

## **Preliminary Phase Diagram Calculations of FLiBe and LiCl–PbCl<sub>2</sub> Molten Salts for Fusion Blanket Applications**

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### **1. Introduction**

D–T fusion reactors require a tritium-breeding blanket to sustain the fuel cycle because tritium is not naturally abundant. Candidate breeder materials include solid ceramics, liquid metals such as PbLi, and molten salts such as FLiBe (2LiF–BeF<sub>2</sub>). PbLi can provide a relatively high tritium breeding ratio (TBR), but its electrical conductivity causes magnetohydrodynamic (MHD) pressure losses in the strong magnetic field of a tokamak. FLiBe largely avoids this issue because of its low electrical conductivity; however, its use is constrained by beryllium toxicity, the potential formation of corrosive HF during tritium extraction, and a TBR that may be marginal for self-sufficiency without a solid neutron multiplier [1,2].

Motivated by these trade-offs, recent studies have reconsidered chloride- and fluoride-based molten salts as alternative breeders, drawing on research on advanced fission reactors, concentrated solar power, and thermal energy storage [1,2]. These systems expand the design space by allowing the neutron-multiplier cation (e.g., Pb or Be) and halide anion (e.g., F or Cl) to be selected in different combinations, with the resulting phase behavior evaluated explicitly through calculated binary phase diagrams.

Building on this literature, this study compares three candidate salts—FLiBe as the reference, LiCl–PbCl<sub>2</sub>, and LiF–PbF<sub>2</sub>—using a common phase-equilibrium framework based on calculated binary phase diagrams. The aim is not to select a final blanket composition, but to identify trade-offs among the candidates and prioritize follow-on experiments.

### **2. Candidate Salts**

FLiBe was selected as the benchmark because extensive property data are available and tritium extraction has been demonstrated. LiCl–PbCl<sub>2</sub> was selected because Pb can contribute to neutron multiplication through (n,2n) reactions while avoiding

Be in the salt. LiF–PbF<sub>2</sub> combines the low parasitic neutron absorption of monoisotopic fluorine (<sup>19</sup>F) with the same Pb-based multiplication pathway. Together, the three systems enable pairwise comparison of anion effects (F vs. Cl) and multiplier-cation effects (Be vs. Pb) relative to FLiBe.

### **3. Methods and Preliminary Results**

#### *3.1 Phase equilibria*

Binary phase diagrams were calculated using the CALPHAD-based Phase Diagram and Equilib modules in FactSage [3]. The MSTDB–TC thermochemical database, loaded as a private database, was used for assessed systems such as LiF–BeF<sub>2</sub> [4]. For Pb-bearing systems not covered by MSTDB–TC, the built-in FTSalt database was used. Where assessed CALPHAD data were unavailable, an ideal-solution estimate based on the melting point and enthalpy of fusion of each pure component was used as a preliminary benchmark for the FactSage calculation.

As an initial benchmark, the LiF–BeF<sub>2</sub> phase diagram was calculated with MSTDB–TC (Fig. 1). The calculated liquidus represents stoichiometric Li<sub>2</sub>BeF<sub>4</sub> at 66.7 mol% LiF as a congruently melting compound near 459 °C, consistent with the electrochemically determined congruent-melting point of 459.1 °C reported for Li<sub>2</sub>BeF<sub>4</sub> [5]. The same measurements place the flanking LiF-rich eutectic at 458.9 °C and 67.2 mol% LiF — within about 0.2 °C of the compound point and not resolvable as a separate feature at the scale of Fig. 1 — while the BeF<sub>2</sub>-rich eutectic occurs near 47 mol% LiF and 364 °C.

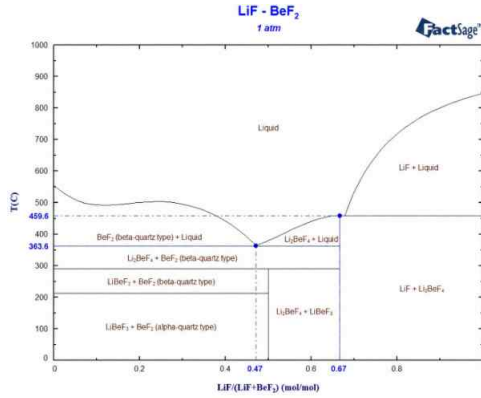


Fig. 1. Calculated LiF–BeF<sub>2</sub> binary phase diagram at 1 atm using FactSage and MSTDB–TC.

In a binary system at fixed pressure, the Gibbs phase rule,  $F = C - P + 1$  ( $C = 2$ ), leaves  $F = 1$  degree of freedom along the liquidus, where liquid coexists with a single solid phase; at a eutectic point, liquid coexists with two solid phases simultaneously ( $P = 3$ ), giving  $F = 0$  — an invariant condition that fixes both composition and temperature and appears in the diagram as a horizontal line. Between the compound composition and each pure end-member, FactSage resolves the corresponding univariant liquid+solid fields — labeled BeF<sub>2</sub>(beta-quartz type)+Liquid, Li<sub>2</sub>BeF<sub>4</sub>+Liquid, and LiF+Liquid in Fig. 1 — bounded below by the two invariant eutectic lines noted above. Below the solidus, further subsolidus invariant reactions are predicted, including LiBeF<sub>3</sub>+BeF<sub>2</sub> and Li<sub>2</sub>BeF<sub>4</sub>+LiBeF<sub>3</sub> fields; these lie well below the blanket's expected operating-temperature range and are not considered further here.

Because MSTDB–TC does not contain an assessed LiCl–PbCl<sub>2</sub> system, the liquidus was calculated with FactSage's built-in FTsalt database (Fig. 2). The calculated minimum occurs at a LiCl mole fraction of approximately 0.42 and a temperature of approximately 390 °C. This result should be treated as a database-based estimate pending comparison with a dedicated experimental or assessed phase-equilibrium source.

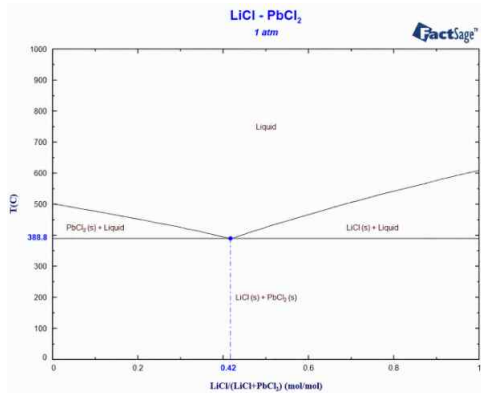


Fig. 2. Calculated LiCl–PbCl<sub>2</sub> binary phase diagram at 1 atm using FactSage and FTsalt.

Unlike LiF–BeF<sub>2</sub>, the LiCl–PbCl<sub>2</sub> system, no intermediate compound is stabilized in the current

FTsalt calculation: Fig. 2 shows only two univariant liquid+solid fields, PbCl<sub>2</sub>(s)+Liquid and LiCl(s)+Liquid, meeting at a single invariant eutectic point where both pure solids coexist with the eutectic liquid — the simplest topology permitted by the phase rule for a binary system. This offers a direct contrast to Fig. 1: a single-minimum, V-shaped liquidus for LiCl–PbCl<sub>2</sub> versus the compound-bearing, multi-segment liquidus for FLiBe.

For LiF–PbF<sub>2</sub>, a physically interpretable liquidus curve was not obtained over the composition and temperature range examined. The calculation settings and additional data sources are being rechecked, and the result will be reported at the meeting.

To validate these calculations experimentally, selected LiCl–PbCl<sub>2</sub> compositions near the calculated eutectic minimum, together with selected LiF–PbF<sub>2</sub> compositions, are being examined by simultaneous thermogravimetric analysis–differential scanning calorimetry (TGA–DSC); the onset and peak temperatures of the observed melting-related thermal events, together with any accompanying mass change, will be compared against the FactSage and ideal-mixing predictions.

#### 4. Conclusion

This study provides a preliminary comparison of FLiBe, LiCl–PbCl<sub>2</sub>, and LiF–PbF<sub>2</sub> for fusion-blanket applications through calculated binary phase diagrams. The FactSage approach was benchmarked using the assessed FLiBe diagram, while the LiCl–PbCl<sub>2</sub> calculation yielded an estimated liquidus minimum that still requires validation against an independent phase-equilibrium source. TGA–DSC measurements of selected LiCl–PbCl<sub>2</sub> and LiF–PbF<sub>2</sub> compositions are underway to validate these calculations experimentally. These results will clarify the trade-offs between chloride- and fluoride-based candidates and help prioritize subsequent experiments.

#### ACKNOWLEDGEMENTS

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