High-temperature corrosion of ceramic construction materials for Dual Fluid Reactor

Abstract

The primary objective of this work is to analyze the corrosion of silicon carbide, considered one of the main construction materials for the Dual Flow Reactor (DFR). The introduction of the Thesis presents the theoretical background related to the discussed phenomena and the mathematical models used. It describes the reactor technology, summarizes the current theoretical and experimental knowledge on selected aspects of using silicon carbide, and the corrosion caused by liquid metals used as fuel and coolant at high temperatures. To broaden the understanding, alloys and compounds of these metals, such as PbLi tested for fusion applications, as well as TRISO fuel studies, were also considered. These provide additional insights into interactions with fission products. Potential undesired interactions with other construction materials and impurities were also discussed. Additionally, the physicochemical properties of SiC, production methods that might influence reaction outcomes, and the mechanisms and effects of oxidation were introduced, especially concerning the possibility of creating a protective passivation layer.

The next section focuses on the simulations conducted. First, models using Density Functional Theory (DFT) are discussed, outlining the methodology applied, pseudopotentials, and system calibration. The research focused on 3C-SiC, the most resilient and resistant polymorphic form of this material. The scope of the studies includes determining the crystal lattice constant, reconstructions of the crystal surfaces (100, 110, and 111), measuring adsorption energy, and analyzing interactions with lead based on density of states and charge density difference. Furthermore, molecular dynamics simulations were performed to study the interactions of these materials, and additional simulations were conducted for analogous interactions involving silicon oxide. This section presents the methodology, used interatomic potentials, and system calibration. Such calculations enable the study of nanoscale interactions, allowing the dominant corrosion mechanisms to be explored depending on temperature and determining diffusion coefficients. Apart from studying various surfaces, grain boundary interactions, the effect of vacancies, and radiation damage were also investigated.

The subsequent section concerns the preparation for the DFR micro-demonstrator experiment. Based on information about other similar circuits, especially TALL-3D, the specifications of individual parts of the facility and their materials were determined, creating guidelines for experimental preparation. In collaboration with experts from the HITEC Nuclear Equipment Institute, a unit design was developed in accordance with current standards. The system consists of two circuits with liquid lead: the first with heating elements, simulating the fuel cycle, and the second acting as a coolant. This section describes all system components, their functions, measurement, and control apparatus. Necessary operational procedures, required for startup, operation, control, and safety verification methods, were also determined. As the first unit of its kind, it will provide valuable insights, including heat exchange, natural convection, CFD model validation, and long-term corrosion studies, serving to verify the results of mathematical models. The micro-demonstrator is both a prototype and a foundation for creating subsequent, already planned, larger and more advanced experiments, which will better reflect the actual reactor configuration. In the context of further research, a review of various types of equipment was prepared, including magnetohydrodynamic pumps and oxygen pumps, which for various reasons were not used in the current version.