries for non fuel pellet materials found in Light Water Reactors

We further aim to design a recurrent neural network to model the changes in the fuel pellet nuclide composition in the depletion process. This project is in the initial stages and training data is currently being generated using computing resources at the PDC Center for High Performance Computing at KTH.

## Methodology

Before lattice codes output few group nodal cross sections, they first have to generate multigroup cross section libraries from continuous energy cross section libraries for each material in each fuel cell. The computational cost of these cross section processing are large. Therefore, we propose the use of a representation model to estimate lattice code multigroup cross section libraries from nuclide concentration data and state parameters.

The model combines Principal Component Analysis (PCA) and fully connected Neural Networks (NN). The model contains three sublayers in a PCA-NN-PCA configuration. The model architecture allows it to handle large multi-group cross section data sets containing cross section data for several dozen nuclides and containing upwards of 50 energy groups. A representation of a forward pass of the model is shown in Figure 1.

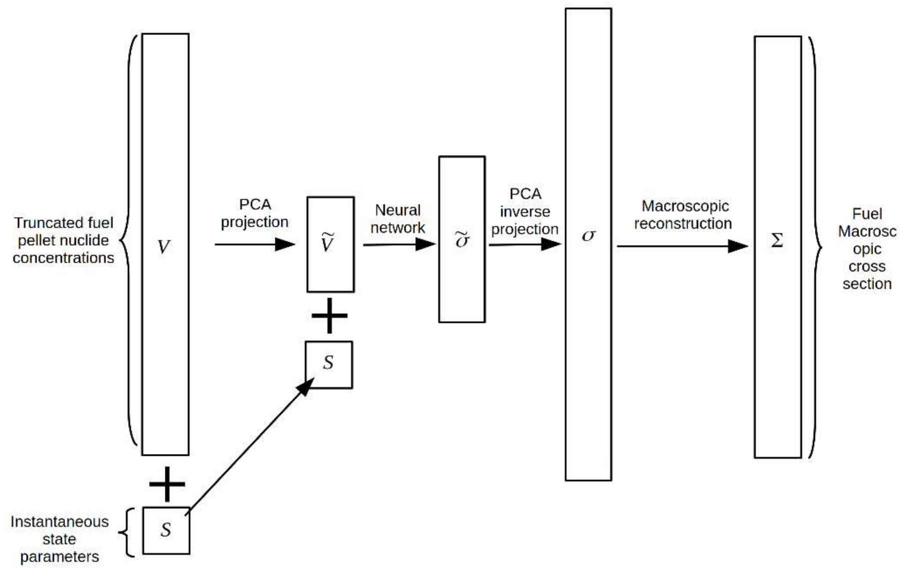


*Figure 1: PCA-NN-PCA forward pass operation*

The use of PCA greatly reduces the number of trainable parameters for the DNN layer and improves model performance. An illustration of the DNN utilized in the model is shown in Figure 2.

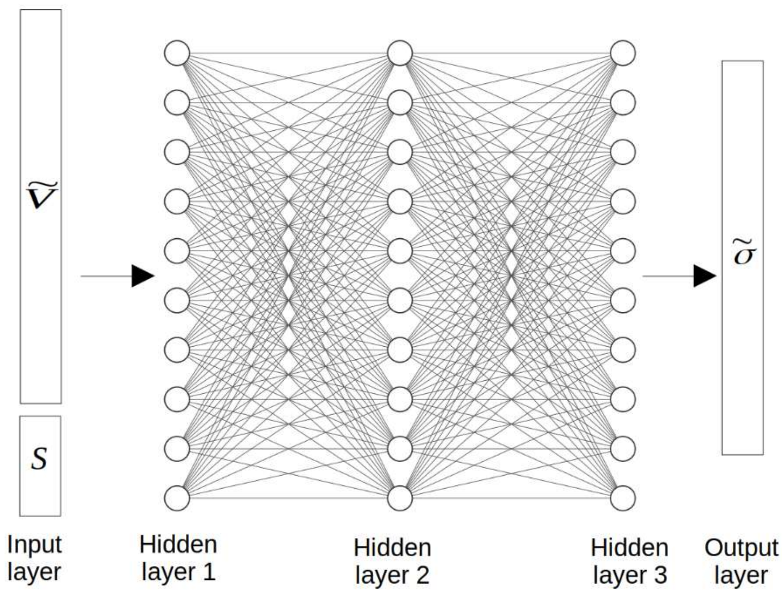


*Figure 2: Fully connected neural network architecture*

As proof of concept, our proposed method is trained on lattice code cross section data for the fuel pellet material in a typical light water reactor assembly. The NEWT model of quarter assembly is shown in Figure 3.

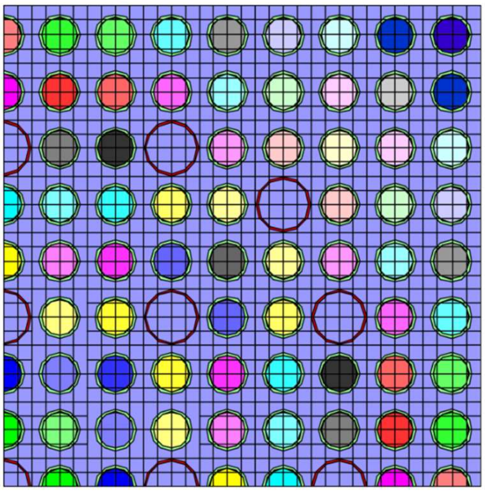

*Figure 3: NEWT model of quarter 17x17 fuel assembly*

The model is expected to be able to generate self shielded cross section libraries in a fraction of the time with acceptable accuracy compared to a reference self-shielding cross section processing code.

## Communication

Ongoing work on this project was presented at the SKC Symposium 2023.

As part of our efforts of better understanding of how nodal data is generated and used, we have communicated with experts from Westinghouse, and with Erwin Müller and Petri Forslund Guimarães who have extensive experience in this area.

## Publications

Chan, Yi Meng, and Jan Dufek. "A deep-learning representation of multi-group cross sections in lattice calculations." Annals of Nuclear Energy 195 (2024): 110123.

# Development of a fully coupled electrochemical and micro mechanical SCC model

Research host:
KTH Royal Institute of Technology
Department of Engineering Mechanics

Postdoctoral researcher:
Michal Sedlak Mosesson

Formal project start:
2020-11-01

Completed:
2023-10-31

Main Supervisor:
Pål Efsing

## Motivation

The study of Stress Corrosion Cracking has until the beginning of the 2000s mainly been associated with describing the in-the-field observations in terms of a large number of laboratory tests that address the impacts of various factors influencing the crack growth rates and cracking phenomenology. Examples of such factors include electrochemical potential, ECP, residual stresses, cold work and carbon content in the grain boundary zones understood to be sensitizated by precipitation of carbides in the grain boundaries rendering chromium mobility sluggish. Over the last 10 years, there has been a number of efforts to enhance the understanding of SCC by modelling the behaviour from both a mechanistic perspective (Shoji et al., Andresen et al., Couvant et al. ) and from a local chemistry perspective (McDonald et al. Saario et al.). By combining these approaches an increased understanding of the interrelated phenomena can be achieved.

SKC has supported the work at the group of Solid Mechanics performed by Michal Sedlak with the support of Prof Bo Alfredsson and adj. Prof Pål Efsing. This work was presented and successfully defended in April 2020. The purpose of the continuations is to create a model for improved prediction of the Stress Corrosion Crack (SCC) growth rate in stainless steel in boiling and pressure water reactor environments. Primary areas of interest for this development are irradiation assisted SCC, influence of cold work on the SCC-susceptibility and SCC in replacement materials such as 316NG (low-Carbon containing stainless steel) and Alloy 690 (high Chromium containing Nickel-based material) which are considered a significant improvement to the previously utilized material but much still remains to be proven for an LTO-perspective.

## Progress

The project was finished during 2023 but there is some remaining work such as editing of articles and ending the running of simulations to be done for two articles. The review process is ongoing.

## Methodology

In the moving Gauss points framework, oxidation module was transformed to an integration point formulation instead of node formulation, still including the duplex/mono -oxide or more complex. The oxide is now modelled with an analytical solution using Euler-Bernoulli beam theory and fracture mechanics. Creep constitutive law was used to obtain the plastic creep strain and stresses during the relaxation phase.

The next stage of the model was to replace the analytical formulation into a local FE formulation containing an oxide growth with slip-planes forming. Determining the damage process of the oxide. This could not be solved every iteration. The local solution was therefore pre-solved and mapped into the global solution.

The fracture mechanics module is enhanced with a crack path module, introducing cohesive elements in the grains with remeshing capabilities was shown to cumbersome and cost ineffective therefore the XFEM ghost node method has been introduced instead. The process introduced the possibility of branching and both inter- and transgranular stress corrosion cracking. The objective cause for the onset of branching is still ongoing research.

The electrochemical module is undergoing changes, the total energy in the model is considered with Gibbs free energy using the chemical potential. The influence from hydrogen embrittlement will also be implemented with Hydrogen enhanced plasticity (HELP) and for decohesion HEDE. The effect on the chromium mobility is also considered.

## Future and ongoing work

1. Collaboration with Dr Elsiddig Elmukashfi from the University of Oxford ,Dr Ageo Meier de Andrade and Prof. Itai Panas from Chalmers. The work involves modelleing the influence of the mobility on chromium and its capability of forming oxides on alloy 690 due to hydrogen diffusion.
2. Implementing a weld model using Bailey-Norton Creep model and phase changes the weld residual stresses can be obtained. The SCC model developed here can then be implemented showing its capabilities. Both in showing the most reasonable locations for SCC and predicting the CGR for different geometries, welds, irradiation degradation and crystal orientations.

## Communication

Two papers are published and two are being finalized. All articles are sent to high ranked international journals in their respective fields and published open-access.

Presented at conference *21TH Environmental Degradation of Materials in Nuclear Power Systems – Water Reactors* (August 6 -10) 2023.

Presented at conference *15th International Conference on Fracture (ICF15) (June11-16) 2021*.

Presented at conference *20TH Environmental Degradation of Materials in Nuclear Power Systems – Water Reactors* (June 17-21) 2022.

## Publications

M. Sedlak Mosesson and P. Efsing, Cohesive zone modelling of intergranular stress corrosion cracking of austenitic steels with moving integration scheme. EFM Ongoing

M. Sedlak Mosesson and P. Efsing, Investigation of fracture in oxide of austenitic steels in light water reactor conditions, due to slip bands from stress corrosion cracking and - fatigue. Scripta materialia Ongoing

M. Sedlak Mosesson and P. Efsing, Modelling of IGSCC with adaptive framework. 20th Enviromental Degradation of Materials in Nuclear Power Systems – Water Reactors, 2022

M. Sedlak Mosesson, B. Alfredsson and P. Efsing, Simulation of Slip-Oxidation Process by Mesh Adaptivity in a Cohesive Zone Framework , *Materials* 2021, *14*(13), 3509; https://doi.org/10.3390/ma14133509

# Influence of Alloying and Neutron Flux on Irradiation Effects in Fuel Rods

Research host:
Chalmers University of Technology
Department of Physics

Postdoctoral researcher:
David Mayweg

Formal project start:
2021-04-01

Completed:
2023-03-31

Main Supervisor:
Mattias Thuvander

## Motivation

The project aimed at improving the understanding of neutron irradiation effects in zirconium-based fuel cladding in a boiling water reactor (BWR) environment (see schematic in figure 1) with a focus on the microstructure evolution at the sub-μm scale. To this end we investigated two cladding tubes (Zicaloy-2 and Alloy 2 – a derivative of Zicaloy-2 with slightly higher Fe and Cr concentrations – both with heat treatment code LK3) at two fluence levels each (from a fueled segment: 38 dpa; and the plenum: 9 dpa). The samples have been used in Oskarshamn 3 from 2001-2007 for 2085 days. Although their composition differs only slightly (see Table *1*) in Fe and Cr their hydrogen uptake is markedly different (Zicaloy-2: 200 ± 29 wt ppm; Alloy 2: 134 ± 9 wt ppm).

*Table 1: Alloy composition of Zry-2 and Alloy 2 prior to irradiation.*

| Material | Fe (wt%) | Cr (wt %) | Ni (wt %) | Sn (wt%) | O (wt %) | C (wt ppm) | Si (wt ppm) | Zr |
|---|---|---|---|---|---|---|---|---|
| **Zry-2 (LK3)** | *0.18* | *0.13* | 0.061 | 1.49 | 0.12 | 143 | 91 | bal. |
| **Alloy 2** | *0.36* | *0.18* | 0.063 | 1.31 | 0.12 | 120 | 90 | bal. |

This unique set of samples allows for investigation of important effects caused by the exposure to real reactor conditions (see schematic in figure 1). Three mechanisms are of interest in our investigations:

1. waterside oxidation on the outer side of the cladding tubes,

2. redistribution of Fe, Cr and Ni by neutron irradiation and their segregation to irradiation-induced defects (these are mainly dislocation loops that form when vacancies or interstitials rearrange; dislocation loops have a specific

nature related to the crystal structure of the metal, in hcp Zr these are a-loops and c-loops that like on prismatic and basal planes respectively); and

3. hydrogen pick-up (HPU) leading to formation of hydrides, which degrade the mechanical properties of the cladding tubes.

These mechanisms have been studied by various techniques used to analyse oxidation and precipitation kinetics (e.g., thermogravimetry), the microstructure (x-ray diffraction, transmission electron microscopy, etc.), composition (atom probe tomography, energy dispersive x-ray spectroscopy, etc.) and mechanical properties for a long time.

The question that connects these three mechanisms is in which manner the alloying element distribution influences oxidation and hydrogen uptake and in what way the oxidation process affects the hydrogen uptake. Since there has been a limited amount of research with respect to the nano-chemistry of fuel cladding that has been used in regular operation in an actual reactor, we try to contribute to filling this knowledge gap by employing atom probe tomography (APT).

An improved understanding of the effect that alloying elements exert on oxidation and hydride formation mechanisms can potentially aid in further optimizing alloy compositions for Zr-based fuel cladding. Such optimized alloys will allow for prolonged operation cycles and hence higher burn-up of the fuel leading to lower total fuel consumption and less down time (also with respect to reducing fuel failures). This in turn will reduce costs and the amount of highly radioactive waste.

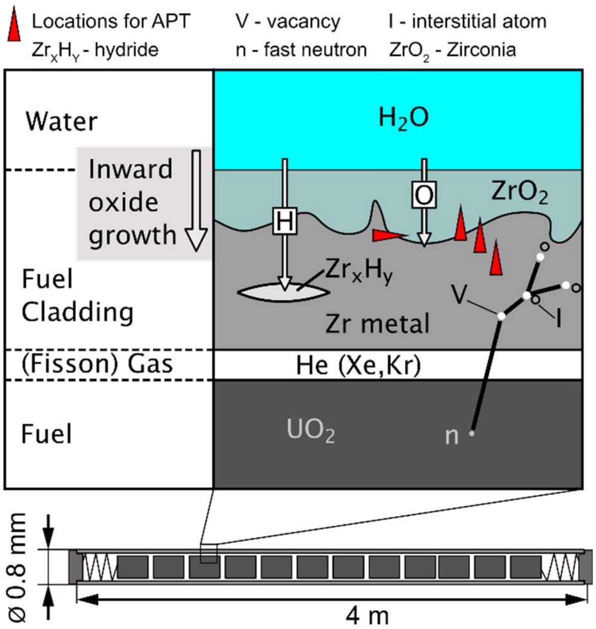


*Figure 1: Schematic illustration of the arrangement of fuel pellets encapsulated in a cladding tube during reactor operation (bottom). At the top a detailed schematic of the water/fuel rod (Zr-alloy)/ fuel pellet (UO2) environment is depicted and processes of interest are illustrated: 1. oxidation (formation of ZrO2) takes place by O transport across the oxide scale, 2. irradiation damage (vacancies and interstitial atoms) caused by fast neutrons, and 3., hydrogen uptake by the metal and leads to hydride formation. Red triangles mark positions that were targeted for specimen preparation for atom probe tomography (APT) measurements.*

## Methodology

The main tool employed in the present research was atom probe tomography in a combination with specimen preparation by focused ion beam (FIB) milling. APT is uniquely suitable to characterize microstructures in three dimensions with a spatial resolution of less than 1 nm and high chemical sensitivity for all elements. The technique relies on a process called field evaporation, which is used to consecutively remove atoms from a very sharp needle specimen (tip radius typically below 100 nm). These atoms are detected in ionic form by a position sensitive detector. From the mass-to-charge ratio the chemical identity of the ions can be inferred and a 3D reconstruction of the evaporated volume is created that enables chemical analysis on the near-atomic scale. Additionally, scanning and transmission electron microscopy (SEM/TEM) measurements were performed to supplement the findings with information on scales from several nm to a few µm.

## Progress

The project was carried out from in April 2021 to March 2023. There was some delay in the experimental work (especially the oxide characterization) due to the untimely breakdown of the atom probe instrument. However, after a new instrument (LEAP 6000XR) was installed at Chalmers Material Analysis Laboratory and became available in early 2023, we were then able to resume this work. We were able to make significant progress in understanding the capabilities and limitations of employing APT to Zr-based fuel cladding. In addition, we used that knowledge and made significant progress in characterization with respect to the three mentioned degradation mechanisms (irradiation damage, HPU and corrosion). Three highlights are showcased below.

### *1.1. Hydrogen analysis by APT*

We successfully obtained a rather unique data set from a specimen fabricated by cryogenic FIB milling, a measure that prevents preparation artefacts related to hydrogen ingress [1] (see Figure 3). In the literature it is proposed that the Zr matrix around intermetallic secondary phase precipitates (SPPs) is a trap for hydrogen (rather than the SPPs themselves) and therefore needs to be taken into account in assessing HPU. The detected hydrogen fraction is below 1 at% and most of it is not even originating from within the specimen but rather from the analysis chamber, which always contains some hydrogen gas that interacts with the specimens leading to detection of hydrogen. In addition, the detection of a relative higher hydrogen fraction inside the SPP is caused by a lower relative field and hence also represents an experimental artifact. Our results are somewhat unexciting in that they do not support the hydrogen trap hypothesis. Nevertheless, they show that additional measures like the use of tracers (deuterium) need to be employed to locate hydrogen traps on the nm scale and hence provide ground for the justification (and necessity) of further pursuing (experimental) work.

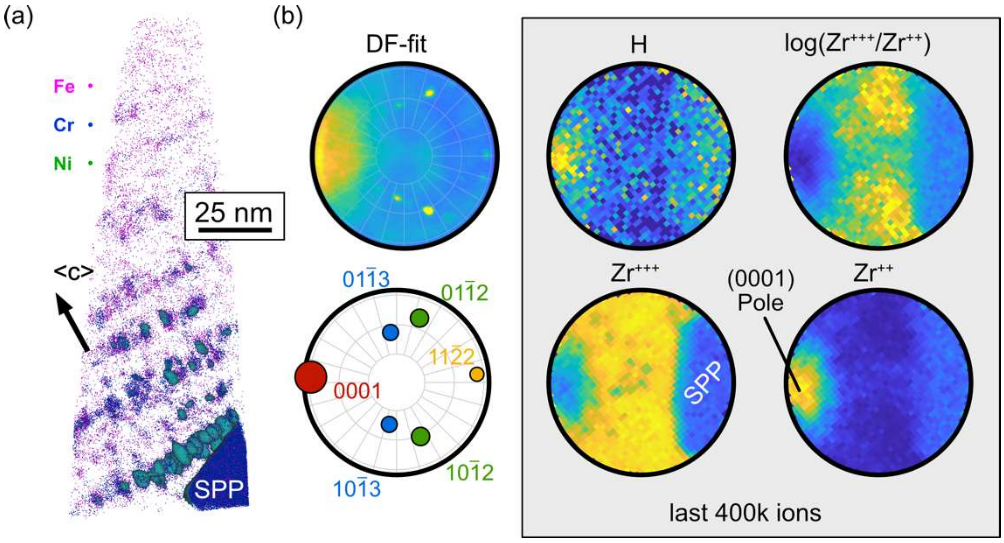


*Figure 3: APT analysis of an intermetallic secondary phase particle (SPP) in irradiated modified Zircaloy-2 with higher Fe and Cr content. (a) is a reconstruction showing the clustering of Cr, Fe and Ni in layers. (b) Crystallographic information and H distribution in and around the SPP.*

### 1.2. Irradiation damage

The emergence of c-component dislocation loops in fuel cladding is associated with accelerated degradation: 'breakaway' corrosion, growth and HPU are correlated with the occurrence of c-loops. Employing APT we found that the segregation behavior of c-loops is strongly differing from what would be expected, namely, that inside such loops, islands of nearly pure Zr are forming (Figure 4). And, since this 'de-alloying' basically counteracts the indented beneficial effects that alloying is used for in the first place, our finding might be a starting point for explaining the role c-loops play in the regime where degradation mechanisms speed up.

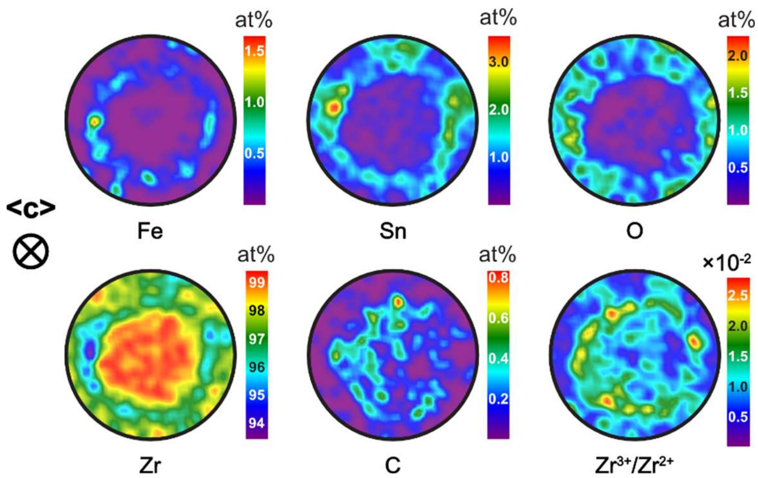


*Figure 4: Color-coded maps around what is believed to be a c-loop. Fe and Sn segregate to the dislocation line. Inside the loop nearly pure Zr remains.*

### 1.3. Oxidation

Zr corrosion is a process in in which zirconia (ZrO2) forms on the surface through Zr reacting with water according to:

$$Zr + 2\,H_2O \rightarrow ZrO_2 + 2\,H_2$$

The ZrO2 formation takes place at the oxide-metal interface. This means that oxygen diffusion through the scale must occur and the velocity of the interface moving inward determines the corrosion kinetics. We used TEM and APT to investigate the oxide and the oxide metal interface. While oxides grown in corrosion experiments show regular columnar grain formation, the representative images in Figure 5 (a) show that oxide scales (which exhibits cracking) from irradiated cladding tubes is much less well defined. In fact, there is no regular pattern observable, but instead large 'patchy' and columnar grains (Figure 5 (a2)) as well as equiaxed grains with diameters of only a few nm (Figure 5 (a3)) are found.

Most APT measurements targeting the oxide-metal interface were not successful since specimens often fractured before the interface was reached. We attribute this low success rate to the cracks inside the oxide weakening the structural integrity of the specimens that experience mechanical loading through APT experiments. Figure 5 (b) depicts a reconstruction of an APT experiment where the oxide-metal interface was captured. In comparison to the reconstruction from the bulk metal seen in Figure 3 it is obvious that the clustering of Cr, Fe and Ni is much less pronounced in the oxygen saturated metal and in the oxide. That dissolution of clusters occurs prior to oxide formation might point to clusters' positive effect on corrosion properties. This novel observation shows the need for a more detailed theoretical understanding as such a mechanism is currently not incorporated in models describing corrosion on the atomic scale. In addition, the proximity histogram shows a slight rejection of Sn at the interface, which also might affect the oxide growth.

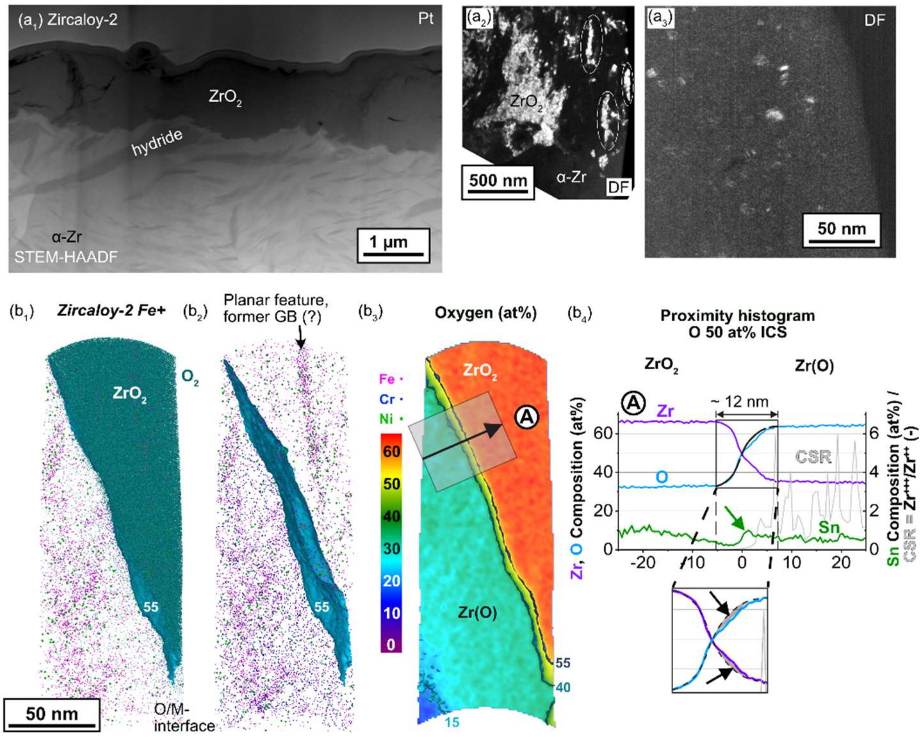


*Figure 5: Oxide metal interface analysis by TEM and APT. (a) (S)TEM images showing an overview (Z-contrast) of the interface as well as the grain morphology. (b) APT reconstruction capturing the interface between ZrO2 and O-rich Zr.*

## Communication

Some work (segregation at c-loops) was presented at APT&M 2023 in Leuven and regular updates given to the MIDAS (Mechanistic Understanding of Irradiation Damage in Fuel Assemblies) community. An overview of work on dislocation loop, oxidation and hydrogen analysis was given at the SKC symposium 2023.

## Publications

Two papers have been published:

J. Eriksson, D. Mayweg, G. Sundell, H.-O. Andrén, and M. Thuvander, "Solute Concentrations in the Matrix of Zirconium Alloys Studied by Atom Probe Tomography," in Zirconium in the Nuclear Industry: 20th International Symposium, ed. S. K. Yagnik and M. Preuss (West Conshohocken, PA: ASTM International, 2023), 149–172, http://doi.org/10.1520/STP1645202200263

D. Mayweg, J. Eriksson, O. Bäcke, M. Thuvander: *Focused Ion Beam induced hydride formation does not affect Fe, Ni, Cr-clusters in irradiated Zircaloy-2,* Journal of Nuclear Materials 581 (2023) 154444, https://doi.org/10.1016/j.jnucmat.2023.154444

Five further manuscripts are in preparation (titles are preliminary):

J. Eriksson, M. Kühbach, M. Rahm, M. Thuvander, D. Mayweg: *An atom probe tomography comparison of the nanoscale chemistry of two Zircaloy-2-type alloys with different iron and chromium content after boiling water reactor operation*

D. Mayweg, J. Eriksson, M. Sattari, H.-O. Andrén, M. Thuvander: *Atom probe tomography study of oxidization of fuel cladding in boiling water reactor operation.*

D. Mayweg, J. Eriksson, M. Sattari, G. Sundell, M. Limbäck, I. Panas, H.-O.Andrén, M. Thuvander: *Formation of pure Zirconium Islands inside c-component Loops in High Burn-up Fuel Cladding*

D. Mayweg, J. Eriksson, M. Sattari, M. Thuvander: *Atom Probe Tomography Investigation of Hydrogen at $Zr(Fe,Cr)_2$ secondary phase particles in Zr-based fuel cladding from reactor operation*

We are also collaborating with *Takashi Sawabe* (CRIEPI, Central Research Institute of Electric Power Industry, Japan) and *Benjamin Jenkins* (formerly University of Oxford, now at University of Rouen, France) to combine our APT results on SPPs from different BWR cladding materials and damage levels to write a paper with working title:

D. Mayweg, T. Sawabe, J. Eriksson, B.M. Jenkins, M. Thuvander: *Redistribution of Fe, Cr and Ni in the vicinity of Secondary Phase Particles under different neutron fluences in Zircaloy-2 and derivative alloys.*