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ARC-2030 SUNRISE Mid-term report

Summary

The SUNRISE centre aims to prepare for the construction and operation of a Swedish lead-cooled research reactor with a target start date in 2030. The work in SUNRISE will not be sufficient to lead to licensing and construction of a reactor and thus it is part of a greater research and development programme with a high profile and significant commercial impact potential. The centre gathers three universities (KTH, Uppsala and Luleå) and a wide range of industrial and societal stakeholders in five work packages that together stake out the path towards advancing lead-cooled fast reactor technology in Sweden. The centre started its operations on January 1 2021 and has since then rather closely followed the plan set out in the application to SSF.

The research advances have so far resulted in four peer reviewed publications and have several results in the pipeline for further dissemination. 45 people have so far joined the centre in different capacities; 19 seniors and 26 juniors, with a mix of MSc students, PhD students and postdocs among the juniors and a mix of professors, associate professors, researchers and industry affiliates among the seniors.

The centre partners have already succeeded in securing funding for the second stage of the greater programme through the Solstice project application which was funded by the Energy Agency by 99 MSEK in 2022. The centre has also secured the planned three year programme access to neutron beam facilities at ANSTO in Australia in late 2022. Additional funding has been secured for the building of local research infrastructure by cash and materials contributions from Blykalla/LeadCold and Alleima. KTH has provided central co-financing to the centre and Luleå University of Technology has provided cofinancing for one PhD project. The centre is thus operating with a significantly higher budget than what was awarded by SSF initially.

The centre and the centre staff have had a truly significant impact in media and society. SUNRISE has been discussed in a very large number of invited popular scientific appearances, some of which are recorded and available: television and radio interviews, news articles, podcasts, a Museum exhibition, panel discussions and debates, and not the least a highly successful Youtube channel operated by one of the SUNRISE PhD students, with millions of views and nearly 40.000 subscribers to date. In short, SUNRISE is very visible in society.

It is with pleasure that we deliver this mid-term report to SSF for the consideration of the evaluation committee.

Pär Olsson – Director of SUNRISE

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List of acronyms (order of appearance)

SUNRISE	Sustainable Nuclear Energy Research in Sweden
SDG	Sustainable Development Goal
SSF	The Swedish Foundation for Strategic Research
SMR	Small Modular Reactor
LFR	Lead Fast Reactor
GenIV	Generation IV
PSAR	Preliminary Safety Assessment Report
WP	Work Package
HLM	Heavy Liquid Metal
KTH	KTH Royal Institute of Technology
LTU	Luleå University of Technology
UU	Uppsala University
SSM	Swedish Radiation Protection Authority
IAEA	International Atomic Energy Agency
ANSTO	Australia's Nuclear Science and Technology Organisation
H2020	Horizon 2020 – the 8 th European research framework programme
FACE	Flow Accelerated Corrosion/Erosion
SEFACE	Separate Effect FACE
CTF	Component Test Facility
COSTA	Corrosion test stand for stagnant liquid alloys
CRISLA	Creep-to-rupture test setup for structural materials in lead allovs
ASGARD	Advanced Steam Generators Assuring Reactor Deployment
TAF-ID	Thermodynamics of Advanced Fuels – International Database
XRD	X-ray Diffraction
SEM	Scanning Electron Microscopy
EDS	Energy Dispersive X-ray Spectroscopy
FIB	Focused Ion Beam
TEM	Transmission Electron Microscopy
TG	Thermogravimetry
DTA	Differential Thermal Analysis
DSC	Differential scanning calorimetry
XAS	X-ray Absorption Spectroscopy
XES	X-ray Emission Spectroscopy
HAXPES	Hard X-ray Photoelectron Spectroscopy
FFLS	Electron Energy Loss Spectroscopy
EXAES	Extended X-ray Absorption Fine Structure
FRDA	Elastic Recoil Detection Analysis
ATE	Accident Tolerant Fuels
SIMFUEL	Simulated Fuel
	Uranium Nitride
	High-Assay Low-Enriched Liranium
	Inprotected loss of flow
UTOP	Transient Over-Power
ULOHS	Unprotected Loss of Heat Sink
RVACS	Reactor Vessel Auxiliary Cooling System
IWR	Light Water Reactor
LME	Liquid Metal Embrittlement
IBE	Lead-Bismuth Eutectic
SSRT	Slow Strain Rate Testing
DFT	Density Functional Theory
MLIP	Machine-Learning Interatomic Potentials
FIV	Fluid-Induced Vibration
SPS	Spark Plasma Sintering
LOM	Light Optical Microscopy
EBSD	Electron Backscatter Diffraction
LFA	Laser Flash Analysis
OMC	Occupation Matrix Control
SQS	Special Quasirandom Structure
LES	Large Eddy Simulation
CFD	Computational Fluid Dynamics
CAE	Computational aided engineering

DNS	Direct Numerical Simulation
ROAAM	Risk Oriented Accident Analysis Methodology
AFA	Alumina-forming Austenite
AFM	Alumina-forming Martensite
CVD	Chemical Vapor Deposition
WRLES	Wall-resolved Large Eddy Simulation
WMLES	Wall-modelled Large Eddy Simulation
PIV	Particle Image Velocimetry
LDV	Laser Doppler Velocimetry
ECTS	European Credit Transfer and Accumulation System
ESNMS	European School on Nuclear Materials Science
IVA	Engineering Science Academy of Sweden
OKG	Oskarshamns Kraftgrupp
CET	Converging Energy Technologies
SWOT	Strengths – Weaknesses – Opportunities - Threats

1. Background, objectives and organization

1.1 Background, motivation and long-term vision

The UN Agenda 2030 calls for solutions to the global climate challenge. The partners of the SUNRISE centre argue that this is best met by developing and deploying a combination of low-carbon power producing technologies, where nuclear power is ideal for providing reliable CO2-free base-load capacity. Currently nuclear power provides nearly 40% of Swedish electricity needs, and has a capacity of 7.8 GW, slightly below the current base-load requirement of 9 GW. The ongoing expansion of wind-power ties up an increasing fraction of the national hydro-power capacity in order to compensate for the intermittency of wind and solar, and is therefore to a lesser extent available for base-load supply. Significant electrification and hydrogenation initiatives and strategies have been launched in Sweden in order to de-carbonize society. The current projections point to a doubling of the electricity consumption in Sweden over the coming decades. With the research that the SUNRISE centre aims at performing, we will work towards addressing the UN sustainable development goals (SDGs) 3, 7, 9, 11, 12 and 13. Development of sustainable nuclear energy has the potential for game-changing positive effects on a global scale, especially with regards to clean and affordable energy for the development of sustainable climate-neutral societies. For the projected transition from fossil fuel based transportation to electric transportation, we need to provide adequate amount of base-load electricity.

Thus, SUNRISE aims to prepare for the construction and operation of a Swedish leadcooled research reactor with a target start date in 2030. The reactor should primarily act as a demonstration first of a kind reactor with lead-cooled technology in the paradigm of advanced small modular reactors (SMR). Once operating, it should provide commercial services to customers as well as opportunities for research and training to academic institutions and research institutes. The services include irradiation of fuels and materials for GenIV reactors and advanced modular reactors and development of safety assessment strategies for a potential global deployment of GenIV lead fast reactors. The reactor will thus function as a demonstration unit for advanced nuclear power technology that can be commercialized on large scale within 15 years.

A three-stage R&D programme is established by the centre partners which will enable Sweden to commence commercialization of lead-cooled reactor technology within the coming 15 years:

- **Stage 1**: Development of R&D platform for materials and components' testing in support of design and safety analysis of a Swedish lead-cooled research reactor and an electrical mock-up prototype. (SUNRISE centre)
- **Stage 2**: Construction and operation of an electrically heated mock-up reactor, along with licensing of the research reactor design developed in Stage 1. (Solstice project)
- **Stage 3**: Construction and operation of a lead-cooled research, demonstration and training reactor. (SUNRISE-LFR)

Stage 1 is the focus of the SUNRISE centre, funded by The Swedish Foundation for Strategic Research (SSF).

Stage 2 has been started already in parallel through the project Solstice, funded by 99 MSEK in 2022 by the Swedish Energy Agency (dnr 2021-019839 Energimyndigheten).

Stage 3 is under initating discussions with the regulatory body (SSM, The Swedish Radiation Safety Authority), as well as with industry stakeholders and government representatives.

The work in stage 1, the SUNRISE centre, is focused on the design and preliminary safety analysis report (PSAR) of the research reactor and supporting research and development in materials, processes, codes and infrastructure.

The timeline of the broader SUNRISE programme, including commercial partner development track is summarized in figure 1 below.





SUNRISE comprises the initial actions above, as already mentioned: the design of the research and demonstration reactor and the R&D on components, materials and manufacturing processes. It also includes some irradiation testing but not with neutrons. Neutron irradiation tests are outside the scope of SUNRISE and are planned for in EU projects (Innumat and Fredmans) as well as under discussion with other reactor operators, such as MIT.

The second stage, Solstice, which includes design, construction and operation of an electrically heated prototype facility has been funded by the Energy Agency and was started during 2022. The facility should be built during 2023-2024 and then run through an extensive experiment and qualification programme to enable the licensing of the Stage 3 SUNRISE LFR. High level discussions on licensing of the research reactor were initiated in

2022 with SSM, the Swedish Radiation Safety Protection Authority, in the form of a series of meetings.

The commercialization tracks, here exemplified by the SMR AB joint venture company between Blykalla (international name LeadCold) and Uniper, are outside the scope of the academic programme leadership and is used to point towards the long-term goal of establishing a Swedish high-tech industry in advanced nuclear energy.

Sweden has a unique position to qualify and commercialize lead fast reactor technology, thanks to breakthroughs achieved in previous research projects funded by SKB, VR, Vinnova and the European Commission. In particular, KTH and (former) Sandvik/Kanthal have developed a class of alumina forming steels that are perfectly corrosion tolerant in liquid lead in a wide range of temperature and oxygen concentrations. In SUNRISE this development continues with other classes of lead-tolerant steels. Moreover, the economy of lead-cooled reactors can be greatly improved by the use of uranium nitride fuel, for which KTH has developed a range of novel manufacturing methods, allowing to obtain fuel pellets with very low porosity in an industrially scalable process. Extensive experience on natural circulation and heat transfer in liquid heavy metals has been built up at KTH and is continued to develop in SUNRISE. Radiation damage effects in candidate structural materials have been extensively investigated and continue here. UU has state-of-the-art expertise in materials chemistry and development of new materials and processes, exposure in terms of ion beam irradiation as well as detailed characterization and the materials under development in SUNRISE for pump impellers are showing great promise. LTU has world leading expertise in advanced materials processing, exposure in terms of wear and fretting, mechanical testing and advanced characterization. The partners are thus very well placed to succeed with the goals of the centre.

We thus argue that Sweden has the capacity to establish a world-unique competence base for development and commercialization of lead fast small modular reactor technology that can provide solutions with true impact for addressing the UN SDG:s and associated Targets.

1.2 Concrete goals and objectives

The clear concrete overarching goal of SUNRISE is that an application to build a research and demonstration reactor based on the design delivered by SUNRISE can be submitted. The centre cannot submit such an application itself, but the participating partners, or a consortium built of them, can do so. In order to reach this ambitious overarching goal there are several key steps that have to be completed. The work in the centre is divided into five work packages and the more detailed work and goals are here given by work package.

In work package 1 (WP1), the concept design of and preliminary safety analysis report (PSAR) for a lead-cooled research and demonstration reactor (SUNRISE-LFR) to be built in Sweden has to be developed and delivered. The detail and completeness level of such a PSAR is under discussion with the Swedish regulatory body (SSM), as well as discussion about who can actually submit it. What is clear is that the SUNRISE centre cannot do it since it is not a legal entity.

In SUNRISE WP1, the following major objectives for the research reactor, here named SUNRISE LFR, are defined as:

- Demonstrate reliable LFR operation
- Demonstrate LFR performance under transients
- Qualify LFR fuels (oxides and nitrides)
- Provide fuel irradiation services
- Provide steam for commercial services
- Provide training and education of nuclear engineers
- Provide irradiation of structural materials

WP1 will deliver a reactor design of such detail that a first level PSAR can be submitted. A first publication details the initial stages of such design [Dehlin-2022]. The contents of the PSAR will be defined in greater detail after further discussion with SSM but will in general follow the IAEA fast reactor licensing guidelines. It has to cover the General design, the Plant systems, the Operation, Radiation protection and Safety analysis. The demands of WP1 in terms of environmental conditions for fuel, clad, structural materials, temperatures, flow velocities, etc will come from WP1 and place demands on the test and qualification procedures in the other work packages.

In work package 2 (WP2), which is focused on steel development and degradation studies – in collaboration with WP3 and WP5 – as well as experiments and modelling of radiation damage.

The goal is to qualify structural steels for use in the research reactor and in extension for use in a fleet of commercial reactors. Most materials developed and studied here will act as overlay welded corrosion and erosion protective materials, that will be fused to already qualified fast reactor materials, such as 316L and 15-15Ti. WP2 will work on materials selection, fabrication and procurement, in cooperation with Alleima. The experimental test matrices will be initially defined and then continuously refined through discussions. New steels will be developed and delivered, for different applications in the reactor. Exposure and mechanical stress experiments will be planned and conducted. Selected complex components will be fabricated for testing in the experimental facilities that are constructed in WP5 (see below). Irradiation of alumina-forming steels and subsequent characterisation and mechanical testing will be performed. We will rely in the centre on ion beam irradiation (from the Uppsala Tandem facility) but may be able to access neutron sources in terms of research reactors as well (to be negotiated – the budget does not cover this). We will work on modelling of different aspects of the steel degradation and compare with experiments carried out.

In work package 3 (WP3), which is the largest work package in terms of manpower, there is an extensive list of tasks and goals. We will continuously work with selection of materials and components for all studies, often in centre-wide discussions at the technical workshops. We will develop new materials for different application areas in the reactor. Of critical importance is development of pump impeller materials and coatings. The processing development that is needed to fuse or clad qualified reactor materials with protective self-healing steels, will be developed here. The main focus for such work is advanced and programmable laser welding, so that once qualified, industrial scale processing can be enabled. Local facilities at LTU for wear and fretting experiments will be adapted for use in a liquid metal environment and materials for such testing will be procured in collaboration with WP2. All materials, compound components, weldments and coatings will be characterized with a wide range of techniques. Post-test analysis will be

conducted on all exposed materials and components. Selected materials and components will be prepared for testing in the larger scale facilities to be designed and constructed in WP5, see below. Post-exposure characterization will be mainly handled by WP2 and WP3.

Work package 4 (WP4) is dedicated to assessing the fuel/cladding/coolant interaction and fuel properties in operational and accident conditions. Uranium nitride is the reference long-term fuel for the SUNRISE reactor, although the plan is to start the reactor with oxide fuel in order to enable nitride fuel licensing in the first years of reactor operation. By coupling experimental and modeling techniques it will be possible to obtain a full description of this system and build a model to support the operational safety in a lead fast reactor. To achieve this, uranium nitride fuel powder and pellets will be fabricated at KTH. With the help of additives from UU in WP3 we will be able to make inactive simulated fuel, that chemically mimic fuel that has undergone irradiation. In order to build reliable models for fuel performance, we need to close the knowledge gaps regarding certain parameters of safety interest. We will investigate fuel/clad/coolant interactions at different conditions (room temperature, operation temperatures, transient temperatures). We will determine how the build-up of fission products cause properties such as the thermal conductivity to evolve. We will prepare samples for high-temperature neutron diffraction experiments in ANSTO, Australia. We will work on thermodynamic modelling of the important phases that appear in the fuel/clad system and investigate whether there is any relevant chemical fuel/clad/coolant interaction that should be modelled from the point of view of reactor safety. We will refine fuel fabrication parameters with spark plasma sintering to perfect impurity, microstructure and porosity control. We will perform mechanical testing and irradiation exposure of fuel materials. We will work with detailed state of the art microstructural characterization tools in all of these aspects.

In work package 5 (WP5), the goal is to develop a combination of modeling tools and an experimental platform that can be used for simulation and testing of flow accelerated corrosion/erosion (FACE) at high temperatures for materials and components that will be used for the reactor design and the licensing process. The aim is to provide test environments suitable for model development and validation data from FACE tests of selected reactor design components in flowing HLM at high linear flow velocities and high temperatures. The work will progress according to a similar materials selection procedure as in the other WPs. The detailed conditions for the test facilities will be discussed in centre-wide workshops. Two testing facilities will be designed, modelled and constructed: a separate effect FACE (SEFACE) facility and a component test facility (CTF). The former to focus on materials' tolerance to FACE and the second to test reactor-relevant scale components over relevant time scales and flow and temperature conditions. The plan is to also construct model-validating minor facilities which will work with scale-prototypic fluids and which can be well instrumented, in order to build detailed and validated models of the conditions in the actual test facilities. Experiments will be planned and carried out and post-test examinations of different kinds will be performed, together with WP2, WP3 and WP4.

1.3 The start-up process

The funding decision by SSF was received near midsummer 2020 and the contract with SSF was signed in early fall 2020. The then president Sigbritt Karlsson established SUNRISE as a KTH centre from 1 Jan 2021 with associated co-funding of 1 MSEK/year from the university. The recruitment of PhD students and postdocs started during the fall of 2020 and by January 2021 the centre was operational. A kick-off workshop was held online on January 19 2021, since this was in the middle of the covid-crisis. At this time, 12 seniors, three PhD students and two postdocs were associated with the centre. During the first year, several more recruitments were completed. By the end of 2021, there were four diploma students, six PhD students and four postdocs working in the centre, with 16 seniors.

The centre agreement discussion started directly between the parties that were decided to be partners in the centre (KTH, UU, LTU, Westinghouse, Blykalla, Alleima (then Sandvik Materials Technology)). Negotiations regarding establishment of the centre agreement were very prolonged and delayed by separate external negotiations between certain industrial partners in the centre that had relatively complicated contract processes ongoing that they insisted on closing first. This delayed getting the centre agreement ready and signed until December 2022. Consequently, the permanent steering group, with representatives from each signatory partner, was not established until the writing of this report (March 2023). The centre has thus operated with the interim steering group until now, consisting of Pär Olsson (KTH, director), Malin Selleby (KTH), Sara Bortot (KTH), Pavel Kudinov (KTH), Marta-Lena Antti (LTU), Gunnar Westin (UU), Denise Adorno Lopes (Westinghouse).

This procedural delay has not, according to our best estimate and understanding, affected the operation of the centre significantly. The centre has been very active in research and outreach and has had regular centre-wide workshops to make sure all participants and stakeholders can follow and discuss the technical progress and the strategy. All workshops have had online or hybrid format to allow participation from all stakeholders. The centre has so far held seven centre-wide technical workshops, at KTH, in Uppsala, in Luleå and in Oskarshamn.

1.4 Organization, leadership, research environments, relation to other grants

The parties in SUNRISE are KTH Royal Institute of Technology (KTH) [centre host], Luleå University of Technology (LTU), Uppsala University (UU), as funded academic partners, and Blykalla, Westinghouse and Alleima (former Sandvik Materials Technology) as strongly contributing industry partners. There is also an advisory body formed of other industrial, societal and academic stakeholders. These are Uniper, Outokumpu, Safetech, Vattenfall, Jernkontoret, Vysus group, Studsvik, Promation (CA), Oskarshamns kommun, The Swedish Radiation Safety Authority, MIT (US), UNSW (AU) and Bangor university (UK). The three international partner universities are contributing in-kind to the research activities in the centre.

The centre is led by the director, Prof Pär Olsson at KTH, together with the core group of Pls that lead the different work packages.

The centre is organised according to the following organigram, shown in figure 2. The centre board is the central unit of governance. The director reports to the board and leads

the activities of the centre. The work is organized in five work packages, see below. The partners with main contribution to the work packages are identified below, and the different types of external stakeholders and collaboration partners that form the advisory body are shown in the bottom.



The centre is staffed with 15 senior researchers at three universities (KTH, UU, LTU), three industry affiliates (Westinghouse, Blykalla, Alleima), seven PhD students (so far), nine postdocs (so far) and many MSc thesis students.

The meeting structure of the centre revolves around the centre-wide technical workshops (8 held so far) that have been online twice in spring 2021, then at KTH and at UU in the fall of 2021. At KTH and then at LTU during spring 2022, at Oskarshamn in connection to CET-2022, and then at UU during the fall of 2022, and recently at LTU in March 2023. Between these workshops, there have been several inter-WP meetings, intra-WP meetings and regular supervision meetings. Outreach actions have been planned and executed in between the workshops as well, most notably the public SUNRISE seminar in April 2022, and the CET-2022 conference in September 2022.

Research environments

The main research environments are located: at KTH in two departments; Physics/Nuclear Engineering (KTH-NE), and Materials Science and Engineering (KTH-MSE), as well as at Uppsala University Chemistry-Ångström (UU-CÅ) and Luleå University of Technology Engineering Sciences and Mathematics (LTU-TVM). These environments and the core staff are succinctly described below.

KTH-NE: Nuclear Engineering (NE), KTH: Participates with Prof Pär Olsson, Prof Janne Wallenius, Assoc Prof Pavel Kudinov, Dr Sara Bortot, Dr Dmitry Grishchenko, Dr Haipeng

Li, Dr Mikael Jolkkonen, technician Max Persson, several MSc diploma students, five new PhD students and six new postdocs. Starting April 1, 2023 also Dr Peter Szakalos and PhD student Christopher Petersson joins KTH-NE from the KTH Chemistry Department to consolidate forces within SUNRISE and in other related projects.

The KTH-NE team has extensive and world-leading expertise in reactor design, reactor physics and thermal-hydraulics, safety analysis, model validation and uncertainty quantification, severe accident modeling and experiments, heavy-liquid metal experiments and modeling, modeling of radiation damage in materials, materials characterization technique development, manufacturing, characterizing, exposing and testing novel composite materials and performing radiation tolerance experiments. The group works in a broad international context with links to a multitude of laboratories in Europe and across the globe. NE currently participates in eight H2020 and Horizon Europe projects in nuclear engineering and one on education, collaborates with several national and international industrial partners in the nuclear and materials science fields, has a state-of-the-art nuclear fuel laboratory where advanced nuclear fuels are developed, tested and characterized; several large nuclear engineering research infrastructures such as the dedicated SUNRISE laboratory that includes the SEFACE (Separate Effect Flow Accelerated Corrosion/Erosion) facility and the CTF (Component Test Facility) under construction, as well as the COSTA (Corrosion test stand for stagnant liquid alloys) facility in which liquid metal corrosion up to 900°C is has been tested, the small scale ECO-Rig (erosion-corrosion testing facility), the CRISLA (Creep-to-rupture test setup for structural materials in lead alloys) facility that is central to the work in WP2 of SUNRISE, and lastly the ASGARD (Advanced Steam Generators Assuring Reactor Deployment) facility which is under construction in collaboration with LeadCold and a Eurostars project. KTH-NE works actively with advanced model, code, and code package development. The division is coordinating the only and very successful Swedish Master program in Nuclear Engineering and has over the last 10 years produced 30 PhDs and over 300 MScs in the field. Recently, we have seen a clear increase in student interest in the Master program and have now the highest number of applicants ever. For the fall term of 2023 we expect more than 60 new students in the Nuclear Engineering Master program.

KTH-MSE participates with Prof Malin Selleby, Dr Huahai Mao, Assist Prof Greta Lindwall (Unit of Structures) and one postdoc under recruitment with world leading expertise in thermodynamic modelling and *ab initio* calculations. Additional support is given from other senior researchers and staff members. The research at the Unit of Structures and Unit of Properties at MSE is oriented towards characterization and theoretical modelling of materials structures and properties. Focus is on the link between atomic-level properties, thermodynamics, phase diagrams and kinetics in multi-component materials systems, in particular metals and cemented carbides. The research groups have also major expertise on structural characterization in the Hultgren laboratory by means of light optical and electron microscopy and high energy x-ray diffraction. Many software codes originate from MSE e.g. Thermo-Calc, DICTRA and several ab initio codes. Through SUNRISE, KTH and Sweden joins the OECD/NEA TAF-ID project (Thermodynamics of Advanced Fuels – International Database) as a full partner. This will allow us access to state-of-the-art thermodynamic data generated over a decade by the leading research institutes in the world and establishes Sweden and SUNRISE as a key international actor in the field.

Chemistry-Ångström at Uppsala University (CÅ-UU) participates with Prof Gunnar Westin and one postdoc (Dr Sarmad Naim Katea, who has now moved on to an industry position), and will recruit one more postdoc in the near future. Prof Westin has over 30 years of experience in all aspects of solution based materials synthesis. A wide range of complex composition and structure materials have been studied from design of metal-organic precursors, via the reactions taking place on heat-treatment, to the target materials in forms of nano-particles, coatings, thin-and ultra-thin films, sponges and compacts. The research group has a dedicated solution processing lab with spin-coaters, specialised furnaces and four glove-boxes for handling of sensitive materials and precursors. Further, the group extensively use various XRD techniques, IR and Raman spectroscopy, XPS, SEM-EDS, FIB-SEM, TEM-EDS, TG/DTA/DSC for microstructural characterisation, as well as a number of advanced techniques including XAS, XES, RIXS, HAXPES, EELS, EXAFS, ERDA, luminescence, in collaboration with UU and international groups. The research ranges from very fundamental designing precursor structures and mechanistic studies to applied, with several processes tried out at pilot or industrial scale, or applied in Swedish industry. These studies have included some 20 Swedish companies. The group has very extensive national and international networks which can be used for microstructural analysis, as well as the very well-equipped Angström laboratory, including the national ion beam infrastructure The Tandem Laboratory, and experts in synchrotron based studies. The group also use the TEM facilities at Stockholm University. UU has its major contribution inside WP3 but is actively working with WP2 and WP4 as well, and will have stronger interactions with WP5 in the near future.

The participation from Luleå University of Technology and the Department of Engineering Sciences and Mathematics (LTU-TVM) is coordinated by Prof Marta-Lena Antti with active support from Prof Farid Akhtar (Engineering Materials), Prof Jens Hardell, Assoc prof Leonardo Pelcastre (Machine Elements/Tribology), Assoc prof Jan Frostevarg (Product and Production Development), two new PhD students, one postdoc, and with several additional researchers and technicians. There is a clear interconnect with the other partners in the centre, and in particular with UU (Prof Westin) inside WP3. There is an integrated research environment that spans across different disciplines and different academic partners.

The research group of Engineering Materials at LTU has been actively involved in cutting edge research on metallic and ceramic materials for applications ranging from structural to functional and hosts advanced and novel research infrastructure. Relevant for this work is the long experience of research on steel, titanium, super-alloys and high entropy materials together with a well-equipped laboratory for analysis and characterization of materials including mechanical properties, microstructure, and chemical composition. The research group has been undertaking several research projects funded by national, European and international funding agencies. Engineering Materials has established strong research network with national and international universities, research institutes and industrial companies. The group hosts TMTest Infrastructure for characterization of high temperature thermomechanical and tribological properties. The Machine Elements group is one of the leading tribology research groups in Europe, possessing competences covering all aspects of tribology and expertise pertaining to machine components tribology, computational tribology, materials related tribology and tribo-chemistry. The group has

earned a strong international position and reputation and has developed an extensive international network based on long-term collaboration with leading research groups and industries worldwide. Over the last 15 years, the research on high temperature tribology at LTU has developed into a research area with strong industrial linkage and relevance. This research at LTU is unique in Sweden and only a few groups are engaged in this field worldwide. The state-of-the-art tribology research laboratory at LTU, "Tribolab", is one of the best equipped tribology laboratories in Europe with >30 test platforms for friction and wear characterization, including several at high temperature, and are now adapted to work with heavy liquid metals.

The activities in LTU are focused in WP3 and are divided into the main research directions as follows: (i) Laser coating of components for liquid lead environments, (ii) fretting and degradation in liquid lead, and (UU): (iii) processing of impeller materials for abrasive liquid lead environment, (iv) oxide coatings on steel, and (v) synthesis of nano-particular metal nitrides for manufacture of sim-fuels.

The two PhD students are fully engaged and integrated into the LTU environment. Paul Gruber is working in two parts, area (i) and (iii) and Daria Kolbas in the fretting and degradation part (ii). In addition, one post-doc worked on synthesis within the sub-areas (iii) and (v) delivering synthesized powders for sintering and studies to WP3-LTU and WP4, and hiring of another post-doc is in progress. The activities are highly interconnected since the laser coatings will be evaluated with respect to fretting performance and the impeller materials are SPS sintered (spark plasma sintering) and studied regarding their mechanical and lead corrosion properties. Metal nitride nanoparticles synthesized in WP3 are sintered with uranium nitride (UN) and studied within WP4 and the impeller materials and coatings on steel will be studied on their lead corrosion and abrasive properties within WP5.

Relation to other grants

The CREATERNITY program at Luleå University of Technology

CREATERNITY is one of the future focus areas at Luleå University of Technology directed towards sustainable material use in a connected and circular economy. The research is multidisciplinary and gathers researchers from a large number of subjects to take a holistic view of industry's and society's sustainability challenges, with an aim to generate new innovations. The research activities involve 14 different projects at present with a wide range of disciplines engaged in collaborative research.

CREATERNITY opened a call for PhD student projects in 2020, with the aim to create an interdisciplinary Graduate School spanning over several research subjects at LTU. The call involved part funding of 200 kSEK/year for a PhD student project for up to four years. A proposal was prepared based on a part of the activities in WP3 of the SUNRISE project, specifically the work focused on fretting and degradation of materials in liquid lead. The idea was to obtain complementary funding to enable the recruitment of a second PhD student at LTU to work in the SUNRISE project. The proposal, Sustainable and Circular Nuclear Energy through Advanced Materials and Tribology Research (CiNEMaT), was granted funding and created the necessary platform for recruitment of a second PhD

student and simultaneously expanding the scope of the activities related to tribology in liquid lead environments. Thus, Creaternity effectively co-funds SUNRISE with 200 kSEK/year.

The Solstice project

The Energy Agency approved step two of the SUNRISE programme by funding the Solstice project by 99 MSEK in February 2022. Solstice is an industry coordinated project with the goal of verifying the Blykalla developed SEALER-technology. The aim is to, financially and conceptually, assure the case for future commercialization of small modular LFR technology. The strategic goal is to establish lead cooled SMR as a sustainable and safe solution for plannable and flexible base power to make it part of a sustainable society working towards circularity. Being financially viable and scalable, the global market can be addressed with products and services like electricity, high-quality heat, hydrogen, biofuels, electrofuels and ancillary services. Advanced and sustainable nuclear, with passive safety and manufactured in automated production, offer all benefits of conventional nuclear but is substantially more versatile and flexible. SMR can become the solution that enables an introduction of large-scale climate-neutral electricity production, and, at the same time, being able to provide additional benefits. The partners of the consortia and interested customers enable in-depth customer requirements, as well as a fast market track. The specific targets of Solstice are to

- 1. Design, construct, commission a 3.3 MW electrically heated facility.
- 2. Qualify processes for manufacturing, engineering and pilot-scale commissioning.
- 3. Verify models for heat transport from reactor core.
- 4. Develop principles for operation and maintenance and the functions of the instrumentation.
- 5. Demonstrate system service connections for the use of high-value process heat.
- 6. Demonstrate and evaluate the concept regarding economics and technology, calculate electricity production cost for different manufacturing options and technical lifetime of components.

The academic partner of the Solstice consortium is KTH and the research planned for KTH is directly in line with and complementary to the work plan in SUNRISE. In essence, with the successful Solstice application, the SUNRISE centre has acted as a seed to the greater programme.

In-situ studies of advanced nuclear fuels (ANSTO programme)

SUNRISE participated in an application to The Australian Nuclear Science and Technology Organisation (ANSTO) for a programme access to their facilities over a timespan of three years (2022-2025). The proposal, focusing on in situ studies of advanced nuclear fuels, was accepted and awarded the requested facility time and access. The program aims to build a mechanistic understanding of the corrosion processes and failure mechanism of accident tolerant nuclear fuels, for light water and for metal cooled reactors, under transient conditions. This will be achieved through four key objectives:

- 1. To characterize the phase evolution and thermal expansion of ATF candidate materials under thermal ramping, oxidation and hydriding, using in-situ neutron diffraction on Wombat.
- 2. To examine cladding failure mechanisms by performing quantitative strain measurements at accident-relevant transient temperatures on Kowari.
- 3. To visualise pellet cracking and coolant ingress events in a damaged fuel pin on Dingo.
- 4. To grow the local ANSTO capabilities in characterising uranium compounds, to enable more advanced, and higher-throughput, in-situ measurements of nuclear fuels in simulated accident conditions.

An ambitious project plan is set in motion and the first samples of UN SIMFUEL have been fabricated and pre-characterised at KTH and are undergoing export to Australia for high-temperature neutron diffraction studies as of March 2023. This entails in-kind facility support to SUNRISE activities worth more than 2 MSEK over the coming three years, not counting associated in-kind manpower. This work feeds directly into and supports the activities in WP4 of SUNRISE.

1.5 Steering group

The steering group is composed of participants from all partners to the centre agreement, i.e. KTH, UU, LTU, Westinghouse, Alleima and Blykalla.

The steering group consists of:

- Sandra Di Rocco (chair, Dean of School of Engineering Sciences, KTH)
- Lina Bertling Tjernberg (Director of Energy platform, KTH)
- Tim Bowden (Head of Department Chemistry-Ångström, UU)
- Margareta Groth (Head of Department of Engineering Sciences and Mathematics, LTU)
- Eva-Lindh-Ulmgren (Head of Materials design, Alleima)
- Merja Pukari (Chief Operations Officer, Blykalla)
- Tage Tarkpea (General Manager, Nuclear Fuel and Engineering, Westinghouse)

Since the centre agreement was not formalized until the end of December 2022, the steering group composition was finalized in early spring 2023 and the first formal steering group meeting will be held in April 2023.

2. The research of the project

2.1 Description of the scientific results

The progress in terms of scientific results are here presented, by work package order.

WP1 Design and safety analysis of a Swedish lead-cooled research reactor

In work package 1, the concept design of and preliminary safety analysis report for a leadcooled research reactor (SUNRISE-LFR) to be built in Sweden is developed. The transient performance of the reactor is to be achieved using a passive safety approach, based on phenomena such as gravity, buoyancy, temperature and radiation. Protection of the public shall be ensured without need to rely on the availability of external power. To this end, the reactor shall be designed with ability to remove residual heat from the core using natural convection of the primary lead coolant, and eventually to remove heat from the primary system to the atmosphere using natural convection of air. By "ability" is meant that the integrity of barriers for release of radionuclides, such as fuel cladding tubes and the primary reactor vessel shall not be challenged during such transients.

The main work is conducted using a three-step process, based on

- 1) Detailed analytical investigation of how basic design parameters are coupled to the performance of passive safety systems.
- 2) Lumped parameter dynamic analysis using the in-house code BELLA.
- 3) Verification with higher fidelity codes, based on e.g. Monte-Carlo and Computational Fluid Dynamics techniques.

The main novelty of this process, compared to state-of-the art approaches, is the introduction of a more detailed analytical investigation on how basic design parameters are coupled to the performance of passive safety systems. The intent is that this shall permit to identify the aspects of the design that drive passive safety performance, and hence allow to focus the design work on a few essential parameters. Moreover, the development of an in-house code for dynamic analysis permits to tailor the code to particular design choices that are difficult to simulate using state-of-the-art codes available to KTH. E.g. SAS4A/SASSYS does not allow to simulate lead-cooled reactors with the steam generator located in the primary system, and APROS does not model feedback from radial and axial expansion of core structures.

Experimental verification of the design is carried out in WP 2-5 of SUNRISE, in the SOLSTICE project funded by the Swedish Energy Agency and the ASGARD project, funded by EUROSTARS.

Analytical approach to safety

In WP1, a significant portion of the first year was dedicated towards developing an analytic method for how to design passively safe lead-cooled reactors starting from first principles. This method was subsequently used to design the uranium nitride (UN) core of SUNRISE-LFR. The work resulted in a published journal paper (Dehlin et al., 2022) and is the foundation for most of the future work within the SUNRISE centre that is directly related to the actual reactor. The reactor core configuration is shown in figure 3.



Figure 3: The core map of the research reactor SUNRISE-LFR.

Fission gas release from nitride fuels

The release of noble gases from the fuel to the gas plenum will influence the dimensioning of the fuel rod. Experimental data are highly scattered and a better understanding of how fabrication parameters such as pellet porosity and impurity concentration influences gas release is necessary. In WP1, a detailed analysis of the data showed that the wide scatter could be attributed to the impact of oxygen impurities in the as fabricated fuel. A semiempirical correlation was developed, introducing a fission gas migration barrier as function of oxygen impurity concentration. This model allowed to reproduce and classify experimental data in a better way than previous correlations, and to predict a burn-up dependent Vitanza threshold for initiation of gas release from uranium nitride fuels [Sheppard-1979].

Fuel management strategy

The current strategy is that SUNRISE-LFR shall achieve its first criticality with a smaller core consisting of HALEU UO₂ fuel. It will subsequently transition to the targeted uranium nitride (UN) fuelled core, which is published in the article cited above, once the UN fuel

has been qualified for use. A strategy for optimising the transition from UO₂ to UN is currently under development based on the fission matrix approach [Morton-1953, Mickus-2020].

Radiological consequences of severe accidents

Closely related to the work conducted when designing the SUNRISE-LFR UN core was the study performed about dispersion of radionuclides from the core in the event of a hypothetical core disruptive accident. One important section of the Preliminary Safety Analysis Report (PSAR) that WP1 will contribute to is the study of how the surrounding environment might be impacted if radionuclides are released from the core. This investigation was performed with the U.S. NRC developed software RASCAL 4.2 and included as a section in the published journal article [Dehlin-2022]. It was shown that even with unrealistically conservative assumptions for the release of radionuclides, e.g., no containment building or filter systems present, the dose limit imposed by the Swedish regulator SSM was satisfied within 1.5 km from the plant. In the anticipated detailed calculations, which will be performed once a more complete design of reactor and reactor building has been performed, will allow for the use of more realistic assumptions and subsequently lower the predicted radiological impact compared with the published one.

Activation of primary coolant

A study into the neutron activation of lead coolant with different amounts of impurity concentrations has dominated the latter part of the second year. The study is currently in the final stages before a manuscript can be submitted to a scientific journal for publication. It concluded that silver contamination poses a significant challenge from a radiological point of view, especially with regards to decommissioning and exempting the coolant from radiological control. It was shown that a final repository will be required even if the initial silver concentration is < 0.1 ppm due to build up of metastable Ag-108^{m1} with T_½ ~ 438 y. This study also investigated if the commonly used assumption that coolant circulation can be disregarded due to the coolant's residence time in the system being orders of magnitude longer than the circulation time is valid. The depletion matrix was combined the combined with a simple advection model and it was shown that for most nuclides there is either no difference or a slight reduction in total activity. The recommendation thus became that the stagnant coolant assumption shall be used for licensing purposes due to it representing the more conservative assumption without exaggerating the coolant activity significantly, compared with the circulating case.

Management and development of BELLA

The multi-point dynamics code BELLA can reproduce the magnitude of mass flow, reactivity, power, and temperature of fast reactors systems, and was developed at KTH [Bortot-2015]. This code can be used for safety-informed design and stability analysis of fast reactor systems, allowing the isolation of essential phenomena and trends of

significance for their safety assessment. Initially, the code was developed on Python and MATLAB Simulink, using the solvers provided by each software.

One of the activities includes re-writing the BELLA code in the Fortran language. This language was chosen because it is easy to learn and provides efficient constructs that are useful for numerical calculations. The initial modules of the code were: neutronics, thermal-hydraulics, and steam generator. These modules were rewritten in the Fortran language and coupled through a main file.

The radial temperatures equations to obtain fuel, gap, cladding and lead temperature are solved in a simultaneous way, using the Thomas method. Regarding the primary Systems, which include hot-leg, steam generator, cold-leg, cold-pool, reactor-vessel and guard-vessel, the model is solved in a sequential way through an explicit discretization. The neutronic model, to obtain the reactor power and heat source, is solved sequentially through an explicit discretization.

Once the initial BELLA Code is coupled, the activity consists of the further development of the code, for the simulation of dynamic transients in liquid metal-cooled reactors. These transients are: unprotected loss-of-flow (ULOF), transient over-power (UTOP), loss-of-heat-sink (ULOHS) and station blackout (ULOF and ULOHS combined) accidents.

In Work Package 1 of SUNRISE, a thermomechanical model of the nuclear fuel was developed by Guan Wang, a visiting PhD student. This module is merged into the Fortran version of the code.

After the coupling, a frozen version of the BELLA Fortran version was obtained and filed on GitHub, to get better control of the code and the future addition or modifications. Also, the manual of BELLA is updated and, a user version is available. This version was used for different users to get improvements.

The last activity related to the BELLA code is the addition of the Reactor Vessel Auxiliary Cooling System (RVACS) module, the activity includes the writing of the model and developing the solution in Fortran language. Once the module is working as a separate module, the next step is coupling with the frozen version of the code and getting a new version of the code.

The new version includes the modules of neutronic, thermal-hydraulic on the primary system and in the reactor core, Thermomechanics on the nuclear fuel, and RVACS. The analysis of the reactor under the different transients and station blackout is currently under way.

References for WP1

- F. Dehlin, J. Wallenius, S. Bortot, An analytic approach to the design of passively safe leadcooled reactors. Ann. Nucl. Energy 169 (2022) 108971. <u>https://doi.org/10.1016/j.anucene.2022.108971</u>
- D Sheppard, C Vitanza, 1979. Fission gas release from LWR fuel during steady state and transient conditions. Paper to be Presented at the Enlarged Halden Programme Group Meeting.Hankø, Norway, 17th-22nd June, 1979. OECD Halden Reactor Project.

- Morton, K.W., 1956. Criticality Calculations by Monte Carlo Methods, United Kingdom Atomic Energy Research Establishment, Harwell, Report T/R-1903.
- I. Mickus, J. A. Roberts, J. Dufek, Stochastic-deterministic response matrix method for reactor transients, Annals of Nuclear Energy 140 (2020) 107103.
- S. Bortot, E. Suvdantsetseg, J. Wallenius, BELLA: a multi-point dynamics code for safetyinformed design of fast reactors, Annals of Nuclear Energy 85 (2015) 228-235.

WP2 Development of advanced steels and radiation damage studies

Liquid metal embrittlement of alumina forming steels

The main work in WP2 has initially focused on investigating the issue of liquid metal embrittlement (LME) [Kamdar-1973, Gong-2022] of the proposed novel steels to be used as protective overlay on the cladding tubes. The susceptibility of Fe-10Cr-4Al steel to LME in low oxygen liquid lead and lead-bismuth eutectic (LBE) environments was investigated using a newly developed slow strain rate testing (SSRT) technique that can be employed at elevated temperatures. This study showed that the Fe-10Cr-4Al steel suffered embrittlement when exposed to LBE over a wide temperature range. The embrittlement, here measured as a reduction in fracture strain, was observed at the melting temperature of LBE and reached a maximum at approximately 375°C. At temperatures above 425 °C, the material's ductility regained its original level. The exposures in liquid lead (pure Pb) showed no indications of embrittlement, but a ductile behavior over the entire temperature range studied (340-480 °C) [Petersson-2023]. This is a crucially important result for the progress in SUNRISE since the candidate protective material is now shown to not exhibit low-temperature embrittlement. This result strengthens the application case significantly.

The effect is here shown by the following two figures that exhibit the LME susceptibility when the material is exposed to LBE, but not to pure Pb, figure 4, and how the effect depends on the Bi concentration in the eutectic, figure 5 [Petersson-2023].



Figure 4: Ductility trough for LBE environment (solid blue line). The red line (light blues dots) is for the experiments in pure Pb. The single sample showing a drop in ductility in the lead is an anomaly and showed no indication of embrittlement when investigated. The anomalous drop to 20.83 % at 350 °C is believed to be caused by a pre-existing defect in the sample.



Figure 5: Relation between Bi concentration (wt%) and the total strain until failure of the Fe-10Cr-4AI material at a strain rate of 10⁻⁵ s⁻¹. Red triangles are tests with a lower strain rate of 10⁻⁶ s⁻¹. A clear drop in total strain to failure is seen at around 4 wt% Bi in Pb.

First-principles based modelling and machine-learning studies of radiation damage in model materials

Austenitic steels, which are face centered cubic (fcc), are widely used in the nuclear industry due to their advantageous physical properties, mainly their good high-temperature strength and creep resistance. For the same reasons, this class of alloys is also a favored choice for lead-cooled fast reactor (LFR) core structural materials. The higher operation temperature and power density in fast reactors require more analysis to understand accurately the behavior of austenitic steels in LFR. In the SUNRISE-LFR reference design, austenitic 15-15Ti steels will be used for the fuel cladding tubes and AFA steels will be used as protective overlay weld for the vessel. At the atomic scale, these alloys are characterized by chemical disorder (i.e., the random distribution of chemical atomic species), and a magnetic disorder at high temperature (i.e., the random distribution of atom magnetic moment intensities and directions). We aim at understanding the effect of magnetic and chemical disorder on the defect properties in this class of alloys using atomscale simulation methods, more specifically first-principles calculations with the Density Functional Theory (DFT) method [Kohn-64], and Machine-Learning Interatomic Potentials (MLIP) [Behler-2016]. Studying both magnetic and chemical disorder at the same time, however, is very challenging, due to the large amount of configurations to explore. Therefore, we started to study the effect of magnetic disorder in pure nickel material, which is a suitable model for austenitic steels given that it is magnetic and has the right crystal structure. Previous studies using fcc Fe as model material suffer from lack stability given that the fcc structure of austenitic steels is stabilized by the relatively high Ni content, and that pure fcc Fe is dynamically unstable. Defect studies in such a model material are thus extremely challenging.

Main results:

- DFT was used to perform molecular dynamics simulations above 800 K, i.e., beyond the Curie temperature where nickel undergoes a second order phase transition from ferromagnetic (ordered) phase to the paramagnetic (disordered) phase. We selected a range of temperatures: 800 K, 1000 K, 1200 K, 1400 K, 1600 K, and 1800 K. Simulations were performed in the NPT ensemble in these three cases: with no defects, with an interstitial defect, and with a vacancy. The paramagnetic phase has been modelled by using the Disordered Local Magnetic-Moment method [Steneteg-2012], i.e., imposing a new initial magnetic moment on all atoms every 8 femtoseconds (given that the molecular dynamic timestep is 2 fs). The results showed quite good qualitative results, but we need to continue these studies as we did not yet observe a clear trend concerning the defect formation energy as function of temperature. Therefore, we are carrying out further simulations in the NVT ensemble based on the average volume found in NPT simulations in the case of the systems with no defects.
- The fitting of a Machine-Learning Interatomic Potential (MLIP) has been initiated using the MiLaDy package [Goryaeva-2019]. MLIP could be very relevant to compute entropy contributions on defect formation enthalpies because they allow to perform much less computationally expensive calculations compared to DFT. At a first step, we aim at developing a MLIP trained on a DFT database to describe nickel properties below the Curie temperature (i.e., in the ferromagnetic phase). To do this, we computed various structural —----- deformations (Figures 6 and 7), elasticity, free surfacen— thermodynamic (molecular dynamics) and defect calculations (formation and migration energy) in nickel to provide a large database to train our machine-learning model. We managed to build a model that predicts

accurately the interatomic forces and stresses but still with a too high error on the energy of the systems (Figure 8). We are performing more calculations on deformations and elasticity to enhance the energy description of our model, and revisiting certain configurations that may suffer from poor convergence (see figure 6).



Figure 6: Deformation calculations to compute the bulk modulus of Ni at zero temperature.



Figure 7: Energy of nickel at zero temperature with high deformations (stresses) applied on the systems. The data in the black square are selected for the training. The remaining are considered as too extreme to be representative.



Figure 8: Force train/test of the machine learning model built at this time.

References for WP2

- M.H. Kamdar, Liquid Metal Embrittlement. Treatise on materials science and technology 25 (1973) 99.
- X. Gong, M. P. Short, T. Auger *et al.* Environmental degradation of structural materials in liquid lead- and lead-bismuth eutectic-cooled reactors. Progress in Materials Science. 126 (2022) 100920. <u>https://doi.org/10.1016/j.pmatsci.2022.100920</u>
- C. Petersson, P. Szakalos, D.D. Stein, Slow strain rate testing of Fe-10Cr-4Al ferritic steel in liquid lead and lead-bismuth eutectic, Nuclear Materials and Energy 34 (2023) 101403.
- P. Hohenberg, W. Kohn, Inhomogeneous electron gas, Phys. Rev. 136 (1964) B864-B871.
- J. Behler, Perspective: Machine learning potentials for atomistic simulations, Phys. Chem. Chem. Phys. 145 (2016) 170901.
- P. Steneteg, B. Alling, and I. A. Abrikosov, Equation of state of paramagnetic CrN from ab initio molecular dynamics, Physical Review B 85 (2012) 144404.
- A.M. Goryaeva, J.B. Maillet, M.C. Marinica, Towards better efficiency of interatomic linear machine learning potentials, Comput. Mater. Sci. 166 (2019) 200–209.

WP 3 Characterization, advanced manufacturing and lab-scale testing of coatings and novel materials

Nuclear fuel tubes. As suggested by Dehlin et al. [Dehlin-2022], the fuel rod design consists of a bulk 15-15Ti (or AIM1) steel tube with a protective layer made from Fe-10Cr-

4AI steel. 15-15Ti provides a base material with high radiation dose tolerance that is qualified as a pressure boundary in fast reactors and will be 500 μ m tick. The FeCrAl coating adds protection against the liquid lead environment due to its corrosion resistance [Dömstedt-2019]. A thickness between 100 – 200 μ m is required to provide sufficient self-healing qualities if abrasion occurs due to erosion or fretting wear while still being thin enough to not impair the neutron flux. Laser cladding using thin wires of 0.2 mm was selected as the coating method due to the clean processing environment, minuscule porosity, strong interface, and ease of producing feedstock material. Conventional laser cladding using ticker wires of 800-1600 μ m diameter is well studied, however, thin wire laser cladding with in-line feedstock is not. Therefore, WP3 conducts process development and optimization of thin wire laser cladding at LTU.

Initially, a model alloy system consisting of 316L stainless steel wire and 316L flat plate substrate was researched to gain first insights into the process. Currently, a publication about these results is being written. In it, high-speed imaging, cross-sectional analysis, and topographical analysis of mainly single tracks was conducted. Several processing modes were discovered such as drop-deposition, which was studied in detail. Dilution of the overlay weld into the substrate was measured as a function of laser power and processing speed and gives a guideline to prevent excessive mixing of substrate and clad material. This will be of great importance to preserve the material properties of both 15-15Ti and FeCrAI. The obtained understanding and knowledge from the single tracks have then been transferred to overlapping tracks to form a closed, continuous surface clad.

Experiments with 200 µm FeCrAl wire (provided by Alleima) started recently. The substrate is still 316L in flat mode but also tube form. Figure 9 below shows the first successful single track using the new material. So far FeCrAl behaves comparable to 316L as cladding material in terms of processing parameters, however, a little more power is necessary to achieve similar dilution, probably due to a difference in reflectivity with respect to 316L.



Figure 9: Laser cladded FeCrAl single track on 316L flat substrate.

Impeller materials. The pump impeller circulates the liquid lead in the nuclear reactor vessel. Due to the high density of lead and high relative velocity between the liquid lead and the impeller-blades, erosion is expected. Therefore, a highly abrasion resistant material that can withstand erosion for a long time even at temperatures over 500 °C is required. Cemented carbides, i.e. composites of a hard metal carbide network and a transition metal binder-phase were identified as the most suitable for this purpose. Such composites are used in demanding metal machining and rock excavation and typically

consist of WC-Co. However, it is also expected that the hard cemented carbide blades require a protective hard coating which also resist possible metal dissolution in a high-temperature liquid metal environment. Hence, the objective for this project is to achieve suitable impeller materials or material combinations that resist erosion by molten lead in the impeller function. In the present study, the aim was to achieve composites of WC or NbC with Ni or Fe binder-phase, as cobalt is generally undesirable in nuclear reactors as it is activated to highly radioactive Co⁶⁰. This is an effort also pursued by cutting tool companies as Co is seen as toxic and a strategic element that should be out-phased from the EU. Furthermore, in order to obtain high hardness and reduce possible damage by dissolution of Ni and to a lesser extent Fe, which are soluble in lead, [Dehlin-2022] a composite with a very low amount of isolated binder-phase in sub-micron grained WC and NbC was the goal. Besides the overall composition the processing parameters are quite decisive on the properties and the prevailing processing techniques are not able to achieve such high quality structures, as far as we can find.[Garcia-2019]

However, by using a solution based process developed by Westin et al. well-adhering Co/Ni/Fe nano-particles or nano-crystalline coatings can be deposited on the carbide grains. [Ekstrand-2003, Ekstrand-2007] Such coated powders yield very homogeneous and high sintering activity allowing for unique high quality composites with extremely low binder phase contents to be prepared.[Naim Katea-2020, Naim Katea-2021] The process is presently explored aiming at high quality composites with submicron WC and NbC grains and down to 2 vol% Ni or Fe binder phase. SPS sintering and mechanical characterisation of the Ni coated WC powders produced at UU were made at LTU. Composites of 99% relative density and submicron WC grains could be obtained with as low binder content as 2 vol% Ni (Figure 10). This WC-Ni composition showed an exceedingly high hardness of 2200 HV₁₀ which is unique for WC-Ni composites. The WC grains forming a strongly connected network and the very low nickel content isolated in pockets may even make this composite a viable impeller material without a supporting coating. Studies on Nb-Ni and WC/NbC-Fe composites are presently pursued and corrosion / abrasive testing in stagnant (WP3-LTU) and high velocity molten lead will be conducted (WP5). Development of WC / Al₂O₃ coatings will commence during 2023.



Figure 10. (Left) SEM image of WC powder coated with 2% Ni nano-dots, (right) SEM image of WC-2%Ni composite.

Tribological testing. In nuclear reactors, small-amplitude oscillatory motion occurs between the fuel cladding tube and spacer wire due to circulation of lead and thermal gradients, which is usually called fluid-induced vibration (FIV). FIV on surfaces that are loaded against each other results in fretting wear which occurs wherever short amplitude reciprocating sliding between contacting surfaces is sustained for a large number of cycles. This leads to plastic deformation, which is followed by cracking involving oxidation of bulk material along the cracks and fatigue [Gong-2022]. Fretting does not necessarily result in extensive material volume loss, but propagating cracks can lead to complete failure of a component. Drozdov et al. [Drozdov-2014] evaluated steels used in the BREST and MTBF reactors and reported that passivation of the samples in lead-bismuth prior to fretting experiments reduced the friction coefficient for all parameters tested. Del Giacco et. al. [Del Giacco-2014] analysed fretting wear in liquid lead of f/m T91 steel, austenitic 15-15Ti steel, and AI surface alloyed T91 (GESA-T91) and showed significant surface wear of varying severity for tested samples pointing to the necessity to consider fretting wear already during the design phase of a reactor. Therefore, fretting/corrosion testing is conducted at Luleå University of Technology (as part of WP3) to understand the damage and degradation mechanisms of candidate materials in a simulated reactor environment.

In the first stage, an existing oscillating high-temperature friction and wear tester was adapted to enable the use of liquid metals as the test environment. Thus, it became possible to test samples immersed in liquid lead at 550 °C in a controlled atmosphere of Ar+5%H2. After repeatability of the experiments was achieved, an experimental campaign involving 316L stainless steel (as the reference nuclear material) and 100Cr6 (as the standard material used in this friction and wear setup) using two contact configurations was carried out. The aim of the test campaign was to perform optimization of the test methodology for the liquid lead environment and the investigation of the influence of lead on the friction and wear processes. The test parameters were based on the predicted reactor operating conditions and computational data available in the literature. Currently, a publication about these results is being prepared. The scope of the publication is friction data, wear volume and volume of the generated tribolayer, analysis of degradation mechanisms, cross-sectional analysis, and surface 3D optical interferometry results. In addition to improving the methodology and describing the effect of lead on friction, valuable insights were obtained on the correlation between the topography and shape of the samples and the wettability of steel with lead.

The next stage of the project is to test the Fe-10Cr-4Al steel received from WP2.



Figure 11: Damage mechanisms of steels after the experiment

References WP3

 F. Dehlin, J. Wallenius, S. Bortot, An analytic approach to the design of passively safe leadcooled reactors, Annals of Nuclear Energy, 169 (2022) 108971. <u>https://doi.org/10.1016/j.anucene.2022.108971</u>.

- P. Dömstedt, M. Lundberg, P. Szakalos, Corrosion Studies of Low-Alloyed FeCrAl Steels in Liquid Lead at 750 °C. Oxid Met 91 (2019) 511. <u>https://doi.org/10.1007/s11085-019-09896-</u>z
- J. García, V. Collado Ciprés, A. Blomqvist, and B. Kaplan, "Cemented carbide microstructures: a review," Int. J. Refr. Metals, Hard Mater. 80, (2019) 40–68. doi: 10.1016/j.ijrmhm.2018.12.004.
- Å. Ekstrand, G. Westin, Highly homogeneous WC-Ni/Co composites produced from WC powder coated with a solution chemical route, Proc. CIMTEC 2002 10th Int. Ceram. Congr. part C, 489 (2003) 1.
- Å. Ekstrand, G. Westin, M. Nygren, Homogeneous WC–Co-Cemented Carbides from a Cobalt-Coated WC Powder Produced by a Novel Solution-Chemical Route, J. Am. Ceram. Soc., 90 (2007) 3449.
- S. Naim Katea, C.-W. Tai, P.-O. Larsson, H. Vidarsson, G. Westin, Nickel dot coating of NbC powder by solution processing, Open Ceram. 4 (2020) 100043.
- S. Naim Katea, C.-W. Tai, P. Ström, P.-O. Larsson, H. Vidarsson, G. Westin, Niobium carbide Nickel-niobium alloy composites from a nickel coated powder: Microstructural development during sintering, Open Ceram. 6 (2021) 100096.
- X. Gong, M. P. Short, T. Auger *et al.* Environmental degradation of structural materials in liquid lead- and lead-bismuth eutectic-cooled reactors. Progress in Materials Science. 126 (2022) 100920. <u>https://doi.org/10.1016/j.pmatsci.2022.100920</u>
- Y.N. Drozdov, A.V. Beznosov, T.A. Bokova, et al. Friction in high-temperature lead coolant. Russ. Engin. Res. 34 (2014) 71–75. <u>https://doi.org/10.3103/S1068798X1402004X</u>
- M. Del Giacco, A. Weisenburger, G. Mueller, Fretting corrosion of steels for lead alloys cooled ADS. Journal of nuclear materials. 450 (2014) 225-236. https://doi.org/10.1016/j.jnucmat.2013.07.005

WP4 Nuclear fuel development and safety

UN and SIMFUEL pellet fabrication for separate effect testing

Uranium mononitride (UN) is an advanced nuclear fuel concept suitable for lead-cooled reactors due to its superior thermophysical, chemical and mechanical properties. Hence, improving understanding and providing predictive modelling of the properties mentioned above, as well as knowledge of its behaviour under nominal and accident conditions is of interest to the SUNRISE project, and the primary goal of WP4.

Firstly, UN powder is fabricated locally in the KTH fuel lab, following the hydriding-nitridingde-nitriding method of U metal [Malkki-2014]. As oxygen contamination is an important parameter to consider when manufacturing UN, alterations have been made to the fabrication process conducting all three reactions subsequently in one step in one day instead of three different stages throughout the duration of three days. Previous reports produced powders with oxygen contamination in the range of 1000 ppm [Mishchenko-2022]. As a comparison, with our improved method the powders produced have significantly lower O wt.%, ranging from 90-135 ppm, which constitutes world record purity for UN powders, to our best knowledge.

UN fuel pellets are then sintered using Spark Plasma Sintering (SPS), and high densities (porosity < 0.2%) are achieved by sintering at 1650 °C for 3 minutes. In figure 12 a SEM image of a UN pellet and the pellet itself is shown.



Figure 12: (left) A UN pellet fabricated using SPS, fingertips included for scale. (right) A SEM micrograph of the UN pellet. Grains are visible as well as some impurities and pores.

For SIMFUEL pellet fabrication, UN and X (X = Zr, Ce, Mo, Ru, Gd, Y, Sr etc.) powders are mixed and pre-milled before sintering to enhance homogeneity and solubility where it is applicable. The SIMFUEL pellets are fabricated to study a simulated burn-up structure, in order to obtain information of the pellets' properties and behavior once fission products are present in the fuel. All surrogate powders mentioned above, except for Zr, are purchased from commercial supplies.

Zr in the form of < 100 nm sized ZrN powder was obtained from WP3-UU, where is it fabricated through a novel carbothermal nitridation route (Naim Katea et al. 2021) according to:

$ZrO_2 + 0.5 N_2 (g) \rightarrow ZrN + 2 CO (g)$

The key factor in obtaining pure nano-sized ZrN is the extremely intimate mixing and stoichiometric control of the ZrO_2 and C obtained through a sol-gel process utilizing sucrose as carbon source. An advantage with nano-phase particles is the faster reaction with the UN host.

Once the UN and SIMFUEL pellets are manufactured they undergo a pre-characterization process to determine their phase presence, morphology, surface structure, grain size orientation, and hardness. The techniques listed here are used to perform the pre-characterization of the pellets: XRD, SEM/EDS, LOM, EBSD, nano-indentation. After acquiring the above-mentioned data, the pellets are subjected to various separate effect tests to firstly create a baseline study of the UN properties under various conditions (temperature, pressure, porosity etc.) and then obtain a better insight of the effect that the simulated fission products have in the UN matrix.

Even though there is a plethora of fission products that can be experimentally examined, elements such as Pu are not accessible for experimental testing in our laboratory environment, and therefore modeling is employed to provide information on materials such as Pu, as well as on the lab materials but on atomistic scale breaching the gap between experiments and modeling, providing a detailed understanding of the underlying physics.

Thermal diffusivity measurements (LFA) of UN and SIMFUEL pellets

The high thermal conductivity of UN with respect to canonical UO_2 is a key advantage we want to exploit. A higher thermal conductivity leads to a smaller thermal gradient in the fuel and thus to a less severe environment in terms of stress development and associated risk of failure. During operation and burn up, the pure UN develops naturally into a multicomponent system through the ongoing fission process and thus the thermal conductivity also evolves. In order to provide predictive models for reactor operation parameters, at least conservative information of this evolution is needed. At the same time, limited data is available in the literature for the most advanced nuclear fuel concepts. Here we present a comprehensive study by coupling separate-effect tests and first-principles electronic structure theory to determine experimentally and to calculate the thermal conductivity as a function of temperature and solid fission product concentrations. The thermal conductivity of UN pellets was estimated using laser flash analysis (LFA) in thermal diffusivity measurements between 298 and 1400 K. The LFA was performed in collaboration with Jönköping University. The results are presented in figure 13 below, where there is a good agreement between the UN pellets fabricated in the scope of this work and the literature values [IAEA-2009, Hayes-1990]. After the UN thermal conductivity results have been obtained and analyzed, the plan is to proceed with (U_{1-x}Zr_x)N composite samples to build predictive models for how the thermal conductivity changes during operation and burn up in the reactor.



Figure 13: Thermal conductivity values obtained from thermal diffusivity measurements of two UN samples (UN01, UN02) and compared with literature data.

Proton implantation on UN and SIMFUEL samples

lon beam implantation of materials poses several advantages as an irradiation method. Firstly, it can achieve rapid damage levels in the materials, emulating the effects on mechanical properties as well as the irradiated microstructure of reactor relevant conditions at a fraction of the time and cost. Secondly, ion implantations operate at very specific and well controlled conditions of temperature, fluence, and radiation dose rate. Therefore, unique phenomena that can be studied such as material damage depending on a single variable and doses higher than the ones that can be reached in a reactor (e.g., dose > 200 dpa). Lastly, ion beam irradiation aids understanding of complex phenomena such as radiation induced impurity segregation, irradiated microstructure evolution, irradiation hardening, and irradiation assisted stress corrosion cracking. [Heidrich-2017]. Literature on proton beam implantation of UN pellets is limited and thus in SUNRISE we have irradiated UN samples with various fluences ranging from 0.1 dpa to 100 dpa in order to examine and study post irradiation effects on the sample microstructure and mechanical properties. The doses have been calculated performing SRIM simulations of 2 MeV protons on UN with predetermined fluences. The irradiation was performed at the Tandem Laboratory of Uppsala University. The next steps are to perform detailed post-implantation characterization with the use of SEM/EDS, EBSD, FIB and TEM. FIB and TEM will be used in collaboration with Chalmers University of Technology.

First-principle atomistic modeling of UN and SIMFUEL

Density functional theory (DFT) calculations were performed to study UN, PuN and (U,Pu)N nuclear fuels using the Vienna Ab initio Simulation Package (VASP) code. In order to improve analysis of the ongoing experiments, detailed atomistic modelling is a very useful tool, and it also opens the door to expand studies beyond what we can do experimentally, here exemplified by studying the effects of Pu in UN, which is unaccessible in our laboratory environment.

The strong correlations among the 5f electrons in the U and Pu atoms were taken into account by adding an onsite Coulomb repulsion (i.e., additional parameters U and J) in the form of Hubbard-type terms in the Hamiltonian. The occupation matrix control (OMC) scheme was used to prevent the convergence of the calculation to a metastable state [Jomard-2008]. OMC calculations were performed using both PBE functional and vdwoptPBE functional. The latter functional has never been used in the literature to study nitride nuclear fuels but is known to provide a better description of ionic compound (like UN and PuN) properties. Therefore, we aimed at investigating the accuracy of the vdwoptPBE functional in the case of nitride nuclear fuels [Klimes-2011]. For uranium nitride UN, we performed OMC calculations with U = 2.0 eV and J = 0.1 eV to determine the lowest-energy occupation matrix [Claisse-2016]. For PuN, the value of the U parameter has been estimated in the literature to range between 1.5 and 2.5 eV. Therefore, we performed OMC calculations for every value of U from 1.5 and 2.5 eV with an energy step of 0.1 eV (i.e., U = 1.5, 1.6, 1.7,, 2.5 eV). Moreover, for PuN, a conflict in the literature exists concerning the number of strongly correlated electrons in Pu ions, most of the studies considered five 5f electrons in Pu, but others claimed only three. We performed OMC calculations in both cases, and we concluded that calculations with three 5f electrons in Pu are not relevant, resulting in very different results by slight variations of the U value, which is not consistent from a physical point of view. Calculations to find the most accurate value of the U parameter for PuN are still ongoing. However, we performed preliminary calculations to determine the lattice parameter of (U,Pu)N with a Pu content equal to 12.5%, 25%, 37.5%, 50%, 62.5%, 75%, 87.5% using the vdw-optPBE functional. For these calculations, we fixed U=2.0 eV for Pu and used the lowest-energy occupation matrix obtained with this U value. We found reasonable qualitative results, but we noticed that the lattice parameters of (U,Pu)N increases compared to ones computed with the PBE functional, yielding in less accurate values of this structural property of (U,Pu)N. The disordered systems used through (U,Pu)N calculations have been generated using the Special Quasirandom Structure (SQS) method [Zunger-1990].

UN high temperature creep testing by SPS

UN creep properties are of interest as they significantly affect the fuel performance and are directly connected to important phenomena occurring during the fuel lifetime, such as fission gas release. However, high temperature (>1200 °C) mechanical testing is usually difficult to perform and expensive. To overcome this issue, a novel design of the die used in the Spark Plasma Sintering (SPS) apparatus was manufactured and utilized to perform high temperature creep testing of a 5 mm in height and 9.3 mm in diameter UN pellet at 1300 °C under 21.5 MPa. Figure 14 shows a sketch of the die design and its component. The choice of the test parameters' values, i.e., temperature and pressure, was done based on recommendations provided by WP1 as the performance of the fuel under the selected values affect fission gas release and, in turn, the design parameters of the fuel.



Figure 14: A sketch of the SPS die design used for creep testing.

During the test, the profiles of the temperature, pressure, and displacement were gathered from the SPS, and the displacement profile was used to calculate the steady-state secondary creep rate from the true strain over time. Figure 15 shows the gathered data as well as the true strain vs time graph that was used for the calculation. The resulting secondary creep rate shows good agreement with the experimental results reported in the literature. The comparison is shown in Figure 16.



Figure 15: a) SPS outputs of the temperature, pressure, and displacement b) true strain over time.



Figure 16: Comparison of the SPS creep test at 1300 °C and under 21.5 MPa with the reported experimental results.

References WP4

- P. Malkki, M. Jolkkonen, T. Hollmer, J. Wallenius, Manufacture of fully dense uranium nitride pellets using hydride derived powders with spark plasma sintering. J. Nucl. Mater. 452 (2014) 548–551. <u>https://doi.org/10.1016/j.jnucmat.2014.06.012</u>
- Y. Mishchenko, S. Patnaik, E. Charatsidou, J. Wallenius, D.A. Lopes, Potential accident tolerant fuel candidate: Investigation of physical properties of the ternary phase U2CrN3. J. Nucl. Mater. 568 (2022) 153851. https://doi.org/10.1016/j.jnucmat.2022.153851
- S. Naim Katea, G. Westin, Ceram. Int. Carbothermal nitridation of solution synthesised ZrO₂–carbon nanocomposites; phase-development from precursor to nitride, 47 (2021) 10828.
- Thermophysical Properties of Materials for Nuclear Engineering: A Tutorial and Collection of Data, 2009. International Atomic Energy Agency, Lanham.
- S.L. Hayes, J.K. Thomas, K.L. Peddicord, MATERIAL PROPERTY CORRELATIONS FOR URANIUM MONONITRIDE III. Transport properties, Journal of Nuclear Materials 171 (1990) 289-299.
- B. Heidrich, 2017. Roadmap for the Application of Ion Beam Technologies to Challenges for the Advancement and Implementation of Nuclear Energy Technologies (No. INL/EXT--17-43130, 1408762). <u>https://doi.org/10.2172/1408762</u>
- S.L. Hayes, J.K. Thomas, K.L. Peddicord, Material property correlations for uranium mononitride: II. Mechanical properties, J. Nucl. Mater., 171 (1990) 271-288. <u>https://doi.org/10.1016/0022-3115(90)90375-W</u>.

- G. Jomard, B. Amadon, F. Bottin, and M. Torrent, "Structural, thermodynamic, and electronic properties of plutonium oxides from first principles," Physical Review B, vol. 78 (2008) 075125.
- J. Klimeš, D. R. Bowler, and A. Michaelides, Phys. Rev. B 83 (2011) 195131.
- A. Claisse, M. Klipfel, N. Lindbom, M. Freyss, P. Olsson. "GGA+U study of uranium mononitride: A comparison of the U-ramping and occupation matrix schemes and incorporation energies of fission products." Journal of Nuclear Materials 478 (2016) 119-124.
- A. Zunger, S.H. Wei, L. G. Ferreira, J.E. Bernard, Special quasirandom structures, Phys. Rev. Lett. 65 (1990) 353.

WP5 Development of experimental and modeling approaches for testing of LFR component performance in high temperature HLM flow

The main result from WP5 focuses on the engineering design of the SEFACE facility, as well as the investigation of time-dependent flow structure in the SEFACE test chamber via large eddy simulation (LES) using computational fluid dynamics (CFD).

Introduction of the SEFACE facility

SEFACE is an experimental facility designed to investigate the flow-accelerated corrosion and erosion (FACE) phenomenon in liquid lead under high relative velocity (~ 4 to 21 ms⁻¹) and high temperature (~ 400 to 550 °C) conditions. SEFACE will provide validation data to support the development of the computational model and conduct FACE testing of advanced structural material candidates in LFR's condition. The overall structure of SEFACE facility is depicted in figure 17.



Figure 17. The SEFACE facility design.

The fundamental design concept of SEFACE facility is based on the rotating disk, where material samples are designed to adhere to the surface of rotating disks. The wall shear

stress profile and flow surrounding the material sample can be systematically characterized due to the direct dependence between linear velocity (v), radial position (r) and rotational speed (ω) of the disc (i.e., $v = r\omega$). In addition, the rotating disc can be positioned asymmetrically such that the inter-gaps between upper and lower stationary disks are dissimilar, which allows concurrent experimentation with varied gap spacings. Figure 18 depicts the asymmetrical design of rotating disk positioning using the latest design of SEFACE test chambers. Using such an asymmetrical configuration enables the investigation of the gap spacing effects on turbulence flow structure and wall shear stress, and hence, FACE performance in a single round of experiment.



Figure 18: Illustration of the SEFACE Test Chambers. Three rotating disks are highlighted in red and each of the rotating disks is positioned asymmetrically such that the effect of gap sizing on turbulence flow and FACE can be studied.

To the best of our knowledge, there is no comparable facility currently or previously in operation that can achieve our targeted operational state. The table below provides a non-exhaustive list of FACE facilities that have been built or are in the process of development across the world.

	Temperature	Velocity	Medium	Reference
CORRIDA, KIT, DE	450-550°C	2 ms ⁻¹	Pb-Bi	(Schroer et al., 2011, 2018)
Lobo Loop, Univ. of New Mexico, US	Up to 700°C	1 to 3 ms ⁻¹	Pb-Bi	(Talaat et al., 2021)
Univ. of Manchester, UK [*]	500°C	Up to 26 ms ^{-1**}	Pb	(Ali et al., 2022)
CORELLA, KIT, DE [*]	450°C	~ 1.5 ms ⁻¹ (U _{rel})	Pb- Bi/Pb	(Fetzer et al., 2021)
Chinese Academy of Science, CN	400°C	~ 1 ms ^{-1**}	Pb-Bi	(C. Li, Liu, et al., 2021)

National Institute for Fusion Science, JP	600°C	0.17 ms ⁻¹ (U _{rel})	Pb-Bi	(Kondo et al., 2011)
CICLAD, CEA, FR	450-540°C	0.14 to 1.756 ms ^{-1**}	Pb-Bi	(Martinelli et al., 2022)
Seoul National University, KR	600°C	0.5 to 3.14 ms ⁻	Pb-Bi	(Choi et al., 2021)
SEFACE Facility, KTH, SE*	400-550°C	4 to 20 ms ⁻¹ (U _{rel})	Pb	-

From the table, one can see most facilities are limited to relatively slow operating velocity. Therefore, there is limited literature of the design on high-speed FACE testing facilities. Computational aided engineering (CAE) tools such as ANSYS FLUENT and COMSOL Multiphysics were used to gather valuable information on the hydrodynamics and structural characteristics. The simulation results are then utilized to aid in the formulation of experimental designs and the selection of operating conditions. Figure 19 shows the design iteration of SEFACE facility. The initial version of SEFACE facility was based on several rotating disks with large diameters and adopts the confined rotor-stator type of geometric design. However, this turns out to induce several operational problems for such a highly rotating apparatus. As a result, most of the FACE experimental facilities are restricted to low-velocity ranges.



Figure 19: Iterations of SEFACE design.

Operational Constraints due to Hydrodynamics

Using ANSYS FLUENT, the operational characteristic of the SEFACE facility can be sought via the steady state simulation with $k - \omega$ SST turbulence model. From the numerical simulation results, several operational constraints were found.

- 1. The axial pressure difference (and significant axial force) across the rotating disks is caused by the asymmetric chamber design (with different gap sizes). As a result, hole perforations must be used to equalize pressure on both sides of the rotating disk, thus reducing the magnitude of bending force on the rotating disks. The same also occurs at the stationary disks, and thus, perforation also appears on the stationary disk.
- 2. A significant radial pressure gradient is created due to the balance of centrifugal and hydrostatic forces caused by the significant rotation. For a confined rotor-stator design, this physical phenomenon is linked to operational issues such as dropping below the vapor pressure near the rotating shaft and increasing the maximum operating pressure up to 10 bar. Because this constraint is related to bulk rotation, the only way to reduce the radial pressure gradient is to decrease the bulk rotational velocity in a confined rotor-stator design version of the SEFACE facility. However, this will result in a much longer experimental time and will also fail to achieve our experimental target flow regime for FACE testing.

As a result, the SEFACE facility has adopted an open chamber design and several inter-diffusion vanes to stop the bulk rotation. This method is effective in reducing bulk rotation in the chamber, thereby alleviating the radial pressure gradient problem. The rapid fall-off of rotational velocity from the disk surface to the bulk of the fluid, on the other hand, increases the efficiency of the SEFACE facility on FACE testing (i.e., it maximizes the relative velocity between the material sample and the bulk).

- 3. The design should adhere to specific torque and power requirements. Because the power is proportional to the third power of the rotational speed and the fourth power of the radius. As a result, the radius of the rotating disk is reduced to reduce torque and power requirements while still allowing sufficient radial space for adhering material samples.
- 4. Chemical saturation problem with corrosion. There should be re-circulation of fresh lead into the testing chamber to avoid the saturation of corrosion kinetics. In the latest design of the SEFACE facility, lead can circulate through the far opening (in the radial direction) of the test chamber, and the pressure perforation holes (in the axial direction).

Figure 20 illustrates the velocity and pressure field at the center cross-section of the latest design SEFACE facility, which has taken account of all previously mentioned operational constraints.



Figure 20: Cross-sectional velocity magnitude (top) and pressure (bottom) for SEFACE test chamber.

Structural Analysis in support of mechanical design of SEFACE

Apart from hydrodynamic, structural analysis is required to confirm the stability of the structural element in the SEFACE facility. Since the facility employs a long shaft with rotating discs in molten lead and a set of stationary structures to create desired flow structure, the concern is the dynamics of the shaft that has a free bottom end, which is not supported by bearings in lead.

The length of the shaft is 1318 mm and maximum rotating speed of the shaft is 1200 rpm. For reliable and safe operation of the facility, it is important to analyze the critical speed and eigenfrequencies of the rotating shaft immersed in molten lead. It is also important to quantify the effect of added mass along with temperature of the shaft. Using rotordynamic analysis, the critical speed and eigenfrequencies of the shaft are determined considering the added mass of lead. The rotordynamic analysis has been carried out using Finite Element Method in COMSOL Multiphysics software. Figure 21 shows the layout of the shaft with bearings and the Campbell plot of the shaft. The first critical frequency is found to be 2640 rpm.



Figure 21: Layout of SEFACE shaft and Campbell plot for the shaft

Further, transient analysis was also performed to calculate the deformations and stresses in the shaft for conditions like mass imbalance on the shaft, vertical deflection and bearing clearances in the shaft support positions. Waterfall plot and orbits of the shaft were studied for the transient events.

Since the maximum operating temperature of the facility is 550 degC, the components like the vessel plate, cold trap and bearing housing will be subjected to differential thermal expansion. Hence, it is required to perform thermomechanical analysis for the design to evaluate the thermal stress and resulting deformation. Based on thermomechanical analysis, the design of cold trap with a single flange and the selection of special types of bolts on the vessel plate were selected.

Development of FACE Model

A preliminary conceptual framework for the computation of FACE phenomenon is presented in the flowchart below.



Information on the intermittent flow structure and wall shear stress can be derived from the large eddy simulation (LES), but at the expense of a small timestep to ensure high accuracy for both temporal and spatial scales of turbulence. Due to the relatively large difference in timescale between corrosion-erosion phenomena and turbulence dynamics, the LES-calculated flow field is typically considered frozen. Using these frozen fields, the damage to the material is calculated in conjunction with the species transport equation to account for feedback such as the oxygen concentration deficit following the oxidation reaction at the material surface. After a certain large timestep, the surface morphology will be updated for species transport. Thus, the new surface morphology will influence the dynamics of turbulence, and hence, a new round of LES computations will be carried out.

Currently, we are at the initial step for obtaining time-dependent flow data in SEFACE facility to support future development of FACE modelling framework.

A representative domain of the test chamber from the SEFACE facility is chosen as the computational domain (10-degree wedge). To obtain time-dependent statistics of the wall shear stress on the rotating disk (to the material sample), a large eddy turbulence simulation (LES) is performed to resolve the time-dependent flow structure and wall shear stress. As with most of the LES models, resolving the flow structure at the near wall region is not feasible due to a similar mesh grid requirement as with Direct Numerical Simulation (DNS), which requires the length scale in the order of O(1) in all directions. In SEFACE, the minimum Reynolds number is at 1.4 million, while the highest Reynolds number can go up to 18 million. Simulating such highly turbulent flows with wall-resolved LES is not trivial, due to the strict requirement to achieve O(1). Therefore, the wall-modelled LES approach is used.

Figure 22 shows the time-averaged dimensionless turbulent velocity profile for dimensionless spatial coordinates (z^+) up to 10000. The turbulent velocity profile follows the universal profile in linear sub-layer ($z^+ < 10$), which indicates that the wall shear stress can be captured with a good accuracy. For relatively high z^+ (>10), the turbulent profile follows the Von-Kármán log-law profile with $\kappa = 0.41$ and $B^+ = 0.5$ up to 1000 [Appelquist-2018]. Note that the z^+ is pointed at the orthogonal direction of the rotating disk.



Figure 22: Time-Averaged Turbulent Boundary Layer Profile.

For the effect of gap size to the flow structure, spiral patterns were seen from the effect of small gap for near-wall flow structure from a preliminary simulation with a larger computational domain (30-degree wedge) as shown in Figure 23.



Figure 23: Q-criterion colored by velocity magnitude on the rotating disk with small gap side.

References for WP5:

- C. Schroer, O. Wedemeyer, V. Tsisar, A. Skrypnik, and J. Konys, "Practical Experience Gained From Operating The Lead-Bismuth Loop Corrida," ICONE-26 proceedings (2018) 16.
- A. E. A. Ali, A. Cioncolini, D. Laurence, and H. lacovides, "Liquid lead flowaccelerated corrosion testing with the rotating cage set-up: A CFD optimisation," Ann. Nucl. Energy 165 (2022) 108620. doi:10.1016/j.anucene.2021.108620.
- K. Talaat, "Design of specimen holders for flow accelerated corrosion experiments in molten lead with numerical evaluation of pressure losses," Nucl. Eng. Des. 385 (2021) 16.

- R. Fetzer, A. Weisenburger, and G. Mueller, "Turbulent flow of liquid lead alloy in oxygen-controlled corrosion erosion test facility," AIP Adv. 11 (2021) 075303. doi: 10.1063/5.0057380.
- C. Li, Y. Liu, F. Zhang, X. Fang, and Z. Liu, "Erosion-corrosion of 304N austenitic steels in liquid Pb Bi flow perpendicular to steel surface," Mater. Charact. 175 (2021)
 doi: 10.1016/j.matchar.2021.111054.
- M. Kondo et al., "Flow accelerated corrosion and erosion–corrosion of RAFM steel in liquid breeders," Fusion Eng. Des. 86 (2011) 2500–2503. doi: <u>https://doi.org/10.1016/j.fusengdes.2011.01.108</u>.
- L. Martinelli, F. Balbaud-Célérier, C. Alémany-Dumont, and V. Botton, "Determination of mass transfer coefficient in flow assisted corrosion of steel in liquid Pb Bi. Rotating cylinder geometry," Int. Commun. Heat Mass Transf. 133 (2021) 105960.
- J. Choi, I. Hwang, and Y. Lee, "Flow Accelerated Corrosion of Stainless Steel 316L by a Rotating Disk in Lead-Bismuth Eutectic Melt," JOM 73 (2021) 4030–4040. doi: 10.1007/s11837-021-04953-y.
- E. Appelquist, P. Schlatter, P. H. Alfredsson, and R. J. Lingwood, "Turbulence in the rotating-disk boundary layer investigated through direct numerical simulations," Eur. J. Mech. BFluids 70 (2018) 6–18. doi:10.1016/j.euromechflu.2018.01.008.

2.2 Participating researchers

In the table below, we list all participating researchers and students, their role, affiliation, status and in which WP(s) they operate. 19 seniors (4 female) and, so far, 26 juniors (7 female) are or have been active in the centre.

Name - seniors	Title	Role	Affiliation	Status	WP(s)
Pär Olsson	Prof	Coordinator	KTH	Active	2, 4
Denise Adorno Lopes	Dr	Industry affiliate, WPL	Westinghous e	Active	4
Farid Akhtar	Prof	Senior researcher	LTU	Active	3
Marta-Lena Antti	Prof	Applicant, WPL	LTU	Active	3
Anders Blennermark	Dr	Industry affiliate	LeadCold	Active	1
Björn Bosbach	Dr	Industry affiliate	Alleima	Active	2, 3
Sara Bortot	Dr	Applicant	KTH	Maternity leave	1
Jan Frostevarg	Assoc	Senior	LTU	Active	3

	prof	researcher			
Dmitry Grishchenko	Dr	Senior researcher	КТН	Active	5
Jens Hardell	Prof	Senior researcher	LTU	Active	3
Mikael Jolkkonen	Dr	Senior researcher	KTH	Active	4, 5
Pavel Kudinov	Assoc prof	Applicant, WPL	KTH	Active	5
Haipeng Li	Dr	Senior researcher	KTH	Active	5
Leonardo Pelcastre	Assoc prof	Senior researcher	LTU	Active	3
Max Persson	Mr	Technician	KTH	Active	2, 4, 5
Malin Selleby	Prof	Applicant	KTH	Active	4
Peter Szakalos	Dr	Senior researcher, WPL	КТН	Active	2
Janne Wallenius	Prof	Senior researcher, WPL	KTH	Active	1
Gunnar Westin	Prof	Applicant WPL	UU	Active	3
Name - juniors	Title	Role	Affiliation	Status	WP(s)
Robin Andersson	Mr	Project office			A 11
		Flojectonice	КТН	Finished	All
Didier Bathellier	Dr	Postdoc	ктн	Finished Active	All 2, 4
Didier Bathellier Elina Charatsidou	Dr Ms	Postdoc PhD student	ктн ктн ктн	Finished Active Active	All 2, 4 4
Didier Bathellier Elina Charatsidou Fredrik Dehlin	Dr Ms Mr	Postdoc PhD student PhD student	KTH KTH KTH KTH	Finished Active Active Active	All 2, 4 4 1
Didier Bathellier Elina Charatsidou Fredrik Dehlin Maria Giamouridou	Dr Ms Mr Ms	Postdoc PhD student PhD student MSc student	KTH KTH KTH KTH KTH	Finished Active Active Active Active	All 2, 4 4 1 4
Didier Bathellier Elina Charatsidou Fredrik Dehlin Maria Giamouridou Paul Gruber	Dr Ms Mr Ms Mr	Postdoc PhD student PhD student MSc student PhD student	KTH KTH KTH KTH LTU	Finished Active Active Active Active Active	All 2, 4 4 1 4 3
Didier Bathellier Elina Charatsidou Fredrik Dehlin Maria Giamouridou Paul Gruber Daria Kolbas	Dr Ms Mr Ms Mr Ms	Postdoc PhD student PhD student MSc student PhD student PhD student PhD student	KTH KTH KTH KTH LTU LTU	Finished Active Active Active Active Active Active	All 2, 4 4 1 4 3 3
Didier Bathellier Elina Charatsidou Fredrik Dehlin Maria Giamouridou Paul Gruber Daria Kolbas Daniel Karlsson	Dr Ms Mr Ms Mr Ms Mr	Postdoc PhD student PhD student MSc student PhD student PhD student PhD student MSc student	KTH KTH KTH KTH LTU LTU KTH	Finished Active Active Active Active Active Active Active	All 2, 4 4 1 4 3 3 3 4

Elias Ljunggren	Mr	MSc student	KTH / RiskPilot	Active	1
Ignas Mickus	Dr	Postdoc	KTH	Active	1, 5
Yulia Mishchenko	Dr	Postdoc	КТН	Active	4
Sarmad Naim Katea	Dr	Postdoc	UU	Finished	3, 4
Eloi Pallares Abril	Mr	MSc student	KTH	Active	1
Sobhan Patnaik	Dr	Postdoc	KTH	Active	4
Alejandria Perez	Dr	Postdoc	KTH	Active	1
Alessandro Persico	Mr	MSc student	KTH	Finished	1
Christopher Petersson	Mr	PhD student	KTH	Active	2
Guillem Sanchis Ramirez	Mr	MSc student	KTH	Finished	1
Faris Sweidan	Dr	Postdoc	KTH	Active	2, 4, 5
Hadi Torkamani	Dr	Postdoc	LTU	Finished	3
Sumathi Vasudevan	Dr	Postdoc	KTH	Active	5
Udyanth Vadiya	Mr	MSc student	KTH	Finished	4
Guan Wang	Dr	PhD student	KTH	Finished	1
Kin Wing Wong	Mr	PhD student	KTH	Active	5
Sarmad Naim Katea	Dr	Postdoc	UU	Finished	3

2.3 Selected publications, awards and conferences

Peer-reviewed publications

- F. Dehlin, J. Wallenius, S. Bortot, An analytic approach to the design of passively safe lead-cooled reactors. Annals of Nuclear Energy 169 (2022) 108971. <u>https://doi.org/10.1016/j.anucene.2022.108971</u>
- J. Wallenius, An improved correlation for gas release from nitride fuels, Journal of Nuclear Materials 558 (2022) 153402. <u>https://doi.org/10.1016/j.jnucmat.2021.153402</u>
- Y. Mishchenko, S. Patnaik, E. Charatsidou, J. Wallenius, D.A. Lopes, Potential accident tolerant fuel candidate: Investigation of physical properties of the ternary

phase U2CrN3. J. Nucl. Mater. 568 (2022) 153851. https://doi.org/10.1016/j.jnucmat.2022.153851

 C. Petersson, P. Szakalos, D.D. Stein, Slow strain rate testing of Fe-10Cr-4Al ferritic steel in liquid lead and lead-bismuth eutectic, Nuclear Materials and Energy 34 (2023) 101403. <u>https://doi.org/10.1016/j.nme.2023.101403</u>

Books and book chapters

• P. Olsson, chapter in: Towards the energy of the future – <u>The Energy Anthology</u>, V&A publishing (Stockholm, 2022).

Awards

• Janne Wallenius – <u>The KTH Innovation Award 2022</u> (500.000 kr award)

Conferences

The table below lists the scientific conferences at which the research results of the centre have been presented so far.

Conference	Location, date	Presenter, Type of talk	WP	Title of talk
TMS 2022	Anaheim, USA, Feb 2022	Elina Charatsidou (Oral)	4	Thermal Conductivity Degradation by Solid Fission Products: Machine Learning Coupled with First Principles Model
Eurocorr 2022	Germany, Berlin	Christopher Petersson (Poster)	2	Slow strain rate testing of Fe-10Cr-4Al ferritic steel in liquid lead and lead- bismuth eutectic
ACerS ICACC2023	Daytona beach, USA, Jan 2023	Gunnar Westin (Invited)	3	Synthesis of amorphous and crystalline oxides from $MAI_3(O^iPr)_{12}$ (M = Ln, Cr) precursors
ACerS ICACC2023	Daytona Beach, USA, Jan 2023	Paul Gruber (Oral)	3	Microstructure and high-temperature mechanical properties of WC-Ni cemented carbides sintered from novel precursor powers

2.4 Future research plans

The centre is driving its research tracks forward according to the plan established in the application, see the detailed task declaration in Appendix A, but with certain minor modifications, as expected. In summary, there are so far no significant negative deviations from the initial research plan. The major deviations are of added value, where additional funding has increased manpower and activity, and where discussions in the technical workshops have added specific tasks and tracks.

Below follows a condensed description of future plans and activities, presented per WP and with main focus on the PhD student work.

WP1: PhD project of Fredrik Dehlin (KTH)

For the remaining years of PhD student Fredrik Dehlin's work within SUNRISE the focus will be on finalizing the fission matrix-based method for optimizing a transition from the UO2 to the UN core. Furthermore, in collaboration with a MSc thesis student he will perform activation analyses of structural components in SUNRISE-LFR, e.g., steam generators and core components, and investigate the potential dose to personnel standing outside of the reactor vessel during normal operation. Moreover, the ROAAM approach to assess various pathways to core damage shall be utilized to analyze the safety of SUNRISE-LFR. Lastly, towards the end of the project when the design has matured further, un-protected transient analyses will be conducted in order to create a safety case which can be added to the Preliminary Safety Analysis Report (PSAR).

WP2: PhD project of Christopher Petersson (KTH)

Christopher will continue to study mechanical properties as well as and corrosion and erosion of the newly developed steels, namely the AFA (alumina forming austenitic) steel and the AFM (alumina forming Martensitic) steel that have been developed and refined in SUNRISE. Two upcoming papers currently in manuscript are "Slow strain rate testing of Fe-10Cr-4AI ferritic steel in Pb with increasing Bi content" and "SSRT on experimental AFA (alumina forming austenites) in Pb and Pb-Bi eutectic". In collaboration with WP5, Kin Wing Wong, a detailed study of erosion kinetics will be performed.

WP3: PhD project of Paul Gruber (LTU)

For the work on laser cladding of nuclear fuel tubes, Paul will optimized processing parameters for FeCrAl laser welding and then progress from flat substrates to tubes. Implement 15-15Ti as substrate material. Test cladded tubes in liquid lead environment.

WP3: PhD project of Daria Kolbas (LTU)

For the work on tribological testing, Daria will devise a testing campaign with Fe-10Cr-4Al self-mating friction pair and perform parametric studies.

WP3: Work led by Gunnar Westin (UU)

Structural impeller materials. We intend to continue the work on the cemented carbides extending the WC-Ni composites to NbC-Ni and WC + NbC-Ni composites investigating the mechanical properties and lead corrosion in collaboration with WP3-LTU. NbC is of interest in the impeller application as it can, when combined with WC, provide a near zero buoyancy in molten lead which will reduce forces on the driving equipment. This part will

be continued by replacing the Ni binder with an Fe binder - this since Fe has a lower solubility in molten in lead. This should be finished before end of 2024.

Coatings for impeller and steel. While the present WC-Ni composites with as low as 2 vol% Ni may work without a hard, corrosion protecting coating, work has started on synthesis of WC coatings. The carbide coatings may also be nano-composites with hard, doped alumina as top-layer for which new synthesis routes will be developed. Previous preliminary results show that such coatings can be very strongly adhering to both carbides and alumina. Furthermore, the CVD precursor systems for Ln-Al-O and Cr-Al-O coatings developed for the now ended SSF-CVD 2.0 is one of the inputs for the solution based routes intended to be used. Here the Ln-Al-O system form nano-composites and the Cr-Al-O system yield spinodal phase separation into Cr-rich and Cr-poor domains which could increase hardness while still being compatible with the FeCrAl(RE)-oxide structure.

To some extent, the WP3-UU having access to a wide range of flexible solution synthesis systems is ready to provide materials on demand, whether it is for WP2, WP3, or WP5. We expect that when results come from the lead abrasive tests there may be changes made to the materials systems.

Sim-fuel nitrides. Nano-sized nitride powders for sim-fuels are synthesised where suitable commercial powders are not found. This can be due to unsatisfactory purity or that small nano-sizes < 100 nm are required to get a good mixing and reactivity with the UN. We have developed routes that likely can achieve such powders for a wide range of nitrides, as well as multi-metal nitrides.

WP4: PhD project of Elina Charatsidou (KTH)

As of now most of the work has been focusing on UN fuel pellets in order to standardize fabrication and characterization of both UN powder and pellets. Separate effect testing has been performed on UN samples such as nano indentation, laser flash analysis, proton implantation. These were conducted to generate a baseline behavior of unirradiated fresh UN fuel pellet and understand its thermal physical and mechanical properties thoroughly before moving into examining more complex fuel composites. Modeling was also used where there is a lack of experimental techniques, or such are cumbersome to perform. In the remaining years of the project period the work will focus mostly on applying these well-established methods to fabricate, characterize and test SIMFUEL pellets and model the physical behavior composites containing elements that are not feasible to acquire for experimental use (e.g. Pu).

Starting from simpler composites of UN and a single phase/element X (X = Zr, Ce, Mo, Ru, Gd, etc.) it will be possible to identify how this particular fission product effects the thermal physical and mechanical properties UN and moving towards more representative SIMFUEL samples where several fission products will exist in the UN matrix it will be possible to examine a simulated burn-up fuel structure and its properties and behavior under various conditions compared to fresh UN fuel, drawing a picture of the UN fuel degradation with fission product concentration.

General WP5: The extension of the SEFACE facility is planned to replace the rotating discs with an impeller to test the components like the impeller in the molten lead, which will be known as Component Testing Facility (CTF). CTF mainly aims to investigate the FACE phenomenon in the pump impeller. Critical speed analysis and transient event analysis for the CTF are to be carried out. Flow simulations representing the actual mass flow rates of the pump and the design of specific internals for the facility are ongoing.

PhD project of Kin Wing Wong (KTH)

More LES simulations are required to obtain accurate flow information for varying gap sizes. The current simulation only takes hydrodynamics into account; additional species transport equations will be added to LES to obtain temporal and spatial dynamics, enabling the calculation of instantaneous corrosion rates on material surfaces. Given the relatively high Reynolds number in the SEFACE facility, turbulent mass transport of species with varying Schmidt numbers may exhibit similar behavior. This needs to be investigated from the LES solution.

Experimentally or numerically, the accuracy of wall-modeled LES (WMLES) for modeling rotating disk flow has not yet been validated. Numerically, wall-resolved LES (WRLES) can be simulated on a generic free-standing rotating disk (without the complicated geometrical feature as in SEFACE); however, an appropriate boundary condition must be found as Neumann/stress-free boundary condition cannot be used in the far-field in radial direction due to the radially increasing velocity component along the disk surface. On the experimental side, the mock-up facility for SEFACE and CTF will provide important validation data to verify turbulence prediction in addition to computational data. Initial collaboration discussions with the KTH mechanics department for PIV/LDV have begun.

In parallel, work on the OpenFOAM-based flow-accelerated corrosion-erosion (FACE) solver has just recently begun, with the coupling of flow dynamics and the material damage (FACE) model being implemented. Initially, the focus will be on the flow-accelerated corrosion phenomenon on pipe geometry under low velocity conditions to facilitate rapid numerical calculation and verification of the approach. With a lower Reynolds number (Re) (i.e., spans from 5,000 – 300,000) than SEFACE facility, the effect of Schmidt number (Sc) on turbulent mass transfer can be compared to that obtained in the SEFACE facility with an extremely high Re (which spans from 2 to 18 million). The relative dependency between turbulent mass transport to Re and Sc can be sought. The said FACE solver's objective is to examine the impact of intermittent flow structure on turbulence-induced material damage. As soon as the FACE experimental data for SEFACE and CTF becomes available, a more dedicated FACE model will be created to account for the erosive effect.

Moreover, we 've recently started our collaboration with WP2 on the ECO-Rig erosioncorrosion testing facility developed by Peter Szakalos and Christopher Petersson, where WP5 will provide CFD simulation on the facility. Since erosion cannot be modelled as a species transport process like corrosion, the experimental data from ECO-Rig will also contribute to the FACE model development that accounts for coupled erosion-corrosion process. In addition, this collaboration can help testing the OpenFOAM-framework in complex geometries, serving as a pilot phase for the geometry of pump impellers in the CTF facility (where moving mesh is required in such case).

Lastly, the same LES simulation sequence needs to be performed on CTF geometry. In addition, the performance of dynamic meshing of surface morphology in OpenFOAM must be evaluated to complete the FACE modeling framework as discussed previously. Another crucial consideration is the effect of roughness on the turbulent boundary layer. When the boundary layer thickness is much thinner than the roughness height on the material surface, the Re no longer controls the friction factor, but only the roughness. As a result, it is possible that the wall shear/friction factor is independent after a certain Reynolds number. The investigation of this effect will be based on both experimental results obtained from the SEFACE and CTF facilities and numerical predictions obtained from the FACE framework.

3. Strategic relevance

Since the time of applying for the SUNRISE centre grant, the political landscapes have shifted significantly. Nuclear energy as a potential game changer for combating climate change has risen to the forefront of the debate. Policies with respect to energy security have been drastically altered in favor of strengthened domestic energy production. In Sweden in particular, but also in many other countries, public support for nuclear energy new build has reached record levels. The SUNRISE centre and its broader development program has gathered massive attention from media, politics, industry and the public. SUNRISE is very well placed to begin to advance a rapid Swedish development of new nuclear technology, inspired by what was done in the 60'ies and 70'ies, and has potential to create a booming industry. In the short term, the SUNRISE development creates a lot of attention and good-will and the changing medial and political landscape has shown itself in a rapid and significant increase in applications to the Nuclear Engineering Master programme at KTH. We have in 2023 had the highest number of primary external applicants ever, and are geared to admit around 60 new students in the fall. This can be projected to lead to a drastic increase in the number of MSc diploma projects that will be carried out in the centre in the coming years and thus significantly increased manpower. In the long term, if the SUNRISE programme is successful and Swedish lead fast small modular reactors are commercialized as an export product, then the impact and strategic relevance of the seed from SUNRISE will skyrocket.

At the same time as the overarching goal of SUNRISE have very high-flying potential impact, there are other near and far term possibilities that can spin off from the research conducted here. In WPs 2 and 3 in particular, we have strong activities on development of new materials, such as bulk phase alumina forming steels of different kinds, which are clearly patentable. Alleima holds the patent for the previously developed FeCrAI steel (Kanthal EF 100) initiated by researchers active in SUNRISE but pre-dating the centre. Novel steels with unprecedented corrosion tolerance and good high-temperature properties can find applications far outside that of the projected goals of SUNRISE. Notable examples are intermediate- and high-temperature environments (e.g. gas turbines), other heavy-liquid metal (HLM) environments (concentrated solar power, Pb-processing and recycling industry) and other generally corrosive environments.

The high quality, low-binder content cobalt-free cemented carbides, developed within WP3, are of great importance for the out-phasing of Co from the metal machining and rock excavation industries which is requested by the EU due its toxicity. Likewise, replacement of WC for the less toxic and less strategically demanding NbC is of importance for the mentioned industries. The leading results obtained in the development of impeller materials should therefore be of great importance for Swedish companies (e.g. Sandvik Coromant, Atlas Copco), as well as for the EU in general. Furthermore, the hard and corrosion resistant coatings being developed will be of great importance for a large range of companies in Sweden and the EU. Some examples are companies working with metal machining, sliding parts, wear parts, fuel-cells, and batteries. The processes are quite flexible and can be optimised for other areas than is the present focus.

As of yet, no new patents have been filed from the SUNRISE research.

A new company has been created, Swedish Modular Reactors AB (SMR AB), as a joint venture between Blykalla and Uniper.

4. The graduate training of the centre

In the Master programme on Nuclear Engineering at KTH, there is a dedicated course on small reactors (SH2611 Small Reactors), given by Prof Janne Wallenius. The SUNRISE LFR is a case study in this course.

In the course at KTH on radiation damage (SH2605 Radiation damage in materials), given by Prof Pär Olsson, the conditions present in SUNRISE and the research and demonstration reactor are used as an example.

Several MSc diploma projects in the KTH Nuclear Engineering Master program have been and will be related to SUNRISE. At KTH, each MSc diploma student always have a KTH supervisor, a KTH examiner, an external reviewer, and sometimes an external industry supervisor. The project work is for the duration of one full term (30 ECTS).

The PhD training programs at the three universities are very similar in structure and thus only the general form is described here. The PhD degree consists of one year of course work plus three years of research. Each PhD student has a main supervisor and at least one co-supervisor. The students are both employed with a salary and admitted as students. The nominal total time is four years, but this can often be extended if the students carry our Departmental duties such as teaching or local technical administration. The students are expected to publish a series of papers (typically four or more) before they can write up their comprehensive summary and defend their thesis in a public dissertation. At the dissertation, there is a faculty opponent, an internationally renown expert in the field, who is mainly responsible for asking questions of the student. Then a thesis grading committee decides on a pass or fail grade after a closed session deliberation. Of the seven students associated with the centre, one has already defended his thesis in a dissertation (Guan Wang, visiting PhD student from the University of Chinese Academy of Sciences). The six currently salaried PhD students are in their first or second years of their doctoral studies.

An international graduate training school on nuclear materials science has been held twice already with co-organisation by SUNRISE: The European School on Nuclear Materials Science (ESNMS). The first instance was held online in Nov 2020 due to covid restrictions and the second installment was held in Nov 2022 on Corsica. Out of the 45 student participants, several PhD students and postdocs from SUNRISE attended the school and the SUNRISE director, Pär Olsson, was the ESNMS chairman. A third installment is planned for 2024, again with co-organisation by SUNRISE. The school awards 2 ECTS for the students who complete the activities.

5. Collaborations

5.1 Scientific collaborations within the centre between participating groups

We exemplify some major collaborative interactions between centre members. Several minor collaborative actions have been and are routinely performed between centre members in different WPs and institutes.

WP2-WP5 collaboration (Christopher Petersson & Kin Wing Wong)

Erosion modelling of the ECO-rig for improved analysis of experiments on erosion.

WP2-WP1 collaboration (Christopher Petersson & Fredrik Dehlin)

Discussion of detailed composition of materials for neutronics studies.

WP4-WP1 collaboration (Elina Charatsidou & Fredrik Dehlin)

The upper temperature limit for thermal diffusivity measurements for UN, as part of the work of WP4, was set by input from WP1. The temperature limit was set to 1100 °C, based on the figure 24 below that shows peak fuel temperatures for the UN fuel during an unprotected transient overpower (UTOP) accident where 0.2 \$ of reactivity was inserted. This corresponds to the extraction of one out of the two control rod assemblies at the point in the operating cycle, which requires the largest amount of control rod insertion.



Figure 24: UTOP transient on UN fuel with a 0.2 \$ reactivity insertion. Calculations were performed independently using the well-established safety analysis code SAS4A/SASSYS-1 and the in-house developed code BELLA.

WP2-Alleima collaboration (Christopher Petersson & Björn Bosbach)

Discussion and collaboration on materials analysis and microstructural characterisation (mainly with SEM).

WP4-WP2 collaboration (Elina Charatsidou, Christopher Petersson & Peter Szakalos)

For the visit of WP4 at Jönköping University for LFA thermal diffusivity measurements of UN fuel pellets, samples of AFA steel were made by WP2, and their thermal diffusivity was measured as well. The LFA measurements agree with previous measurements of diffusivity of the particular AFA steel and extend the data to results significantly above 300 °C (see figure 25).



Figure 25: Thermal diffusivity measurements of new AFA steel in the range of 25-800°C.

WP4-WP3 collaboration (Elina Charatsidou, Sarmad Katea & Gunnar Westin)

ZrN powder was manufactured at Uppsala University and then transferred to KTH in order to fabricate SIMFUELs of various compositions $(U_{1-x}Zr_x)N$. The pellets are then used in separate effect testing similar to what pure UN was subjected to, and the results of these tests can provide information in how the presence of simulated fission products (here Zr) affects the physical, mechanical and thermal properties of the fuel compared to fresh UN. From this we can obtain a better understanding of the fuel properties during burn-up.

WP3-WP2 collaboration (Daria Kolbas, Jens Hardell & Christopher Petersson)

Collaboration of tribological testing team of WP3 with materials development team of WP2. A meeting was held at LTU to exchange experience on liquid lead testing and the safety of lead handling. WP2 provided FeCrAl alloy for the WP3 fretting tests.

WP4-WP3 collaboration (Faris Sweidan, Elina Charatsidou and Farid Ahktar, with technicians)

High-temperature creep tests were conducted at LTU by members of WP4 in collaboration with WP3. In their Gleeble facility. This was complementary to the high-temperature creep test scheme that was developed at KTH and the national SPS centre at Stockholm University.

WP3-UU and WP3-LTU. The collaborations between the WP3 nodes at UU (Westin, Naim Katea) and LTU (Akhtar, Gruber) are presently focused on the development of cemented carbides for impellers. Synthesis routes are developed and carbide powders are coated with binder phase metals at UU. The powders are then SPS sintered and studied on mechanical properties at LTU. This study will continue with various types of composite compositions. Meetings and discussions are conducted continuously as well as during the larger quarterly meetings. Mechanical and stagnant Pb corrosion tests on protected coatings developed at WP3-UU are expected in the coming part of the Sunrise project.

Collaboration with WP5 on the abrasive wear by lead on materials developed for the impeller materials will start as soon as the testing rig is finished.

Collaborations with WP2, WP5 and WP3-LTU on protective oxide coatings deposited to enhance and smoothen the natural oxide layer formed on FeCrAl(RE) steels where needed in e.g. pipe bends and other places where high velocity lead flow is expected.

5.2 Scientific collaboration between different disciplines and departments

- WP4 collaborated with Tandem Laboratory at Uppsala University conducting proton implantations using 2 MeV proton beam on UN fuel samples. A joint paper, also with Chalmers University of Technology for FIB/SEM and TEM analysis will be written.
- WP3 UU and WP3 LTU collaborated on manufacture and mechanical testing of cemented carbides where UU make nano-coated carbide powders and LTU sinter them using SPS into compacts and study their mechanical properties. A joint paper is in manuscript.
- WP4 collaborated with Jönköping University conducting thermal diffusivity measurements using LFA on UN fuel samples. A joint paper is in the planning stage.
- WP4 collaborated with Luleå Technical University conducting compressive creep tests measurements using Gleeble on UN fuel samples.
- WP4 collaborates actively with Stockholm University conducting compressive creep tests measurements using SPS on UN fuel samples as well as fabricating UN and SIMFUEL samples using SPS.
- WP3 UU and WP4 collaborated on synthesis of simfuel nitrides which were mixed with UN and sintered and tested at KTH.

5.3 International collaboration, including participation in EU projects

There is an intense collaboration with University of New South Wales (UNSWI in Australia, and with the ANSTO center, is ongoing. We are in a joint proposal which has been accepted for access to the research reactor at ANSTO.

We are working in collaboration with MIT (US) on ion irradiation and coupled irradiationcorrosion experiments. Samples of our materials have been sent to MIT for a first round of irradiation testing and in a second campaign, the MIT researchers will install a device in the Uppsala Tandem ion beam facility.

We participate in several ongoing EU projects (PATRICIA, ENTENTE, PASCAL, Orient-NM, Innumat, Fredmans, OperaHPC, ASSAS, SASPAM, McSafer, ...). Some are on their last years while the newer batch of such were initiated around the time the SUNRISE centre started its activities, so there is no explicit link to SUNRISE in any of the current projects, but in Fredmans and Innumat there are clear paths for collaboration and synergy. For the next Euratom round, with deadline in November 2023, there will be clear and possible synergies between SUNRISE and a few EU-project proposals. Notably the cofunded European partnership on nuclear materials can be an important venue for SUNRISE to stake a claim and to provide access to our developed facilities to external researchers in order to synergize strongly. There is a collaboration with AC2T research GmbH in Austria for high temperature hardness testing of cemented carbides (funded by the Austrian COMET Program (project K2 InTribology, no. 872176), carried out at the "Excellence Centre of Tribology" AC2T research GmbH).

Promation (Canada) actively collaborates with SUNRISE on additive manufacturing and laser welding of alumina forming steels.

5.4 Collaboration with industry and/or other parts of society

In SUNRISE there are several active industry affiliates. Of particular note are:

- Denise Adorno Lopes from Westinghouse, leading the technical work in WP4, who also has a formal affiliation with KTH as "affiliate faculty".
- Björn Bosbach from Alleima, who is contributing actively to the work in WP2 and WP3 and who participates and engages actively in the technical workshops and in direct collaboration with reserachers in SUNRISE.
- Anders Blennermark from Blykalla, who leads the PSAR activity in WP1 and actively participates in the centre work, technical workshops and more.

SUNRISE is collaborating with Blykalla in the testing of a prototype of a steam-generator for Blykalla's SEALER reactor. The steam-generator is developed by Blykalla and the UK company TSP Engineering within the ASGARD project, co-funded by EUROSTARS. It is planned that TSP Engineering will manufacture the prototype in 2023, after which it will undergo freezing tests in the SUNRISE laboratory under construction at KTH.

SUNRISE is also contributing with manufacturing of alumina forming steel samples for irradiation testing in foreign research reactors, where the irradiation campaign is defined and funded by Blykalla.

6. Continued work after the project is finished

As described earlier, in Figure 1 above, the SUNRISE centre can be seen as the seed in a greater programme context. There is an ambitious plan laid out for continued work beyond the lifetime and current funding of the centre. Thus, we fully expect the centre to continue after 2026. There is already now funding for the Solstice project, see below, for activities until 2028.

The outcomes of SUNRISE will feed directly into the Solstice project, which aims at qualifying the safety approach and structural materials developed within SUNRISE, in an integrated, electrically heated proto-type of a commercial lead-cooled reactor (named "SEALER-E" by Blykalla, or "Solstice" by SUNRISE). The Solstice project is coordinated by SMR AB, with Uniper, Blykalla and KTH as main participants. The facility will be built on the site of OKG in Oskarshamn. KTH is responsible for developing and installing the instrumentation of Solstice/SEALER-E. Moreover, it is planned that researchers and PhD students from KTH will lead and participate in experiments carried out in Solstice/SEALER-E.

The preliminary safety analysis report produced in WP1 of SUNRISE will be utilised by LeadCold in an application for permit to build SUNRISE LFR (named "SEALER-D" by Blykalla), the lead-cooled research and demonstration reactor with an intended thermal power of 80 MW.

Steels developed and tested within WP2, WP3 and WP5 of SUNRISE will be used by Blykalla in its commercial fleet of SEALER-55 reactors and has great export potential for other LFR development projects around the world.

Data on uranium nitride SIMFUEL obtained within WP4 of SUNRISE will be used for demonstrating the safety case of SEALER-55 and other lead-cooled reactors operating on nitride fuels.

7. Budget of the centre

The centre was initially awarded 50 MSEK by SSF, whereof 3% (1.5 MSEK) is reserved for utilization/exploitation. This budget is summarized in Table 1 below. The submitted application had a budget of 60 MSEK and in the first year following the grant approval, SUNRISE managed to secure that difference in support from KTH centrally, from LTU through Creaternity and from Blykalla in cash and materials contribution. The total budget could thus return to nearly 60 MSEK. For clarification, the exploitation funds are included in "Other costs" in Table 1. The SSF-external funds are not shown in these table since they are not reported to SSF and cannot be extracted from the system. The additional support goes mainly into materials and equipment (since the SSF grant has a cap on 10% of the total budget for that) and a smaller part to PhD student salaries (Creaternity support mainly).

Year	Seniors	PhDs	Postdocs	Other	OH	Total
				costs		
2021	1610	2512	655	1090	1478	7346
2022	1658	3881	1330	2270	2203	11342
2023	1707	3302	1330	1332	2257	9929
2024	1758	2706	655	910	2066	8096
2025	1810	2788	993	894	1995	8479
2026	1864	718	675	880	1178	5315
Total	10406	15908	1391	7376	11178	50507

Table 1. SSF centre budget. All costs in kSEK. The minor over-budgeting here presented will be covered by KTH co-financing.

For the first years, the centre has underspent somewhat with respect to the budget, see a summary in table 2 below. This is mainly due to initial delays in recruitment, mostly due to the dampening effect of the covid crisis, but then for 2022 due to the start-up demands of the Solstice project, for which certain staff in SUNRISE was assigned to work in both SUNRISE and for Solstice in parallel.

Table 2. Actual expenditure and planned such. All costs in kSEK. The column "Diff" shows
the difference between the budget and actuals (negative is over-spending with respect to
the budget). The column "Acc.Diff." shows the accumulated difference over time.

Year	Seniors	PhDs	Post docs	Other costs	ОН	Total	Budget	Diff	Acc. Diff.
2020	8	92	0	116	36	254	0	-254	-254
2021	1057	1366	593	645	1281	4941	7634	2693	2439
2022	1830	1831	614	1969	2154	8397	11342	2945	5384
Total	2895	3289	1207	2730	3471	13592	18976	5384	

The plan for the continuation of the centre, from 2023 to 2026, is to get back on budget. Roughly half of the mismatch will be naturally recovered in time since it was due to delays in the recruitment of juniors. The other half can be used for additional junior salaries. In this way, the lack of expenditure in time, mainly due to the start of the Solstice project, will be highly beneficial for SUNRISE in terms of added manpower. The Solstice activities which have caused roughly half of the mismatch are well aligned and complementary to the SUNRISE research.

Utilization/Exploitation funds have so far not been used, but one study is approved by SSF and ordered from RISE. This is a pre-conceptual techno-economic study on the potential of using the high-temperature steam (530 °C) from the SUNRISE LFR for bio-mass pyrolysis and generation of a non-electric value stream. The utilization plan in terms of budget is detailed in Table 3.

	. Origoning and plannod admization projecto		
Year	ltem	Cost (kSEK)	Status
2021	N/A	0	
2022	N/A	0	
2023	RISE high-T pyrolysis study	250	Ongoing
2023	CO2 capture proof of principle study	500	Planned
2024	Market analysis	250	Planned
2024	SUNRISE LFR siting study	200	Planned
2025	Patent costs	150	Planned
2026	Patent costs	150	Planned
Total		1500	

 Table 3. Ongoing and planned utilization projects

For the planned activities, the costs are rough estimates.

8. External information and public outreach activities

SUNRISE has so far had a truly significant media impact with many interviews, reports and popular science lectures on TV, radio, newspapers, the web, podcasts, museum exhibits, panel debates, etc.

PhD student Elina Charatsidou (WP4) has created a YouTube channel called '<u>Elina</u> <u>Charatsidou – Your Friendly Nuclear Physicist</u>', talking to and educating the public on nuclear energy matters. Several of the videos on the channel discuss the work done with UN fuel and at the fuel lab in general. The videos related to SUNRISE have over 150k views, and the overall channel has a reach of over 2.5M views with nearly 40k subscribers. The channel was started in the summer of 2022.

PhD student Fredrik Dehlin (WP1) has been involved in the following external activities related to SUNRISE:

- Two Swedish speaking podcast interviews has been conducted. The first one <u>Strålande tider podcast: Avsnitt 3 – Den nya generationen med Fredrik Dehlin</u> was an almost hour-long discussion about SMR, Generation-4, the work we are doing in SUNRISE and why we are doing it.
- The second one <u>Ekomodernistpodden: 29 Fredrik Dehlin doktorand fördelen med</u> <u>blykylda kärnkraftsreaktorer och SMR</u> contained a similar discussion as the first one, but in a slightly shorter 30 min format.

Furthermore, Fredrik Dehlin has given two seminars to external organisations. The first seminar was given to the environmental organisation ELMA – Erfarenheter och Lärande av Miljöarbete on 2021-10-19 and the second seminar was given to the organisation Svenska Mekanisters Riksförening on 2022-04-26. Both seminars discussed SUNRISE in detail and, among many things, our motivation for selecting lead as coolant in our reactor design.

PhD student Paul Gruber and Prof Jens Hardell of LTU were interviewed by <u>SVT</u> <u>Norrbotten</u> on February 12 2023 and by <u>Swedish Radio P4</u> on February 26 2023 regarding SUNRISE.

Prof Janne Wallenius (WP1) has presented aspects of the SUNRISE project at conferences in Romania, France and Norway. He has given numerous interviews in public media, such as Ny Teknik, Dagens Industri, Sveriges Radio, Aftonbladet TV and Sveriges Television.

Prof Pär Olsson (Director) has been in a large number of interviews on television, radio, podcasts and the web. A few examples are given below:

- Interview about SUNRISE and Solstice by <u>Swedish Radio</u> February 15 2021 with Janne Wallenius and Pär Olsson.
- Article in forskning.se about SUNRISE on Feb 22 2021.
- Article in <u>Tidningen Energi</u> about SUNRISE and Solstice on May 11 2021.
- Interview by <u>Fjärde uppgiften</u> regarding nuclear energy and SUNRISE research on March 18 2022.
- Interview in <u>Studio Ett, Swedish Radio</u> about the proposed change in nuclear legislation to allow for small reactors on January 11 2023.
- <u>National television (SVT)</u> broadcast a popular scientific seminar arranged by the Engineering Science Academy (IVA) where Pär Olsson presented GenIV research and the SUNRISE programme; seminar on Nov 30 2022, national broadcast on Jan 13 2023.
- Prime time national news (Rapport) reports about renewed interest in nuclear engineering education at KTH on Mar 7 2023.
- Panel discussion participation at inauguration of <u>exhibition on nuclear energy</u> at Tekniska Museet in Stokholm on March 16 2023.

He has also given several invited lectures about SMR, SUNRISE, new nuclear technology, GenIV reactors; to various associations, the 1st AP Fund (national pension fund), various

companies, the French Embassy, the Technical Museum (where Sunrise models and materials is now part of an exhibition), etc.

Pär Olsson wrote a chapter in a popular scientific book on energy, <u>The Energy Antology</u>, published in collaboration with the KTH Energy platform and Vetenskap & Allmänhet on July 14 2022.

A public SUNRISE seminar was held at KTH on 27/4 2022 with the participation of researchers from the centre as well as a panel with members from SSF (CEO Lars Hultman), Vattenfall (VP Desiree Comstedt), OKG (CEO Johan Lundberg), politics ((now) State Secretary Daniel Westlen (L)). Presentations and a full recording are available via the centre's website: <u>www.sunrise-centre.se</u>

SUNRISE was a co-organizer of the high-level conference <u>CET-2022</u> (Converging Energy <u>Technologies</u>) in Oskarshamn 21-23/9 2022. About 200 participants listened and discussed over three days to a large list of speakers with e.g. the EU Commissioner for Energy, IAEA Director General, etc. All information, all presentations and recordings of the entire conference are available at the website.

9. SWOT analysis

We here present a SWOT analysis for the centre.

	Strengths	Weaknesses
1.	Excellent senior staff with good complementarity	 Ambitious work plan that may be challenging to complete in all details
2.	Excellent junior staff recruitments (MSc, PhD, postdoc)	 Person-dependent expertise in a few fields of research – in case staff
3.	Team-building spirit and excellent relations between staff in centre	moves away, replacements can be difficult to arrange
4.	Very good internal support in management at the three universities	 Relatively skewed gender balance (25/75) - but difficult to improve much given recruitment basis
5.	Excellent collaboration network with invested partners and stakeholders	4. Limited access to research reactors
6.	Very promising initial progress in centre research with important breakthroughs	
7.	Good connections to government and governmental agencies (e.g.	
8.	SSM is part of advisory body) Ambitious outreach program and	
	range of activities	
9.	Excellent track record in attracting funding	
	Opportunities	Threats
1.	Opening up new collaboration paths due to impossibility to access e.g. BOR-60	 The war in Ukraine and impossibility to collaborate with facilities such as BOR-60
2.	High visibility in media, society and politics – excellent potential to attract beneficial attention	 High visibility in media, society and politics – may be sensitive to political or and future financial
3.	Rapidly growing sphere of influence	backlash if opinions shift
4.	In nuclear energy research Subject field under rapid expansion locally and internationally	 Difficulties in attracting and retaining excellent junior staff, especially at postdoc level (the best ones are very attractive to the high-tech industry)

Appendix A.

Task and work descriptions for the five work packages in SUNRISE, taken from the application.

Task	Title	Work description	Schedule
1.1	General design	General operational and safety objectives of the research reactor are defined, and a general design is elaborated allowing to meet these objectives. The designed reactor should also function as a demonstration unit for a future commercial fleet of lead-cooled SMRs that can be deployed within 15 years. Priority is given to passive safety features and simplicity of operation and maintenance rather than to maximizing irradiation performance parameters. An intrinsic aim is that the research reactor should be possible to construct in three years, in order to reduce costs. Among the computational tools to be used for the design are Serpent, SAS4A, BELLA, STAR-CCM+ and ANSYS.	M1-M6
1.2	Plant systems	All reactor systems are listed and a conceptual design of the systems required for carrying out a detailed safety analysis is completed.	M7-M18
1.3	Operation	Operational modes of the reactor are defined, including monitoring, control, maintenance, inspection and testing procedures. Operational limits and conditions are determined. Emergency operating procedures, guidelines for accident management, core management and fuel handling, management of ageing and human factors are also to be addressed.	M19-M24
1.4	Radiation protection	Component activation is calculated using MCNPX and radiation protection measures for operational and maintenance procedures are defined.	M19-M42
1.5	Safety analysis	Detailed safety objectives and acceptance criteria specific to systems and components for different classes of events and types of analyses will be specified. Deterministic and probabilistic safety analysis of a set of enveloping transients is made based on a compilation of initiating events and hazards obtained by failure mode analysis. Deterministic codes such as SAS, BELLA and RSAC are used for analyses of anticipated operational occurrences, design basis events, beyond design basis events and selected severe accidents. A Risk Oriented Accident Analysis Methodology (ROAAM+) will be applied [9]. PhD exchange with WP5.	M19-M42
1.6	SAR compilation	In this task the documentation produced in tasks 1.1-1.5 will be logically aligned with in-kind contributions from industry and compiled into a SAR that can be submitted to SSM.	M42-M48

 Table 1.1 Task and work descriptions for WP1. Milestones follow from the Schedule.

 Table 2.1
 Task and work descriptions for WP2. Milestones follow from the Schedule.

Task	Title	Work description	Schedule
2.1	Selection of materials	Continuous selection of materials of high priority for LFR components, to be tested in experiments. Down-selection and additional materials may be added during the project.	M1-M36
2.2	Selection of experimental matrices	Define test matrices for exposures, irradiation, component manufacture and coatings. Will be performed and updated in yearly rounds.	M3-M40
2.3	Development and manufacture of new advanced steels	A range of reactive elements and concentration variations will be used to produce FeCrAI steels that can be tested in parallel for erosion and fretting resistance in WP3 and WP5. Characterization of microstructures in collaboration with WP3. PhD exchange with LTU and UU in WP3.	M1-M48
2.4	Preparation of exposure experiments	Selected materials will be prepared for different types of exposure, performed in WP3. PhD exchange to UU and LTU (WP3).	M10-M14
2.5	Manufacture of complex components	State of the art metallic additive manufacturing techniques will be employed to manufacture pump impeller and other complex geometry components for coating in WP3 and test in WP5. PhD exchange with Sandvik/Kanthal.	M20-M32
2.6	Irradiation at MIT	Combined irradiation/corrosion experiments will be performed at MIT. PIE analysis will be performed on-site as well as in WP3. PhD mobility to Boston, MIT.	M6-M36
2.7	Modeling of swelling in advanced steels	Direct vs multiscale modeling of swelling will be performed for the advanced steels developed in the project. Supercomputers will be heavily employed.	M12-M48
2.8	Modeling of embrittlement of advanced steels	Irradiation induced embrittlement of FeCrAI alloys will be modelled using a multi-scale modeling framework.	M36-M60
2.9	Pb/Al ₂ O ₃ interaction	Will be investigated in WP3 extensively and have modeling support here. PhD exchange with UU and LTU in WP3.	M6-M18

 Table 3.1
 Task and work descriptions for WP3. Milestones follow from the Schedule.

Task	Title	Work description	Schedule
3.1	Selection of components	Select components of high priority for LFR and their designs to be tested in experiments	M1-M3
	Development of	Development and characterization of; -Coated powders and sintering of two carbide compacts -FeCrAlO and Al ₂ O ₃ coatings -Addition of FeCrAl-O and Al ₂ O ₃ coatings to FeCrAl-steel and cemented	M1-M12 M6-M18 M12-M24
3.2	new materials	carbide compacts, including intermediate layer: TiN and graded structures -Development of B containing material for control rod. -Development of new coatings, e.g. LaCrO ₃ and metal-Al ₂ O ₃ nano-	M12-M30 M30-M40
		composites, and/or further optimised carbide / nitride composites and intermediate coatings. PhD exchange with KTH and WP2.	M40-M60
3.3	Materials characterization of new materials post Pb-heating	Detailed microstructural and mechanical characterization of materials developed in 3.2 before and after heating in Pb at 500 and 750 °C, and in selected cases 1000 °C in order to screen and rank suitable materials for the selected components.	M12-M72
3.4	Development of small-scale erosion/corrosion test rig	Design, fabrication, assembly, trial-testing and validation. PhD exchange with KTH and WP5.	M4-M16
3.5	Adaption of wear tester	Design of specimen holder and container, development of test methodology including safety measures	M6-M12
3.6	Test campaign	Testing newly developed materials and wear quantification	M16-M40
3.7	Post-test analysis	Analysis of surface damage and material removal mechanisms as well as changes in mechanical properties and chemical composition/ microstructure. PhD exchanges with all three partners.	M18-M42
3.8	Post-processing of wear data	Adapt wear data for be used in predictive models.	M18-M48
3.9	Welding process development	Test and optimize welding process for selected materials. PhD exchange with KTH and WP2.	M18-M36
3.10	Weld evaluation	Performing test campaign on welded samples with the selected materials.	M36-M54
3.11	Post-test analysis of weld samples	Weld characterization after exposure to harsh environment.	M38-M56
3.12	Characterization of large-scale tested materials	Determination of characterization plan. Material cut up and performing characterization. PhD exchange with KTH and WP5.	M56-M72

 Table 4.1
 Task and work descriptions for WP4. Milestones follow from the Schedule.

Task	Title & staff	Work description	Schedule
4.1	Fuel Fabrication and Characterization	Fabrication of all fuel material to be used, including different densities, compositions and fuel geometry to be analyzed. Characterization included are OM, SEM/EDS, EBSD, X-ray diffraction, ICP-OS. Other techniques maybe included	M1-M36
4.2	Fuel/Clad/Cool. interaction annealing	Assemble of interdiffusion samples and annealing over several temperatures and times	M7-M36
4.3	Fuel/Cladding/ Coolant interaction	Characterization for phase identification of the interdiffusion samples. Characterization included are OM, SEM/EDS, EBSD and X-ray diffraction. Other techniques may be included. PhD student	M12-M40
	characterization	exchange with UU and WP3.	
4.4	Leak rod test design/ assemble	Design and specification of different defects geometry to be evaluated, and production of such cladding material. Fuel loaded rods will be subject to annealing in static Pb, while blank rods will be test in the high-temperature loop. PhD student exchange with WP5.	M36-M48
4.5	Leak rod test post-run characterization	Destructive characterization of the tested rods with cut cross sections from different distances from the imposed defect. PhD exchange with WP5.	M42-M60
4.6	Thermophysical properties of UN fuel doped surrogate radionuclide	The dependence of the thermal conductivity of (U,X)N and phase stability will be investigated investigated as a function of burnup and porosity. Characterization included are DSC, Laser flash, X-ray, Neutron diffraction. Other techniques may be included. PhD mobility to UNSW (Aus) and exchange with UU and LTU in WP3.	M7-M60
4.7	Thermodynamic modelling	Calphad modelling of elements, binaries, ternaries and higher order systems supported by DFT calculations and experiments.	M1-M60

Table 5.1	Task and work	description for	r WP5.	Milestones	follow from	the Schedule.
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Task	Title	Work description	
5.1	Selection of components	Select components of high priority for LFR and their designs to be tested in experiments.	M1-M3
5.2	Preliminary component analysis	Define prototypic for components flow and turbulence characteristics based on preliminary CFD analysis	M3-M9
5.3	Development of modeling approaches	ment of gapproaches done in WP3 and WP5. PhD student exchange with LTL and WP3	
5.4	Design of SEFACE	Design of a separate effect small scale FAC/E facility (SEFACE) to for model development. PhD student exchange with LTU and WP3 .	M3-M14
5.5	Design of CTF	Design of a component test facility (CTF) to provide data for model validation	M6-M18
5.6	Design of SEFACE-M and CTF-M	Design of scaled mockups SEFACE-M and CTF-M for characterization of turbulence in relevant conditions and code validation	M3-M12
5.7	Construction of SEFACE-M	Construction and commissioning of SEFACE-M facility.	M12-M18
5.8	Construction of CTF-M	Construction and commissioning of CTF-M facility.	M12-M20
5.9	Construction of HLM SEFACE	Construction and commissioning of SEFACE facility (for WP3). PhD student exchange with LTU.	M14-M24
5.10	Construction of HLM CTF	Construction and commissioning of CTF facility.	M20-M32
5.11	SEFACE-M tests	Carrying out tests in SEFACE-M to provide model closures, calibrate and validate turbulence modeling approaches for SEFACE HLM.	M18-M30
5.12	CTF-M tests	Carrying out tests in CTF-M to provide turbulence model calibration and validation data.	M20-M32
5.13	Post-test model development	Post-test model development and calibration using data from SEFACE- M and SEFACE. PhD student exchange with LTU and WP3.	M36-M60
5.14	CTF tests	Carrying out tests in CTF to provide data for validation	M32-M60
5.15	Model validation	Post-test FAC/E-HLM model validation against CTF data	M32-M72