Thermochemical Modeling of Multi-component Salt Systems for Generation IV Nuclear Reactors

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Abstract

Computer assisted process simulation is a key tool for the development of generation IV molten salt nuclear reactors. In order to select suited salt mixtures and their treatment during operation, it is necessary to have a thorough knowledge of the multicomponent phase diagrams as well as the underlying phase equilibria. A self consistent high quality thermodynamic database including all salts (ThF_4, PuF_3, LiF, BeF_2, CeF_3, ...) is therefore a must.

In the case of ThF_4 base systems, this work has been started in the frame of the French National program (sponsored by CNRS) on molten salt reactors called “Programme Concerté de Recherches sur les Réacteurs à Sels Fondus”. Results will be presented concerning the modelling of the LiF-ThF_4 and LiF-BeF_2 binary systems and LiF-NaF-XF_3 (X=Ce, La and Pu) ternaries. The modified quasichemical model has been used to describe the molten salt, because it allows the introduction of chemical short range order (formation of complexes). Th has three different coordination numbers in the LiF-ThF_4 system depending on the concentration. For low ThF_4 concentrations, Th has a 8-fold coordination in the liquid. For higher contents, the coordination becomes 7 before forming dimer complexes with a nominal composition of $Th_2F_{10}^{2-}$. Liquid BeF_2 has also a complex polymer-like structure which is also present in multicomponent systems. The implications of this complex chemical behaviour for the thermodynamic modelling will be discussed.