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MSR Fuel Cycle and Thermo-Dynamics Simulations

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The Molten Salt Reactor (MSR) is unique, with respect to other Gen IV concepts as well as current LWRs, in the fact that the liquid fuel comes with a slew of safety-relevant features, which are chemically distinct from those otherwise encountered. These features are often neglected in the scope of neutronics-based investigations into the topic, where more heed is paid to the isotopic composition rather than the elemental or chemical one.

The overall aim of the present work is to investigate the chemical behaviour of an MSR depending on the setup, fuel cycle as well as initial fuel composition. In order to achieve this analysis, EQL0D, a MATLAB based fuel evolution routine, as well as a Gibbs'energy minimization program (GEMS) are employed. While EQL0D uses inputs such as fuel composition, geometry and reactor power in order to produce an isotopic composition, GEMS can be used on this obtained composition in order to make a prediction on the chemical speciation of the salts present in the system. When the speciation is known, more qualified statements on the volatility, miscibility as well as influence of the redox conditions on the system can be made.

In this paper, simplified MSFR-like systems are used for the neutronics simulation in order to generate representative fuel compositions which can be passed on to GEMS. There are a total of four cases, with all combinations of the fertile isotopes Uranium-238 / Thorium-232 as well as chloride-/ fluoride-based carrier salts. For each case, a separate equilibrium composition is generated by EQL0D, which is used as an input for GEMS to perform a speciation on the most important elements of the system. From there, it is possible to add less prevalent elements to the chemical-thermodynamic simulation to make a prediction as to their chemical state, and therefore volatility, or sweep through various conditions such as temperature or redox environment to investigate which elements are primarily at risk of being transformed into a different state that affects their safety-relevant parameters.

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