# Summary

The purpose of this thesis is to discuss the use of liquid metals in next-generation nuclear fission and fusion reactors. Liquid metals can be employed as coolant (fission machines) or as coolant/breeder/carrier for the tritium exploitation (in future fusion rectors), since they present good thermo-physical and nuclear properties with respect to water. Due to the complexity of the systems where liquid metals have to be used, suitable multi-physics tools must be developed to correctly retrieve the inherent physical aspects of their employment. Several European initiatives are today supporting the research and development of this tools, as for instance, the EUROfusion consortium and the PASCAL project (where the FALCON consortium is heavily involved). Thus, the work here presented aims to verify, test and develop tools and new models for the multi-physics assessment of advanced nuclear system based on liquid metals. For this reason, two areas of activity are discussed: modelling of Liquid Metal-Cooled Reactors for future Generation IV reactors within the context of reactor physics and thermal-hydraulics assessments, and modelling of radioisotope transport in liquid metals in fusion systems.

The first part of this thesis regards the use of liquid metals in future fission nuclear reactors. The activities have been carried on with the scope to pursue the verification activities of the FRENETIC code, a multi-physics tool that has been being developed in the last years at Politecnico di Torino. Currently, the FALCON consortium and the PASCAL project are supporting the design of the ALFRED reactor in order to exploit Lead Fast Reactors technology. As a consequence, the benchmark of FRENETIC has been performed on the ALFRED core, analysing both steady state and transient coupled scenarios. To accomplish this, a temperature-dependent cross section library has been built using the Monte Carlo code Serpent-2. As second verification activities for the neutronic module, FRENETIC has been benchmarked against the SIMMER code using the same set cross sections calculated by Serpent-2.

With the aim to broaden the application domain of FRENETIC, a methodology to generate the data to simulate also secondary contributions to the total thermal power as photon heat deposition and the KERMA of neutrons has been developed. The generation of photon data (i.e, the attenuation coefficients, the deposited energy per particles, the cross section of $(n, \gamma)$ interactions) has been carried out

to retrieve also the thermal power due to KERMA of neutrons and photons by a high-level detailed Serpent-2 model of the EBR-2 Sodium-cooled Fast Reactor. A previous benchmark coordinated by the IAEA on the EBR-2 reactor (SHRT-45R) has been chosen, to test also several strategies of spatial homogenisation in Serpent-2 due to the high complexity of the core configuration.

As final activity in the framework of the European project PASCAL, a preliminary design of a design-oriented-code, EFIALTE, for the deformed fuel bundle in Lead Fast Reactors has been assessed. EFIALTE is part of the suite of design-oriented-code (TEMIDE, TIFONE, ANTEO+), whose development is currently coordinated by ENEA Bologna. Its application encompasses the End-Of-Life condition and/or the accidental scenario of a fuel rod displacement. Specifically, the core solver of this code has been derived and implemented, solving the mass and momentum conservation equations - including the transverse momentum equation, accounting for possibly different pressures among sub-channels located at a given axial location.

Concerning the fusion-related activities, the design of an extractor of tritium from the PbLi by suitable numerical models to assess the tritium permeation has been carried out. The PbLi is the liquid metal breeder which is foreseen in one of the concepts of the WCLL Breeding Blanket for the future EU DEMO reactor. Several technologies are being investigated, and one of the promising solutions is based on Permeator Against Vacuum (PAV) technology. The first part of the work consists in the development of a new model for the evaluation of the permeated flux from the carrier (the PbLi) by means of an extractor where a pressure drop is established across a metallic membrane. Two regimes of permeation have been focused: the Surface-Limited, when the permeation is strongly conditioned by surface effects of the membrane, as the recombination and dissociation. The other one is called Diffusion-Limited and it is established when the the surface effects are faster than the diffusion in the bulk of membrane. The model has been developed starting from previous works and the physics modelling has been extended to the case of liquid-membrane-vacuum treating the transport from the liquid metal bulk towards the wet side of the membrane as the source of permeation.

The above-mentioned model has been used to perform efficiency analyses on the PAV mock-up that has been designed starting from the constraints of geometry prescribed in TRIEX-II facility (ENEA Brasimone). An experimental campaign was foreseen to test the technology with hydrogen. Unfortunately, due to the outbreak of COVID-19 pandemic in the 2020, the tests have been postponed beyond the ending of this PhD. The design of the mock-up has been conducted by a preliminary sizing of the vessel and holed plate where the pipes (the membrane) are located. The assessment have been performed with analytical formulas for thin shell and plates, and then verified with a set of FEM analyses considering the operational and accidental conditions. A set of CFD analyses have been assessed to study the effects of the mass flow repartition (i.e, the turbulence level in each single pipe) on the extraction efficiency, as well as the surface conditions.

Finally, the application of the developed model has been exploited on the extractor up to EU DEMO scale. The Tritium Extraction and Removal System has been sized to achieve the required extraction efficiency foreseen in DEMO with a methodology to design the membrane, the vessel encumbrance and the number of pipes has been developed. The sizing have been carried on by changing the operative conditions, in order to find the best solution for the permeation.

Results for the fission part have shown good agreement for the activity on the FRENETIC code. On the ALFRED reactor, the benchmark between Serpent-2 and the deterministic tool has highlighted an improvement of the accordance ($k_{\text{eff}}$ and thermal power distribution) when the geometry simulated in FRENETIC corresponds to the one of the Monte Carlo simulation. Furthermore, the verification of the neutronic solver of FRENETIC with respect to the SIMMER core has shown good results in terms of neutronic flux solution, showing the good capability of FRENETIC to simulate the neutronic flux with the diffusion theory. Regarding the EBR-2 reactor, the correctness of the methodology for the generation of photon data, as well as the spatial homogenisation optimisation, has been demonstrated. The thermal fission power and the neutron KERMA power have been correctly retrieved. On the contrary, the photon flux was not well reproduced by FRENETIC, and this discrepancy arose from the incapability of Serpent-2 to provide the photons multiplicity production which led to an underestimation of photon flux. Concerning EFIALTE, the solver has been tested with promising results on a simple undeformed test case: the exchange of flow rate is correctly retrieved when a proper driver is provided as boundary condition.

For the fusion-related activities, the new model for the permeation has been compared with another permeation model (purely diffusion-limited), showing great accordance between the evaluation of the extraction efficiency. The model is capable to encompass both surface-limited and diffusion-limited permeation regimes when the respective set of permeation properties are introduced in the model. As a consequence, the evaluation of extraction efficiency of the mock-up based on the PAV technology has been carried out together with its design. The study has also shown the main effects due to the main variables (membrane condition, temperature, pressure of H/T and PbLi mass flow rate) on the permeation efficiency. With this information, the design has been extended to EU DEMO scale, where the operating conditions of the extractor have been selected by means of a methodology developed to be compliant with the prescribed constraints of the design of extraction system.