Young Molten Salt Reactor (YMSR) conference

Politecnico di Milano, Lecco campus, June 6 - June 8, 2022

Book of Abstracts

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The YMSR conference is organized by the SAMOSAFER project*. SAMOSAFER is a European research project, funded by the European Commission, focusing on the development and demonstration of innovative safety barriers for a more controlled behaviour of Molten Salt Reactors during severe accidents.

A "young" conference is organized at the premises of Politecnico di Milano, in the city of Lecco - along the Como lake - in Italy, from June 6 th to June 8th, 2022. The conference is tailored to PhD students, PostDocs and young researchers interested to present and discuss their research on Molten Salt Reactors. During the conference, senior scientists from the SAMOSAFER project will provide feedback and transfer experience to the young people. In addition, students attending the SAMOSAFER online school will have the opportunity to present the capstone project assigned to them.

The topics of interest include, but are not limited to, neutronics, fuel cycle, thermal-hydraulics, multiphysics transient simulations, safety studies, operation and control and experimental facilities related to Molten Salt Reactor technology.

Organising committee:

Sandra Dulla, Politecnico di Torino
Karin van der Graaf, Delft University of Technology, Project Manager SAMOSAFER project
Jan Leen Kloosterman, Delft University of Technology, Coordinator SAMOSAFER project
Stefano Lorenzi, Politecnico di Milano

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Summary

Evaluation of NICKel-based Materials for MSR applications: ENICKMA irradiation project

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Abstract. The Molten Salt Reactor (MSR), as one of six generation IV reactors, exhibits great potential for future safe and economic use of nuclear energy and is gaining more and more attention worldwide. To support the research and development of the Molten Salt Reactor technology, a MSR research program has been established at NRG. The main objectives of this program are (i) the characterization of irradiated molten salt fuel, (ii) the investigation of interactions between fuel & structural materials and (iii) the assessment of the behaviour of structural materials candidates under MSR operating conditions.

Material selection and qualification is an important feature for the development of the MSR technology. Like other generation IV reactors, MSRs will operate under harsh conditions for structural materials: operating temperatures in the range of ~500-800 °C, exposure to corrosive environments and neutron irradiation. For MSR materials selection, it is essential that the mechanical properties and dimensional stability are retained under both operation and abnormal conditions.

Various present conceptual MSR designs consider the use of Ni-based alloys as MSR structural materials due to their excellent high-temperature properties and corrosion resistance. However, Ni-based alloys are known to be sensitive to thermal neutron irradiation due to the transmutation of Ni itself and of B, present in trace amounts, which result in the production of He, among other products. The presence of He in metallic structures is well-known for causing embrittlement and overall deterioration of mechanical properties. Since irradiation data of Ni-based alloys is limited, the ENICKMA irradiation project (Evaluation of NICKel-based Materials) was initiated as a part of the NRG's MSR research program. The aim of the experiment is to study material degradation behaviour under neutron irradiation and the underlying mechanisms of degradation. This project is financed by the Dutch government (Ministry of Economic Affairs) subsidized nuclear research program.

The present work provides an overview of the scope, planning and status of activities carried out within the ENICKMA irradiation project. In total, 100 tensile and fatigue specimens from 7 different materials (6 Ni-based alloys, 1 stainless steel) are currently under neutron irradiation for 9 cycles in the High-Flux Reactor in Petten, at a temperature range between 650-750 °C. The irradiation will be completed by the end of 2022. The total fluence received by the samples will be such to achieve a He-production of roughly 10 times more than experimental data published in recent sources. In parallel to the irradiation, annealing treatments at 650 ºC and 800 ºC, for durations of up to 9 months and 1 month, respectively, are performed, in order to improve the understanding of the interplay between thermal exposure and helium embrittlement. Mechanical tests such as tensile, low-cycle fatigue, tension stress relaxation and small punch testing, as well as microstructural analyses by means of optical microscopy, SEM and TEM are part of the ENICKMA testing scope. Tests will be performed on as-received, annealed and irradiated materials. Preliminary tensile testing results, obtained for specimens in the as-received and annealed at 800 ºC conditions are discussed.

Experimental Investigation of Freezing Phenomena in Forced Convection Internal Flow

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Abstract. Melting and solidification of the fuel salt plays an important role in the design and safety of the Molten Salt Fast Reactor, such as the design of the freeze plug and the analysis of accident scenarios where the solidification of the salt might be a risk. An example of such an accident scenario is the sudden solidification inside the steam generator, which may lead to clogging and result in a dangerous situation. As such, there is the need to have a proper understanding of this phenomenon, and to improve the current numerical modelling capabilities for transient freezing, specifically in forced convection flows with a sudden wall-temperature drop. To do this, detailed and comprehensive experimental measurements of the transient growth of the ice-layer with well-defined boundary conditions are required.

However, while extensive experimental studies have been performed for melting under natural convection conditions, very limited experimental measurements have been performed for freezing under forced convection conditions. Moreover, most of these experimental studies, whilst presenting very interesting findings from a theoretical point of view, did not include precise measurements of the solid-liquid interface position nor of the velocity field and as such are ill-suited for numerical benchmarking purposes. To this end, this paper presents the ESPRESSO (Experiment for Re-melting and Salt Solidification) facility.

The ESPRESSO facility features a water tunnel capable of generating both laminar and turbulent flow fields. At the bottom wall of the test section, a cold-plate is located capable of reaching a minimum temperature of -20 °C from which the growth of the ice-layer will be initiated. The cold plate was custom designed and build in order to achieve the highest possible heat transfer from the fluid above into the cold plate in order to facilitate the growth of an ice-layer even for high flow rates. Moreover, the temperature distribution along the cold-plate is measured during operation, such that a more accurate representation of the experimental conditions may be included in future numerical validation campaigns. Apart from a description of the experimental facility and a future outlook, the present work will include measurements of the velocity field and transient development of the solid-liquid interface in laminar flow using planar PIV (particle image velocimetry), as well as a comparison of these measurements with theoretical predictions from literature. As such, this paper aims towards the generation of a more comprehensive, precise and reproducible experimental database for the transient growth of an ice-layer in forced convection flow, suitable for numerical validation studies.

Density and thermal-conductivity measurements on chlorides for molten salt reactor technology

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Abstract. Future applications of nuclear energy will strongly benefit from the closure of the fuel cycle, reducing the natural resource needs andthe amount of the generated radioactive waste to be disposed. Although plutonium from used UOx fuels can be recycled as mixed oxide fuel (MOx), as it is currently done for the EDF fleet of reactors, significant improvement in fissionning all the Pu isotopes and minor actinides can be achieved with the introduction of fast-spectrum advanced reactor systems. A molten salt reactor (MSR) using chloride salts is a very promising advanced reactor system aiming to reuse and valorise plutonium from the spent fuel and other sources. Chloride salts are often retained for the fast spectrum concepts, as they provide harder neutron spectra and higher solubility of actinides. For the design and safety assessment of this reactor, the knowledge of thermodynamic and thermo-physical properties of actinide chlorides and their mixtures is required. However, few experimental data on the characteristic of potential fuel salts are available.

This work focuses on the optimization of techniques to determine some thermophysical data of molten chloride salts selected as the MSR fuel salt candidates, such as density and thermal conductivity.

As the main goal is to perform measurements on PuCl3 -containing molten salt mixtures, the applied techniques have to comply with several constraints, such as high temperature and volatility of molten salt samples, reduced amount of the material and the need to work in a glove box with inert atmosphere with very low O2 and H2O concentrations.

Techniques for measurement of density and thermal conductivity in plutonium containing molten chloride salts are currently in the final testing phase and the progress will be presented. For the density measurement, a set-up based on the Archimedean principle was recently developed at JRC. In this paper, measurements were carried out to optimize and validate the method on several inactive salt mixtures, including CeCl3 and NaCl-CeCl3 as a simulant to PuCl3. The measurement method was successfully demonstrated paving the way of the experimental set-up towards the installation in an active glove box.

Thermal conductivity measurement are carried out using laser flash techniques in gas-tight crucibles that were specially designed for this purpose. Inactive quenched salts such as FLiNaK, LiCl-KCl and MgCl2-KCl were enclosed in those crucibles. X-Ray measurements at room temperature were accomplished to analyse the behaviour of the salt in the closed crucible. The purpose is to identify and avoid the presence of void zones in the salt, which has been found as key to achieve reliable thermal conductivity measurements.

Round Robin 1.0 on Chemical and Thermal Property Characterization of Molten Salts

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Abstract. Under the informal umbrella of the Molten Salt Thermal Properties Working Group (MSTPWG), Oak Ridge National Laboratory (ORNL), UC Berkeley, and the University of South Carolina organized a Round Robin on Chemical and Thermal Property Characterization of Molten Salts. Properties of two salt mixtures (FLiNaK and ~50% NaCl-KCl) were measured by different groups using a diversity of methods and instruments. The results for each property were inter-compared to understand the ability to reproduce measurements, the appropriateness and limitations of each technique, and the possible sources of error.

The goals of this round robin exercise were: (1) development of standard procedures, (2) generation of calibration standards and standard materials for working with molten salts, (3) generation of verified properties (for FLiNaK and NaCl-KCl), (4) quantification of error, identifying the sources of error, demonstrating the reproducibility, identifying the limitation of the measurement techniques and (5) sharing of best practices across the experimental groups in the performance of these measurements.

The round robin focused on creating a research community within which best practices can be shared. Blind-blind peer review of procedures were facilitated by the organizers. A total of 22 organizations, from 7 countries, collaborating in this round robin effort have collaborated to the Round Robin.

ORNL provided 100 g batches of purified FLiNaK and purified NaCl-KCl that were stored and distributed by UC Berkeley. The participants were provided of an identification number by UC Berkeley allowing for the open distribution of measurement results, without identifying the institution where the work was performed. The results of the round robin testing were statistically analyzed by the organizers of the round robin.

The results of the Round Robin measurement of density, elemental analysis, melting point, viscosity, and thermal diffusivity will be presented, and a discussion of variability and error analysis and error reporting will be provided.

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Acid/Base Behavior and Buffering Capacity in Molten Fluoride Salts

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Abstract. The concept of solvoacidity (acid-base characterization based on the Lewis definition of acids) has been used to systematically describe molten salts and characterize properties across solvent compositions. Fluoroacidity (pF), a measure of the activity of dissociated F- anions which is relevant to molten fluoride salts, is a composition-dependent metric which may be useful in understanding corrosion in molten salt systems. Experience from the MSRE led to the hypothesis that more fluorobasic salts with a higher activity of F- have a greater capacity to stabilize corrosion products by solvation in the solvent and are therefore more corrosive. More recently, modeling results from our collaborators at UC Berkeley have shown that chromium in various oxidation states can incorporate into the polymer network of the melt, so a higher activity of F- is not necessary for solvation of corrosion products. Solvation of chromium may take place by both dissociated fluorides (dsF) and by oligomers. The dominant solvation mechanism was found to depend on the oxidation state of chromium. Cr2+ is approximately equally solvated by dsF and oligomers, whereas Cr3+ is predominantly solvated by dsF. Experimental studies of chromium diffusivity in molten fluoride salts of various fluoroacidities are underway to examine the effect of fluoroacidity on corrosion product behavior. Studies will attempt to validate the simulation results, giving evidence of the differences in behavior of the Cr2+ and Cr3+ oxidation states of chromium in solvents of differing pF.

Within the analysis of the simulation study, we have also introduced the concept of acid-base buffering capacity in molten fluoride salts. From the simulation study, we found that characterizing pF simply by the count (or more accurately, the activity) of dsF leads to different conclusions than characterization of pF by the presence of conjugate acids in the melt—bridging fluorines (which indicate oligomeric behavior) and under-coordinated cation centers. Acidity contributions can come from both bridging fluorines and under-coordinated cations, and one contributor might dominate depending on the melt composition. When chromium is oxidized and solvated in a melt, it can be solvated by dsF or by oligomers, resulting in either an increase in under-coordinated cation centers, or an increase in bridging fluorides. If a melt has a high concentration of bridging fluorines or has cation centers amenable to under-coordination, the melt will have the capacity to produce dsF in response to the consumption of dsF by solvation of a Cr cation. This we call acid-base buffering capacity. Buffering capacity is a function of the degree of polymerization and the strength of association of ions in a melt. This theory can help us understand how salt structure changes when corrosion products are present, aiding in fundamental understanding of corrosion in molten fluoride salts. This presentation will include a discussion of the theory of acid-base buffering capacity with molten fluorides, along with experimental results from chromium diffusivity studies in melts of varying pF.

Thermodynamic assessments of the LiF-ZrF4-BaF2, NaF-ZrF4-BaF2, KF-ZrF4-BaF2 systems

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Abstract. In the framework of the safety assessment of Molten Salt Reactor designs, understanding and modeling of the thermal stability and retention capability of the fuel salt solution is a key point for the operability and licensing of this technology. The behavior of different fission products in solution with the carrier salt needs to be described in detail to anticipate dispersion of volatile elements to the environment in an accidental scenario, or parasitic compounds that could precipitate and neutron poisoning reactions which could affect the long-term operation in an active reactor.

Barium and zirconium have been described as some of the most abundant fission products of the uranium fueled reactors. Even if they are both considered as short-lived radionuclides (with the notable exception of the isotope 93Zr, half-life: 1.5 million years), the high potential of precipitation as multicomponent systems has been observed in the literature and current the generation of Light Water Reactor. The fluoride fuels investigated for the Molten Salt Reactors, with the references LiF-ThF4-UF4, NaF-ThF4-UF4 and KF-ThF4-UF4, present particularly oxidative conditions and the behavior of the fission product has to be predicted. In this work, the most stable fluorides salts of the two fission products, respectively BaF2 and ZrF4, have been thermodynamically described in equilibrium with LiF, NaF and KF by CALculation PHAse Diagram (CALPHAD) combining experimental studies by calorimetry and X-Ray diffraction with modeling. The thermodynamic assessments of the LiF-ZrF4-BaF2, NaF-ZrF4-BaF2, KF-ZrF4-BaF2 systems have been established using the modified quasi-chemical model in the quadruplet approximation. These systems have to be considered in the safety assessment of the fluorides fueled Molten Salt Reactors.

Thermodynamic assessment of the corrosion products between molten salts and reactor structural materials.

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Abstract. Within the framework of Generation IV Nuclear Reactors, the Molten Salt Reactor (MSR) design allows the nuclear fuel (dissolved in a molten salt) to circulate inside the reactor core and the primary heat exchanger units. This implies that the radioactive fission products (which may exist in different physical states) also circulate in the primary circuit and can interact with the internal structural material, here steels (Fe,Ni,Cr). The knowledge of the corrosion products on molten salt behavior is important for the evaluation of MSR performance. In this context, phase diagrams are essential to understand the effect of changing composition, pressure and temperature conditions on the material behavior. For complex multicomponent systems such as in MSRs, the CALPHAD method (CALculation of PHAse Diagram) is a reliable approach for modelling the thermodynamic properties and phase diagrams of this system.

The present work aims at the development of a CALPHAD database for predicting the thermodynamic properties of the corrosion products which may form between the molten salt and the structural materials. The Modified Quasichemical Model is used to describe the Gibbs energy of the liquid phase. For this work, the reference fuel is composed of molten chloride salt of (NaCl+MgCl2) and (PuCl3+AmCl3). Thermodynamic models already exist for the system NaCl-MgCl2-FeCl2-NiCl2, which reproduce well the available experimental results. However, there is no model and very less or no experimental data available on the corrosion interaction of the salt with Cr.

This work describes the current state-of-the-art on the thermodynamic database for molten salt-steel component interactions. The thermodynamic assessment of the pseudo-binary systems of NaCl-CrCl2, NaCl-CrCl3 and FeCl2-CrCl2 will be presented. To encounter the lack of thermodynamic data, ab-initio calculations coupled with a quasi-harmonic approach were performed to estimate the data for the intermediate solid compounds for NaCl-CrCl2 and NaCl-CrCL3 binary systems. The comparison between the calculated phase diagrams and the available experimental thermodynamic data is presented. A good agreement is obtained. Utilization of this database in the CEA code “MOSARELA” to perform thermodynamic calculations for molten salt is also discussed.

Towards the definition of Hastelloy N properties catalogue for the preliminary design of MSFR primary confinement

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Abstract. The confinement of the molten salt fast reactor core region needs to withstand a harsh environment: high temperatures and high temperature gradients, high impinging fast neutron flux resulting high fast fluence and high dpa, corrosive environment. Experience with the molten salt reactor technology narrowed down the material selection for this key component to nickel-based alloys, i.e., Hastelloy. Nevertheless, the operational conditions envisaged in the molten fast reactor require the revision and extension of available correlations for the thermophysical and thermomechanical properties of such materials, and of their behavioral models as well (e.g., void swelling and creep under irradiation). In this work we thus focus on the critical review of material properties and behavioral models for Hastelloy N (which has been identified among the most promising material candidates), with the twofold goal of setting up a preliminary material properties catalogue for design purpose and of identifying gaps in available knowledge, to be filled by future experimental works and/or conservative design assumptions.

CFD simulations of the Molten Salt Fast Reactor

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Abstract. The Molten Salt Fast Reactor (MSFR) is a fast-spectrum molten salt reactor (MSR) concept, where the fuel salt flows freely through a quasi-cylindrical core (two meters high and two meters in diameter), instead of circulating through pipes like in the historical MSRs. This reactor presents several specificities compared to solid fuel reactors, in particular: the strong density feedback depending on the turbulent, chaotic, temperature field in the core; the turbulent transport of the delayed neutron precursors through the core. These two aspects require the use of coupled thermal-hydraulics / neutronics tools to model the MSFR core.

In the Commissariat aux Energies Atomique et Alternatives (CEA), a coupled tool combining the deterministic neutronics code APOLLO3 ® and the CFD code TrioCFD is used. This coupled tool was first used to model a two-dimensional simplified study, used as a benchmark between SAMOSAFER partners. The code is also used for the modelling of the first molten salt reactor built, the Aircraft Reactor Experiment, in order to reproduce some of the historical experiments made in the reactor. The modelling of the MSFR, for which several coupled simulations were already performed on different codes, appears to be the next logical step for the validation of the coupled tool.

In a first stage, several thermal-hydraulics studies of the steady-state MSFR flow were performed, using TrioCFD. The thermal power distribution was taken from a Monte Carlo calculation. The Reynolds number of the steady-state flow in the MSFR being approximately one million, Reynolds Averaged Navier Stokes (RANS) models as well as Large Eddy Simulations (LES) were performed. Different geometries were considered, from one sixteenth of the core to the full core.

Our RANS model was compared to steady-state simulations realised by other SAMOSAFER partners. The RANS model showed almost no sensitivity to the geometry considered, the results for one sixteenth being very similar to the full core results. The RANS simulations were also used to determine several turbulent parameters (Taylor microscale), in order to optimize the meshing for the Large Eddy Simulations. The Reynolds number being very high, a fine mesh is required to compute directly at least 80% of the turbulent kinetic energy in the LES modelling. Furthermore, the LES simulations are very sensitive to the geometry used, requiring to perform full core simulations in order to correctly model the eddies in the centre of the core. These two aspects contribute to the high computational cost of the Large Eddy Simulations. They are nonetheless necessary, comparisons between Large Eddy Simulations and RANS simulations having revealed important differences in the mean velocity field. These simulations also revealed a very turbulent instantaneous velocity field with several recirculation zones, leading to early estimations of the power and temperature instabilities in the MSFR core.

Hybrid Data Assimilation methods: application to the DYNASTY experimental facility

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Abstract. Theoretical modelling through Partial Differential Equations is a widespread tool for designing and optimizing engineering systems. However, the main limitation of this approach is the associated computational cost of the numerical solution, which prevents quick repetitive solving, for instance, necessary in control applications. Moreover, mathematical models have limitations related to the hypothesis used to derive the model and the uncertainty of the parameters (e.g., heat transfer coefficient at the boundary, nuclear cross sections or material properties).

Nuclear reactors are complex engineering systems which must satisfy tight criteria to operate, and it is necessary to have an accurate estimation of each characterizing quantity of the system, like temperature, power, neutron flux or coolant velocity. Generation IV nuclear reactors usually have a hostile environment due to high temperature, radiation, or corrosion issues, and it is not simple to measure every physical field. In particular, Molten Salt Reactors (MSR) cannot include in-core measurements, and only the boundary is available to place sensors due to the fluid nature of the fuel. Moreover, some fields cannot be easily measured, making a data assimilation process not feasible. However, thanks to the strong coupling of the system, the measured quantities may give an inkling about non-measurable ones. Therefore, it is legitimate to investigate the possibility of getting, for instance, some information on the coolant velocity or the reactor power from the temperature (easier to be measured).

Since the estimation of the physical fields is a crucial part of the safety of nuclear plants, there is a need to provide suitable tools with an efficient and accurate procedure. These requirements are satisfied by Hybrid Data Assimilation (HDA) methods, which integrate Reduced-Order Modelling techniques into a Data Assimilation framework. This integration leads to reduced solution time, the accuracy of the models kept to the desired level and the possibility of using the experimental data as an update to the a priori prediction of the model. These techniques look very promising, and in literature, there are several works concerning their application to simple numerical cases, showing outstanding results. Therefore, they are mature enough to be tested on actual complex facilities and validated with experimental data. This work aims at being the first step in a deep validation phase to assess their efficiency and reliability. In particular, this work considers three techniques: the Generalized Empirical Interpolation Method (GEIM), the Parametrized-Background Data-Weak (PBDW) formulation and an algorithm for Indirect Reconstruction (IR) of fields. The selected test case is DYNASTY (DYnamics of NAtural circulation for molten SalT internallY heated), an experimental facility for studying natural circulation built at Politecnico di Milano, considering, for the time being, only synthetic data (the results are preliminary only). Nevertheless, they show the potentiality of the methods, even for complex systems. It is a matter of future developments to use experimental data to assess the efficiency and reliability of the HDA techniques.

Normal and abnormal states investigation of molten salt experimental loop using CFD

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Abstract. Experimental Molten FLiBe Salt Loop (MSL) in the Research Centre Řež, Czech Republic, is currently undergoing a renovation. This experimental molten salt loop was designed for construction material development, components development and testing, and corrosion tests.

The MSL renovation is based on the risk-based design approach. Important part of this approach is to reliably define working and critical conditions of the MSL. To investigate and consequently to define those working and critical conditions of the MSL computational fluid dynamics simulations are used. In the chosen software – ANSYS Fluent – a model of MSL has been prepared. The quality of this model was checked, and sensitivity analysis for mesh quality was performed. Moreover, another sensitivity analysis was done for heat transfer coefficient between insulation and air.

A number of different normal and abnormal states were identified including, but not limited to the following: startup (MSL filling before the experiment), regular operation with natural circulation, regular operation with forced circulation, regular shutdown (MSL draining after the experiment), abnormal shutdown, heating cutoff without draining, and insulation failure during operation.

From this list of working and critical conditions several of them was chosen, investigated, and described. For example, for the regular operation with natural circulation of molten FLiBe in the MSL an optimal heating distribution on the heating segments was found in order to achieve maximal mass flow rate through the loop while obeying all the limitations. As well as for the regular operation with natural circulation, the investigation of the regular operation with forced circulation was performed. For several flow rates, a heating distribution on the heating segments with minimal differences between hottest and coldest place of the MSL were found.

One of the abnormal states investigated was the heating cutoff without draining. From that investigation, a place where molten FLiBe salt would start to freeze as first was identified and time when it would start to happen was measured.

The results of these investigation will be used for the risk-based design of the MSL renovation and consequently, on the regular basis for the risk-based operation, experiments, and maintenance of the MSL.

A Numerical Method for Melting Phenomena in MSFR

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Abstract. In recent years, Molten Salt Reactors (MSRs) have gained new momentum thanks to their high potential for innovation in the nuclear industry. Currently, the European project SAMOSAFER (2019-2023) is aimed at ensuring that Molten Salt Fast Reactors (MSFRs) can comply with all the expected safety essentials. In terms of passive safety, a strategy currently envisaged in accidental scenarios is to drain by gravity the molten salt – which acts both as fuel and coolant –, in an emergency draining tank, ensuring both a subcritical geometry and a proper cooling. To activate the draining system, a freeze plug, made by inert salt, is expected to open by melting when the temperature in the core reaches a critical value.

For this reason, it is interesting to be able to quantify the physics of melting phenomena within the salt used in the reactor. The aim of this work is to propose a method for the numerical modelling of the melting process in a freeze valve, on the basis of a compromise between accuracy, computational efficiency, and simplicity of implementation. The model is subsequently implemented using the open-source software OpenFOAM. Since the scope of the project will eventually be to integrate the model into a multiphysics solver developed for the reactor-scale simulation of MSR, the study takes into account the compatibility for this application.

After a careful review of the literature, different numerical methods for the latent heat modelling in the context of the finite volume method were tested by using OpenFOAM. As a result of this analysis, a novel way of combining two temperature-based, fixed-grid numerical methods for the latent heat modelling, namely the Apparent Heat Capacity method (AHC) and the Latent Heat Source Term method (LHST), is proposed. Moreover, the energy equation is then coupled with the Navier-Stokes equation for the liquid phase. The resulting solver was tested and verified against well-established analytical and numerical solutions, showing good accuracy within tolerance without compromising the overall computational cost.

Afterwards, the code was applied to simple case studies related to the freeze valve system, showing the flexibility of the solver for the intended application. Three scenarios are simulated on a valve-like geometry, represented by a squared cylinder with a diameter of 200 mm, and assuming that the valve is positioned right below the leg of the heat exchanger. The first case is stationary, and the aim is to analyse the position of the solid-liquid interface during normal operation of the reactor. The second and the third case are melting transients, and the aim is to keep track of the melting rate and of the shape of the solid-liquid interface, first with adiabatic boundaries, and then with more complex boundary conditions. The results of such preliminary simulations demonstrate the feasibility of the developed code to efficiently simulate the macroscopic behaviour of melting phenomena in MSR.

Implementation of a new point reactor kinetics calculation strategy for MSR neutronic-thermalhydraulic dynamics in the system-code CATHARE

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Abstract. Molten salt reactors (MSRs) constitute a promising class of generation IV nuclear reactors, potentially enabling safe, abundant, and long-term low-carbon energy production. Academic studies, industrial projects, and national research and development programs are carried out worldwide to advance knowledge and technology of MSRs, aiming for Alvin Weinberg's vision to become a reality.

To perform design and safety analyses of MSR-systems, modeling and numerical simulation of their neutronic-thermalhydraulic dynamics, which present distinctive features from traditional solid-fuel nuclear systems, are essential. Among these features, the migration of delayed neutron precursors (DNPs) in the circulating fuel, and the deposition of radioactive decay heat throughout the fuel circuit, require to adapt system-scale calculation codes originally developed for solid-fuel reactors.

Several strategies have been proposed to account for these features in system-scale neutronic-thermalhydraulic simulations, notably regarding the neutronic and DNP dynamics. They range from direct resolution of appropriate multi-group diffusion formulations of neutronic and DNP dynamics, to marginal adaptations of classical punctual reactor kinetics (PRK) models, such as the one-time correction of the effective delayed neutron fractions accounting for DNP migration. Other strategies employing classical PRK models include models featuring continuously-updated effective delayed neutron fractions, addition of terms representing the core-exiting and re-entering of DNPs in the PRK equations, or employment of a moving mesh to spatially track the DNPs, among others. A modified PRK model, obtained by adjoint-weighting the neutron and DNP balance equations accounting for fuel circulation, has also been proposed, and various forms of the quasi-static method, wherein PRK effective parameters are periodically updated, tested.

In this work, we present a new calculation strategy for system-scale MSR neutronic-thermalhydraulic simulations based on a partial adjoint-weighting procedure. It relies on the separation of the neutron flux into an amplitude and a shape function, and focuses on the amplitude function (obeying a first-order differential equation obtained by adjoint-weighting the neutron flux balance equation), but it features a fully-fledged spatio-temporal representation of DNP groups concentrations. At each time-step, the DNP concentrations in all mesh cells are updated by solving their time-discretized balance equations (which account for fuel circulation), and the power/amplitude PRK equation is solved using effective (punctual) DNP concentrations, obtained by weighting the actual (spatially-distributed) DNP concentrations by a precomputed adjoint-informed spatial profile. The conventional PRK equations bearing on the effective DNP concentrations are discarded. Furthermore, the effective delayed neutron fractions are continuously-updated on the basis of the fractions of DNPs inside the core. This strategy is implemented in the system-scale code CATHARE, and is compared to a more classical modified PRK model, including terms representing the core-exiting and re-entering of DNPs in the classical PRK equations.

Establishing a molten salt phase change benchmark - preliminary results

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Abstract. Molten salt reactors (MSR) are characterized by complex physical phenomena that do not occur in conventional nuclear reactors. One such phenomenon is phase change of the fissile salt, which can happen both in a controlled manner and as an unwanted incident. Understanding of the phase change processes that can take place in freeze valves, drain tanks, or heat exchangers is of utmost importance to reactor designers. In some designs, safety of the reactor depends primarily on the melting of the freeze plug. Excessive cooling in the heat exchanger can cause the salt to freeze and thus limit the output power. In order to predict the behavior of the entire system, the salt's thermophysical properties, as well as the heat transfer characteristics of the phase change process must be thoroughly known. This can be achieved with the use of separate and integral effect tests, and computer simulations. However, due to the scarcity of experimental facilities investigating melting and solidification of salts intended for use in MSRs, it is predominantly the numerical models that are used to predict the salts' behavior on a macroscopic level. The different models, due to the lack of validation possibilities, should be compared with each other to determine the relative margin of error of the computational fluid dynamics (CFD) codes. An attempt to create a systematic benchmark framework for comparison of the modelling capabilities of the salt melting of different codes is being made by the Technical University of Denmark (DTU) and Delft University of Technology. A simple, two-dimensional model of a freeze valve based on the Molten Salt Fast Reactor (MSFR) design has been developed. With each step of the benchmark, an additional level of complexity is added to the model to pinpoint what the possible sources of discrepancies between different codes are. A thorium-lithium fluoride-based salt plug is being melted from the top, utilizing the MSFR's core decay heat, assuming a total loss of power accident. The fuel salt's internal heating is considered. The influence of the heat conduction in the piping is studied. The Boussinesq approximation is included in the model to study the effect of buoyancy and natural circulation on the melting process. Lastly, the movement of the liquid salt above the plug is implemented, as the freeze valve is located very close to the reactor core, in which the salt is not considered stagnant. Temperature, liquid volume fraction, as well as velocity fields computed by different codes are compared. An outline of the benchmark is presented and preliminary results of the simulations performed at DTU using the commercial CFD software STAR-CCM+ are shown. In DTU's simulations, a Volume Of Fluid model is used to account for the multiphase nature of the problem. The phase change is described using an enthalpy-porosity approach. First results indicate that the addition of the piping changes the results significantly, and that the natural convection plays a non-negligible role in the process of melting from above.

Status and perspectives of the Molten Salt Fast Reactors analyses with the SIMMER code

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Abstract. The Molten Salt Fast Reactor is a concept developed by the European Union based on a liquid fissile salt circulating through the reactor core. The design is currently under development by the SAMOSAFER project, in the framework of the HORIZON-2020 program. The peculiarity of the concept, with a flowing fluoride salt that acts as both fuel and coolant, poses important challenges from the computational point of view, that require ad-hoc adjustments for existing simulation codes, if not completely new approaches. The main challenge is the tight coupling between the neutronics and the thermal-hydraulics of the core, which is much stronger than in conventional nuclear designs.

Suitable codes should be able to consider the unique case of flowing neutron precursors, which are generated in one position but release the delayed neutrons somewhere else; this calls for an additional (with respect to solid fuel core designs) streaming term in the delayed neutron precursors balance equations, which directly couples the thermal-hydraulics to the flux shape. Another peculiar concept is the bubbling system: the injection of helium bubbles into the liquid fuel will improve the fission product removal (both gaseous and solid) but will also have a strong impact on the reactivity (locally and globally) due to void feedback. This further increase the coupling between thermal-hydraulics and the neutronics, as dimension, distribution and behavior of the bubbles influence the flux shape.

KIT has been working in the past years to adapt the coupled code SIMMER to model these phenomena. SIMMER is a multi-dimensional, multi-velocity field, multiphase, multicomponent, Eulerian, fluid dynamics code coupled with a space and energy dependent neutron kinetics module and a structure model. It has been developed as a tool for studying core disruptive accident scenarios in Liquid Metal-cooled Fast Reactors (LMFR), but thanks to its flexibility it has been successfully employed for applications outside of its focus: light water reactors, general multiphase problems, steam explosion problems.

SIMMER has been developed and validated with most of the MSFR-related features already included, as liquid fuel motion is a condition that has to be dealt with when modeling core disruptive accidents: this includes advanced models for fuel movement, bubbling (with multi-velocity field), solidification and melting, material stratification... Karlsruhe Institute of Technology (KIT) has also developed in the past a set of code modifications for the modelling of the MSFR concept: the changes act on both the neutronics section, considering the neutron precursors flow, and the thermal-hydraulics part, with new equations of state for the fissile salt.

This work summarizes the activities that KIT plans or is currently carrying on with SIMMER about the MSFR, in the framework of the SAMOSAFER project. These include the assessment of the bubble model against experimental activities and CFD codes, the revision and update of the code modification set, the modeling of the core in Loss Of Heat Sink transients, the modeling of the core draining and cooling in the Emergency Draining Tank..

Benchmarking, Point-Kinetic Verification, and Application of GeN-Foam towards Multiphysics Simulation of Molten Salt Reactors

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Abstract. In light of the growing need for detailed analysis of up-and-coming reactor technologies, several codes are under development with the aim of simulating multiphysics phenomena. These codes are largely unproven and unqualified, and as such they must be tested prior to being used for this purpose. This work takes on the task of assessing a particular OpenFOAM-based multiphysics code (GeN-Foam) for potential use in both design and deterministic safety assessment of the Compact Molten Salt Reactor (CMSR) developed by Seaborg Technologies. It begins with an evaluation of the code against the MSFR benchmark developed at CNRS. The code is found to pass the benchmark without issue; thereby its fidelity with respect to several MSR-specific phenomena is established insofar as the benchmark results can be considered accurate. Next, a quite recent neutronic verification scheme is applied to the code, based on the extraction of the point-kinetic component of a transient solution. The phase response to a reactivity perturbation is found to be correct in this respect, while a discrepancy is found in the amplitude response. Finally, the code is applied to the CMSR. A set of multiphysics simulations are performed of this full-core 3-D porous media model. A mesh independence study is performed on the fully-coupled steady-state solution and a sensitivity study is also performed with regard to the calculation of βeff with DNP transport. Transient simulations are performed of bulk reactivity insertion, loss of moderator cooling, and unprotected loss of flow. Results fall well within reasonable expectations and the general safety benefits of molten salt reactors are exhibited. With this, GeN-Foam is positively assessed for continued use in the design and licensing campaign of the CMSR.

Calculation tools for the simulation of the MSFR physics

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Abstract. Molten Salt Fast Reactor (MSFR) is a 4th generation nuclear reactor concept. The system studies being at the preconceptual level, the development of simulation tools is a key point to support design, operation and safety studies. Due to molten salt reactor (MSR) specificities, in particular the use of a circulating fuel, the stiff coupling between neutronics and thermal-hydraulics requires dedicated calculation codes to simulate the multi-physic phenomena and thus to support the studies mentioned above.

The objective of this work is to perform systemic study of alternative versions of the MSFR, focusing on small modular designs. These studies should emphasize possible cliff effects, safety aspects or design optimisations. To begin, the first parameter to analyse is the influence of the size of the fuel circuit at different levels of power. To do so, this work is based on coupled neutronics thermal-hydraulics associated with various constraints, such as chemistry during the enrichment adjustment process.

In order to use high fidelity component modelling from Framatome, the TFM-OpenFOAM code developed at CNRS has been adapted in the StarCCM+ code. The two simulation codes provide a high-fidelity Computational Fluid Dynamic (CFD) modelling together with the TFM neutronics model based on a fission matrices approach for neutron kinetics. The latter consists in generating a stochastic code fission matrices plus a time matrix in order to combine accuracy and a reduced computational cost.

The studies led by CNRS use OpenFOAM for the CFD thermal-hydraulic calculations, a well- adapted open-source code that has been modified to include the neutron kinetic. This code can perform various calculations from steady state to normal and accidental transients such as load following, reactivity insertion and over-cooling.

As mentioned above, the TFM-STAR code presented in this conference has been developed in collaboration between CNRS and Framatome to use the industrial CFD code StarCCM+ developed by Siemens. The implementation has been validated using a code-to-code comparison with TFM-OpenFOAM. Its use will bring some useful alternative features not included in OpenFOAM. For instance, it has computer-aided design (CAD) and meshing features but it also allows more easily to add components or other physic phenomena. Finally, the optimisation process and preliminary results will also be presented for a small modular version of the MSFR.

Application of PCM Model Validation on Isotopic Prediction and Uncertainty Reduction

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Abstract. This work develops a method, denoted as Physics-guided Coverage Mapping (PCM) to support model validation in designes of advanced reactors. Model validation is required by the regulatory bodies to approve the use of computer models to simulate system conditions over the wide range of operational conditions, both during normal and off-normal conditions, i.e., transient and accident scenarios. The goal of model validation is to develop confidence in the model predictions for the application, under design stage, via a concerted use of analysis results and measurement from scaled-down experiments, designed to replicate the key physical phenomena that occur in the application. The validation process combining the analysis results and measurements is intended to improve the predictions of application responses of interest, implying a reduction in the predictiion uncertainty, as compared to its prior value which is propagated and quantified through the simulation only. A crucial challenge in the isotopic validation of advanced reactors is that this quantified prediction uncertainty is unreasonablely high by simply propoagting the nuclear data uncertainties throughout the neutronics simulation. This is because the advanced reactors usually have different fuel types from the conventionals, e.g. molten salt reactors (MSRs) use liquid fuel, Accident Tolerance Fuels (ATF) use different fuel and/or claddings materials, all of which may cause difficulty in setting safety margins in fuel transportation, safeguard accounting, etc. The safety analysis of the advanced fuels requires accurate prediction on the fuel composition, such as activity, masses, or concentrations of isotopics, during and at the end of the irradiation based on the data from conventional fuel concepts. PCM is employed under this circumstance to support the safety and performance evaluation of the advanced fuels by predicting isotope concentrations and the associated uncertainties across the burnup based on a few measurements of irradiated conventional fuel. PCM methodology proposes an information theory-based approach to design mathematical mapping kernels that are capable of transferring biases and their uncertainties directly from the predictors to the application responses in a manner that can be rigorously defended. It precludes the need for sensitivity coefficients and only requires forward model executions, and can be applied using non-informative priors for the sources of uncertainties. Focusing specifically on the isotopic prediction, PCM constructs a mapping kernel, in the form of a joint probability density function (PDF), between the predictor, a few isotopic concentrations at certain burnup that can be measured (e.g., at end of cycle), and the application response, isotopic concentrations across burnup, based on the simulation results, and predicts the response with uncertainty evaluation by mapping the measurements of the predictors. The demonstrative study employs PCM to predict isotopic concentrations of a representative PWR assembly across burnup using a few isotopic data measured at EOC. Results show 70% to 95% reduction in uncertainty of isotopic concentrations across burnup predicted by PCM comparing to the prior uncertainty when all sources of uncertainties, including cross-section data, geometry, enrichment, fission yields, etc., are propagated throughout simulation.

Design and optimisation of a breeder MSFR using U/Pu cycle

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Abstract. The current fleet of nuclear reactors provides affordable, abundant and low-carbon electricity. In the meantime, the technology in operation (mainly light-water reactors) faces several challenges. First, it makes a suboptimal use of the natural resources by mostly relying on the 0.7% of 235U present in uranium ores. Second, it produces highly radioactive long-lived matters (minor actinides) that it cannot easily dispose of. It can hardy perform more than a monorecyling for plutonium, leading to an open fuel cycle. Third, the accumulation of strict safety measures that followed Fukushima accident leads to complex and so expensive systems for water-cooled reactors. This paper describes the design of a reactor that could tackle all aforementioned issues: a molten salt fast reactor (MSFR) using U/Pu cycle in chloride salts.

Molten salt reactors (MSR) are one type of reactors among the six selected at the international level by the Generation 4 International Forum to focus studies on. It has the unique feature of a liquid fuel that can also be the coolant, offering several advantages (e.g. excellent intrinsic safety) and possibilities (e.g. online-reprocessing). Since 2008, the reference for MSRs is the MSFR concept initially developed at CNRS (LPSC, Grenoble, France). It has been studied and optimized for 15 years as a 3GWth breeder using the Th/U cycle in fluoride salts, and shows very good performances. However, it might not be the most optimal one to reuse existing matters. The worldwide use of U/Pu cycle led to the accumulation of depleted uranium, and spent nuclear fuels containing transuranic elements (TRUs). Said TRUs, with the exception of plutonium, are currently considered as wastes even though they contain fissile matters. They have a low solubility in fluoride salts while chloride salts can accommodate for large quantities of them, leading to the idea of using a MSFR based on chloride salts, object of this work. Moreover, it can use available depleted uranium as the fertile matter required for the reactor to breed.

The design of a reactor involves many different tasks. Some of them are considered here, corresponding to the first pre-conceptual steps of the system.
First, the changes of solvent and fuels require significant adjustments of the design: the one of the MSFR of reference cannot be directly used. Heat extraction requirements and safety considerations have to be evaluated. Then, elements that are soluble in lithium fluoride may precipitate in chloride salts and reciprocally, so thermodynamical computations to obtain the chemical form of all elements have to be performed. The scheme of the reprocessing dedicated to chloride salts needs to be defined afterwards. Finally, the consequences of the deployment of such reactor on the available resources should be assessed; feedback from scenarios of deployment could be considered to enhance the design.

This paper will first discuss on the optimisation of the reactor from a thermo-hydraulic and neutronic point of view, including considerations on safety. It will continue with the definition of the fuel treatment unit, to finish with preliminary studies on the deployment capabilities of such reactors.

Nuclear data uncertainty quantification in Molten Salt Fast Reactors

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Abstract. Due to its unique features with respect to other Gen-IV designs, the deployment of the Molten Salt Fast Reactor requires new experiments, calculation tools, safety and construction standards.

Among its peculiarities, this kind of reactor is featured by the adoption of some uncommon nuclides, like F19, Li7, U233 and Th232, which constitutes the circulating fuel salt. Due to their importance, the assessment of the impact of the uncertainties in their raw nuclear data on the macroscopic parameters of the core, e.g., the effective multiplication constant, is of paramount importance for both design and safety aspects.

The aim of this work is to employ computationally efficient techniques to propagate the uncertainty from the raw nuclear data to some relevant neutronic quantities, like keff, βeff and the breeding ratio, using the Monte Carlo Serpent 2 code.

First, the legacy Generalised Perturbation Theory (GPT), available in Serpent, will be employed to perform a first-order sensitivity study and uncertainty propagation, in order to select the nuclides in the core which contribute the most to the overall uncertainties in the output responses. Both integral parameters like the effective lifetime and local quantities like the collapsed and homogenised cross sections will be considered in the study.

For these top contributors, the brute-force Total Monte Carlo (TMC) approach will be used to estimate their statistical distribution, which then will be used as a reference. These distributions and their variance will be then compared to other techniques commonly employed in uncertainty propagation, with the objective of assessing their accuracy and computational performances.

Then, the eXtended Generalised Perturbation Theory (XGPT), a reduced-order TMC approach recently implemented in Serpent, will be applied to these nuclides in order to construct surrogate statistical distributions of the output responses, to verify if its accuracy is adequate to convey the most important features of the reference TMC output.

Finally, the same calculations will be run using non-intrusive techniques, which would allow to use any code without further modifications. Among these methods, we will focus on the fast TMC (fTMC), on the GRS method and on the Unscented Transform (UT). For each of these methods, suitable perturbed, random nuclear data files will be generated using the open-source SANDY code.

The first approach, fTMC, allows to estimate the variance of the output responses of interest thanks to a reduction of the number of neutron histories in each simulation, while the GRS requires to run two sets of simulations, each set featured by an identical random seed, in order to estimate the output variance from the two batches. Finally, the UT method allows to approximate the response variances by means of an approximation in the original input statistical distribution.

Parametric Study of Two-Zone Breed and Burn Molten Chloride Fast Reactor

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Abstract. The Molten Chloride Fast Reactor (MCFR) was selected as one of the six advanced Generation IV nuclear reactor by the Generation IV International Forum. MCFR's use a nuclear fuel dissolved into a molten chloride salt. The salt is used both as the fuel carrier and coolant. The low vapor pressure and high thermal capacity of molten salts allow for operation under atmospheric pressure. Having a liquid fuel removes the integrity issues related to solid fuels and allows for the homogenization of the species in the fluid. By operating with a fast neutron spectrum, the fission probability of many actinides as well as the average neutrons produced per fission increase. Using a chloride salt results in better neutron economy compared to fluorides and was used in this investigation. Using the breed and burn (B&B) mode of the fuel cycle utilizes the neutron leakage from the core by implementing a blanket to convert a fertile material into fissile. This alleviates the need for waste reprocessing since the bred fuel covers the losses of the waste fuel. Removing the reprocessing step greatly reduces the cost of operation for the MSCR. Using chloride requires a large reactor to minimize neutron leakage. A breeding blanket will also minimize the required size by using the leaked neutrons to generate fuel. In this study, the MATLAB based EQL0D v3 procedure coupled to Serpent 2 code was used to simulate operation of the B&BMCFR. The EQL0D procedure is a dedicated tool for MSR fuel cycle simulation, which allows for continuous or step-wise treatment of the salt composition. There are three degrees of freedom that can be adjusted in the selected reactor design, fuel volume, blanket volume, and the rate of salt refilling and removal from the core and blanket. A parametric study was performed to find the most efficient geometrical design of the reactor by balancing the total salt volume with the achievable burn up of the nuclear fuel while criticality is maintained. The effect of the fuel removal rate from the core on a simple infinite reactor was investigated first to understand the relationship between reactivity and burnup. Later, the finite reactor with a blanket was analyzed. The rate had an effect on the overall burn up inside the reactor and on the efficiency of breeding in the blanket. At too slow a rate the breeding material in the blanked began to fission the generated fissile material, leading to a loss of fuel and neutrons. The balance was thus between maximal burn up and an optimal breeding ratio. Having an ideal removal rate then allowed for the investigation of how the reactor size and the blanket size affect the neutron population, burn up and breeding efficiencies of the reactor. A larger breeding blanket will generate more fuel but resulted in a longer retention time of material, resulting in the consumption of the bread fissile material. A large reactor is more capable of higher burn up and of power production but at a financial cost.

Monte Carlo Simulation-based efficient exploration of the model of a Molten Salt Fast Reactor for the identification of abnormal operating conditions

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Abstract. The deployment of the Gen-IV Molten Salt Fast Reactor (MSFRs) requires the demonstration of its enhanced safety features with respect to other reactor concepts. To this aim, a power plant simulator including the primary system, the secondary system and the balance-of-plant has been developed in the framework of the SAMOFAR EU project. This simulator allows to describe the plant (transient) response to a variety of (normal and abnormal) operating conditions.

The aim of this work is to propose a Monte Carlo simulation-based method to map the system behaviour with respect to uncertainties and variations in physical and operational parameters and in components' states, by means of an efficient (adaptive) exploration of the MSFR power plant state space.

The proposed approach comprises the following steps. First, a set of physical (input) parameters that are found to strongly influence the behaviour of the plant simulator (e.g., the fuel and intermediate salt mass flow rates) is selected, together with their ranges of variation. Second, several possible combinations of physical parameters values are generated by (adaptive) Monte Carlo sampling and the corresponding time-varying (transient) behaviour of the MSFR is simulated. Finally, the time evolution of some relevant (output) plant parameters (e.g., reactor thermal power, fuel and intermediate molten salt temperatures, …) are analysed in detail to: (i) identify normal and abnormal system (output) configurations; (ii) retrieve those combinations of the reactor (input) physical parameters that are capable of leading the system into abnormal operation states.

The final aim will be to exploit such maps to develop (prompt, on-line) incident detection methods for safer MSFR plant operation.

Modeling flow blockage accident in graphite-moderated MSRs

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Abstract. Xenon 135 evolution affects the dynamic behavior of thermal nuclear systems due to its large absorption cross-section. In solid fuel reactors, the produced Xenon 135 has a limited mobility. This allows for a simplified, local modeling of its concentration evolution in the fuel. In liquid fuel reactors, Xenon migration requires models to account for additional phenomena.

The present work describes the development of a reduced order model, suitable for the analysis of Xenon behavior in graphite-moderated MSRs, also accounting for the Xenon transport within the salt, as well as Xenon migration into the graphite pores.

This work analyses a single channel of a MSR adopting a multiregion CFD approach within the flowing liquid salt and the porous graphite structure, exploiting the thermal/mass transfer analogy, coupled to Monte Carlo neutronics. The numerical model is used to build a reduced order model suitable to reconstruct the Xenon concentration distribution in salt and graphite.

Study of the impact of compressibility modelling during reactivity insertion transient in Molten Salt Fast Reactor

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Abstract. The MSFR (Molten Salt Fast Reactor) is a project concept of 3 GW th breeder molten salt reactor. In this kind of molten salt reactors, the fissile and fertile nuclei are dissolved in a circulating salt that acts both as fuel and as coolant. Here, coolant doesn't mean cool the fuel but transport the heat produced by the neutronic power from the fissile zone to the power conversion loops. Two versions of this concept are studied: a fluoride fuel salt with the Th/U cycle and a chloride fuel salt with the U/Pu cycle. In the fluoride reference concept, the global temperature reactivity feedback is around -8pcm/K. This strong negative reactivity feedback (for a fast spectrum reactor) takes into account two effects: Doppler Effect and coolant density effect, each one being approximately half of the total reactivity feedback.

Contrary to the solid fuel in FNR (Fast Neutron Reactor), in the MSFR, the fuel is nearly in its most compact geometry. That is why a large-scale compaction, which is one of the source of most of the severe accidents in FNR, cannot occur in this type of reactor. Conducting studies of the reactor behavior in the case of postulated severe transients in parallel with the risk analyses (which aim at identifying the initiating events) is very important in order to make some efficient progresses in the design of the system by integrating safety at an early stage of the design process and also to convince the safety authorities of the safety level of innovative reactor design such as molten salt reactors. In the case of the MSFR concept, no control or shutdown rods are foreseen, which requires a good justification of the behavior of the core without such a device. Thus in connection with the safety function "control of reactivity", some bounding postulated events are investigated in this work, no matter their likelihood, in order to study the physical phenomena entering into play. In order to perform these studies, a calculation plateform, MIRRACl, has been developped. It consists in two independant calculation tools: MOSAICS, including an incompressible flow calculation tool and COCCINELLE, a compressible flow calculation tool.

In the case of extreme reactivity insertion, at the beginning of the transient, the salt cannot freely expand and go out of the critical zone. The pressure increases and the density feedback effect is slower to act if the compressibility is taken into account. A criterion has been developped in order to shift from MOSAICS to COCCINELLE. Some sensitivity studies are performed to assess the impact of the time when this criterion is reached on the behaviour of the core. This compressible behaviour of the fuel salt leads to extreme transients and a goal of this work is to identify what plant conditions (such as the power of the core) and reactivity ramps can lead to compressible transient during a reactivity insertion in order to prevent them if their consequences are not easily manageable by design provisions.

Probabilistic safety margin evaluation of MSFRs design basis accidental scenarios

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Abstract. This work has been developed during a project for the course "Artificial intelligence and advanced simulation for and safety, reliability and maintenance of energy systems" held by Professor Francesco Di Maio at Politecnico di Milano (AY 2021-22). The objective of this analysis is to show, through order statistics, one of the possible ways to extract point estimators and confidence intervals of key parameters in MSFRs accidental scenarios. The starting point is a deterministic code developed by Politecnico di Milano using Dymola software. This model can be directly used as the data source, but it would take too much computational effort to perform the required number of runs. Therefore, the next step is to use Artificial Neural Networks to condense the system behavior through a univocal mapping between representative input-output relations and speed up the simulations by few orders of magnitude. Four main scenarios are selected to undergo this process, for which four individual ANNs are properly trained and tested. The first one is the accidental insertion of either positive or negative reactivity due to the failure of the chemical reprocessing unit, while the other three are transients involving respectively the pump of the primary loop, the pump of the intermediate loop and the compressor of the turbine in the power conversion loop. To assess the potential damage of these accidental transients, the choice is to focus on representative temperature values throughout the whole plant. Different failure modes are selected from literature in order to choose the proper temperature nodes and the respective safety limits. Liquid fuel in the primary loop is affected by either solidification or dissolution of the constituent fluoride salts, so that inlet and outlet core temperature are chosen as representative. The same failure modes, coupled with different safety limits, characterize the fluoroborate salt circulating in the intermediate loop. One failure mode is also selected to cover the turbine operating in the power conversion loop, which must be protected from thermo-mechanical stresses, in particular blade creep and thermal shock. The freeze valve drain, which should otherwise be considered a failsafe mechanism, is added to the set and an activation limit is given in the form of specific heat received during the transients. Once the problem setting is concluded, a proper number of runs for each scenario are simulated using the deterministic code and fed to the respective ANN for training and testing. A Monte Carlo code is then used to sample failure magnitudes following both a uniform distribution as a baseline and a more realistic gaussian distribution, with bounds and moments chosen through expert judgment. Every time the kernel samples an input value, the proper ANN is called so that the total runtime is greatly reduced: from several seconds to run the deterministic code just once, to less than a minute for ten thousand Monte Carlo simulations. Thanks to this it is possible to achieve a great precision in confidence interval estimation due to the possibility of collecting many code realizations in a small timeframe while avoiding the burden of a full output distribution evaluation.

Temperature coefficients of reactivity in Molten Salt Reactor Experiment calculated with direct method using Serpent 2 Monte Carlo code

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Abstract. Full core Monte Carlo calculations of the Molten Salt Reactor Experiment (MSRE) are performed using Serpent 2 and the influence of different temperatures on the effective multiplication factor are investigated around a global temperature of 900 K. For simplicity, no spatial dependence of the temperatures within the different materials are taken into account, which is considered valid for zero power operation. Only the case of U-235 fuel is considered. An input file from literature was adapted such that the vessel has, in this simplified model, a closed shell and its effect of expansion can be taken into account. A python function was written which generates an input file for Serpent 2 as a function of the different temperatures. The expansion of all materials is considered individually, as well as the Doppler effect and the thermal scattering inside the graphite moderator. The direct method was used by running multiple calculations. Changing one temperature at a time gives the individual coefficients, and changing all temperatures gives the total temperature coefficient.

The vessel temperature coefficient of reactivity is positive, since an expansion of the vessel will allow more fuel to enter the reactor, but this happens delayed in time after reactivity insertion. The graphite temperature coefficient describing thermal scattering causes the neutrons in the thermal energy regime to become faster for higher graphite temperature. This causes a reduction in reactivity, which is in contrast to what can be found, according to literature, in some single region Molten Salt Breeder Reactor designs utilizing the Thorium fuel cycle.

The calculated coefficients of reactivity in the MSRE are compared to the experimental values found in literature and good agreement was found for both the fuel component (Doppler effect plus thermal expansion) and the total coefficient (sum of all contributions). The fuel component is calculated to be -8.7 +/- 0.5 pcm/K and the total coefficient to be -14.1 +/- 0.4 pcm/K. This compares well with the measured values from Oak Ridge National Laboratory, which gave for the fuel -8.8 +/- 4.1 pcm/K and for the total coefficient -13.14 +/- 0.36 pcm/K.

Analysis of the source term in circulating fuel reactors: preliminary results of the SAMOSAFER Benchmark

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Abstract. Molten Salt Fast Reactors (MSFRs) are nuclear reactors employing a circulating fuel salt, which simultaneously acts as coolant. This unique feature has recently drawn the interest of the nuclear scientific community and MSFR has been identified as the reference circulating-fuel reactor in the frame of Generation IV International Forum. Its design has been developed in the context of EVOL and SAMOFAR European projects and is currently under study in SAMOSAFER project. The main advantage over solid-fuelled reactors is the possibility of continuous reprocessing of the fuel salt during reactor operation, which allows removing fission products and controlling the eutectic composition and reactivity. These tasks are fundamental to preserve the physico-chemical properties of the fuel and so to ensure safe operation of the reactor. However, the continuous reprocessing conceived in the design of MSFR implies several technological, safety and design challenges, e.g., the treatment of highly radioactive streams. In this view, an accurate evaluation of the radioactive source term in the fuel is needed for the design of the reprocessing units. The usual simulation tools for depletion calculations adopted by the nuclear scientific community are tailored for solid-fuelled reactors and cannot account for the mass exchange processes that characterize a circulating-fuel reactor. This work aims at the development of new burnup simulation tools for the source term evaluation and it is based on an extension of Serpent Monte Carlo burnup code suitable for the modeling of the mass exchange processes occurring in MSFR. In the framework of this work, reactivity control and eutectic control algorithms have been implemented in the latest release of Serpent, namely the 2.1.32 version, together with a new batch algorithm for thorium mass control. This new extended tool has since been verified by means of a comparison with analytical solutions of Bateman equations.

Enabling techniques within OpenMC for dynamic models of molten salt reactors

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Abstract. We present how the flexibility of OpenMC has greatly improved our ability to simulate and design molten salt breeder reactors. We will present our findings from testing different CAD model import tool chains as well as integration of dynamic constructive solid geometry (CSG) in OpenMC for reactivity control throughout multi year burnup. We show how nuclide addition and refueling operations as well as online removal of fission products can easily be integrated into the OpenMC burnup depletion scheme simulations, and how scripting of dynamic CSG made it possible to optimize the reactor core dimensions. This shows why OpenMC is well suited for the class of molten salt reactors.

Thermochemical modelling of LiF-CsF-ThF mixtures for MSFR application

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Abstract. The molten salt reactor (MSR) is an innovative nuclear reactor concept selected by the Generation IV International Forum (GIF) for being particularly promising in terms of sustainability, non-proliferation, resource saving, safety and waste management. European projects are strongly focused on this technology, leading to recent international cooperation between private and public entities for the development of the Molten Salt Fast Reactor (MSFR), a 3000 MWth reactor concept in which a mixture of molten halides serves as both nuclear fuel and coolant.

In order to achieve a proper performance, the composition of the MSFR fuel salt is subjected to a set of requirements on conventional aspects, such as physical and chemical properties or interaction with structural materials, and other constraints specific to the nuclear industry such as neutronics properties and reactor safety issues. The research for the most suitable mixture of molten fluorides for MSFR is based on a systematic procedure involving both experimental and computational approaches. The thermodynamic and thermophysical properties must be evaluated considering the accuracy of the adopted methods, to provide reliable results in compliance with industry requirements.

The aim of the present work is to emphasize the feasibility of fluorides mixtures as the working fluid for the MSFR. To achieve this goal, a systematic approach to evaluate the MSFR fuel salt is described, highlighting the reasons why this type of halide is suggested as the most suitable choice for this reactor concept. The considered system includes actinides and fission products, both in fluoride form, as well as lithium fluoride, the solvent selected for the MSFR. Numerical studies are performed using the equilibrium thermodynamics software Termochimica, were different of fluoride mixtures are preliminarily studied, in particular for LiF-CsF-ThF mixtures, analyzing the effects of variations in stoichiometry and temperature.

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Radiolytic production of fluorine gas from MSR relevant fluoride salts

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Abstract. The production of fluorine gas from the gamma radiolysis of fluoride salts is an important safety and operational aspect to be accounted for in fluoride salt based molten salt reactor (MSR) designs. These aspects particularly relate to safe storage practices of the spent 'frozen' salt and operational requirements for auxiliary chemical waste and re-processing systems. The Nuclear Research & Consultancy Group (NRG) in Petten (Netherlands) has set out with its partners to investigate radiolytic fluorine production from the fluoride salts, BeF2, LiF, FLiBe-UF4, UF4 and ThF4, under the NRG experimental programme denoted as SAGA-01. Radiolytic fluorine production from a given salt is reported as the salt G-value and measured as number of fluorine molecules produced per 100 eV of energy absorbed (molecules F2/100 eV). To the knowledge of the authors, there are no published G-values of these salts in current literature, with the only work of similar nature (but different salt matrices) being that of Oak Ridge National Laboratories (ORNL, USA) in the period 1965 to 1995. In the NRG SAGA-01 experiment, the fluoride salts were irradiated within an experimental rig which allowed for spent fuel from the High Flux Reactor (HFR) in Petten to act as a gamma source. The SAGA-01 irradiation was conducted for just over 41 days with total absorbed gamma doses in the range of ~ 50 – 195 MGy (depending on salt sample). By measuring the fluorine gas pressure within the salt capsules during irradiation, it was possible to quantify the radiolytic fluorine production of the salt samples - with the exception of UF4. The maximum G-values of the salts were found to be G(BeF2) ~ 0.0076, G(LiF) ~ 0.0034, G(FLiBe-UF4) ~ 0.0042 and G(ThF4) ~ 0.018.

Development of In-Pile Electrochemical Corrosion Measurements and Waste Management of Molten Fluoride Salts

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Abstract. The renewed interest in recent years in using nuclear energy as a low-carbon energy source has brought with it a resurgence of research efforts into the development of commercial molten salt reactors by various public and private parties around the world. NRG, in collaboration with national and international partners, aims to contribute to the understanding of the behavior and properties of molten salt fuels as well as to the development of MSR-related technologies and operational experience.

In the SALIENT (SALt Irradiation experimENT) experiment series, we are studying the behavior of molten fuel salts in contact with different materials such as graphite and metallic alloys, both in pile and in out-of-pile lab-scale experiments. In the MSR Waste project we are investigating potential pathways for the disposal of (irradiated) spent fuel salt. In this contribution, we will discuss the design of the irradiation facilities and some of the (preliminary) results of the abovementioned research projects.

In 2017, the first molten salt irradiation experiment since the 1960s was started at the high-flux reactor (HFR) at NRG. In the SALIENT-01 experiment, several (open) graphite capsules filled with samples of fluoride fuel salt were irradiated. After 540 full-power days of irradiation, the experiment was removed from the reactor in 2019, allowed to cool down and subsequently subjected to post-irradiation examination (PIE). During PIE we performed analysis of the fission gases, gamma-spectroscopy scans of the experiments and in-cell microscopy of slices of the salt and capsules.

While past irradiation experiments focused mainly on the interaction between molten salts and graphite, the focus of the SALIENT-03 experiment under preparation is to investigate molten salt corrosion of (sealed) Hastelloy-N capsules. The aim of this experiment is to study the fission-product distribution and corrosion behaviour during PIE by means of head-space gas analysis, Knudsen-cell analysis, gamma-spectroscopy and in-cell microscopy of the salt and the capsule material. Additionally, one of the capsules is outfitted with a pressure transducer and a set of electrodes for carrying out on-line experiments and data gathering during irradiation.

These research efforts are supported by lab-scale experiments of molten salt electrochemistry and infiltration tests of graphite samples submerged in molten salt.

Spent fuel samples of halide salts are not currently accepted as a suitable waste form for storage by the relevant (Dutch) authorities due to the possibility of halogen gas formation caused by gamma-radiolysis. As a result, it is necessary to develop a route for transforming the spent halide fuel salt samples into acceptable, stable waste forms such as oxides. To this end, we are currently investigating several potential processing routes such as aqueous processing, vitrification or stripping of fluoride at high temperatures with fluoride getters such as SiO_2 or B_2O_3.

Numerical methodology for the analysis molten salt natural circulation systems

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Abstract. In the year 2002, as an international effort for the development of nuclear technology, the Generation IV International Forum (GIF)selected a series of new nuclear reactor technologies which were believed to represent the future of nuclear energy. One of the main areas of improvement for this new generation of reactors designs lies within the safety features, often trying to recur to passive phenomena to ensure a proper compliance with the safety functions. The Molten Salt Reactors (MSR) is no exception to this objective, and designs involving natural circulation are being considered, for example, for the Decay Heat Removal System, but the behavior of natural circulation using molten salt as working fluid is yet to be more thoroughly analyzed. This work is focused in the development of a comprehensive numerical methodology for the study of these types of systems for its application in MSR design. This methodology is devised to analyze and evaluate different natural configurations regarding its feasibility for the desired applications, focusing mainly in its heat removal capabilities. To achieve this type of analysis a description of the dynamic behavior of the system is required, followed by a stability analysis, with a special consideration in the detection of bifurcation phenomena. Moreover, due to the high amount of configurations to be tested in a design stage, an instance for the reduction of the associated computational cost is needed, for which the use of Reduced Order Models (ROM) has been applied. The numerical toolkit to implement this methodology is based in the OpenFOAM software for Computational Fluid Dynamics (CFD) simulations, coupled together with MATLAB-Python routines to extend its capability for the desired analysis. The different steps of the implementation have been tested against a numerical benchmark of a differentially heated cavity, with good agreement with results from the literature, both in terms of the thermal-hydraulic behavior and stability analysis, as well as the application of ROM for the reduction of computational cost. Then for a preliminary assessment of the performance of the tool a simple 2D case of a simple natural circulation configuration known as Rayleigh-Bénard convection has been used, which results from an enclosure heated and cooled from the bottom and top surfaces respectively. The dynamic states of this system have been analyzed within a range of parameters, both geometric and thermal-hydraulic. Steady-state and oscillating solutions has been observed, as well as hysteresis phenomenon in the vicinity of certain bifurcation points. A bifurcation diagram is produced, showing the transition between the different solutions. The numerical tool has shown a good performance both for the description of the thermal-hydraulic system as well as for the stability analysis. The application of the ROM implementation allows reducing the processing time to describe the different dynamics behaviors of the system but a systematic application for the detection of bifurcation points is still under development. The amount of different dynamic states for the simplified case analyzed allows highlighting the need of this type of robust and systematic methodology.

Preliminary Experimental Campaign for the Coupled DYNASTY-eDYNASTY Facility

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Abstract. In the development and design of Gen-IV nuclear reactors, the study of natural circulation is significant because it can provide a passive runaway system to remove the decay heat during shutdown operations. Natural circulation is of primary focus in designing the Molten Salt Fast Reactor (MSFR), a Gen-IV reactor type characterized by an internally distributed heat source, which plays a relevant role in the decay heat removal system (DHRS) of the reactor. The DHRS of the MSFR requires a secondary intermediate loop as a safety barrier between the reactor and the environment, which should also operate in natural circulation.

Studying natural circulation on a coupled system with a homogeneously distributed heat source is challenging, both from the modelling and experimental point of view. In particular, the latter requires a purpose-built facility with two loops that can both operate in natural circulation with a distributed heat source. To this aim, the DYNASTY (DYnamics of NAtural circulation for molten SalT internallY heated) and the eDYNASTY loops were built and coupled in the energy labs of Politecnico di Milano. In the facility, DYNASTY acts as the primary loop of the MSFR by using an externally distributed heat source, whereas eDYNASTY acts as the secondary loop of the MSFR, having a localized heat source represented by the heat exchanger coupling.

This work shows the first preliminary experimental data acquired from the coupled DYNASTY and eDYNASTY loops using water as a working fluid, considering both heating and cooling transients (with the heat source turned off). This work considers different heating configurations according to the DYNASTY leg used as the heat source. These preliminary experiments keep the cooling fan switched off to analyze the coupled facility heat losses and the heat exchanger coupling effectiveness. The results collected are the fluid temperatures and the mass flow rate.

These first experimental results show the transient evolution of the mass flow rate and the temperature starting from zero power conditions up to steady-state conditions when the heaters turn off to analyze the facility behavior during the cooling transient. The coupled facility results show similarities with the corresponding experiments of the uncoupled DYNASTY results in the heating transient observing lower maximum DYNASTY temperature values. The cooling transient reports the main differences for the vertical heater configuration, which shows oscillations in the mass flow with flow inversion.