Fluoride materials for fuel and cooling systems of the IV generation reactor

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Fluoride systems have been described as one of the possible fuels for molten salt reactor application [1-3]. Besides the lowest melting point another criterion is the same important for the salt fuel: a concentration of fissile material. To optimize the molten salt fuel parameters the computer models of fluoride systems are to be built.

Computer model is based on the detailed geometrical description of a diagram: dots, curves, surfaces, phase regions. As a result it permits to use a phase diagram (PD) as an instrument to solve different applied tasks of heterogeneous design and physics-chemical analysis [4-8].

E. g., construction of the arbitrary taken diagram's vertical or horizontal cuts is provided with a table containing the detailed information of the surfaces and phase regions sections. For the given center of masses it is possible to receive a vertical diagram of the material balance, and the isothermal state of arbitrary taken isopleth could be illustrated by the horizontal diagram of material balance. By means of PD computer model, it is convenient to compare and analyze the contradictions between the methods to determine eutectical and peritectical fragments borders of three-phase region [9].

The LiF-KF-LaF_3 system [3], as a prototype of the possible fuels for molten salt reactor application, can be made as the modification of T-x-y diagram with binary compound decomposed before melting and appeared on the ternary liquidus [10] and T-x-y diagram with incongruently melting binary compound [11].

Computer Model of T-x-y Diagram LiF-KF-LaF_3 System

The kinematical method is used for the unruled and ruled diagram surfaces simulation. In this case, a diagram surface is presented as the pseudo-ruled one, that is, a space curve, given by the interpolation polynomial, moves along the analogously given directing curves [4-8].

Data for binary systems LiF-KF [12], KF-LaF_3 [13-14], LiF-LaF [15] concerning the melt temperatures of initial components (LiF≡A, KF≡B, LaF_3≡C), points coordinates of binary eutectics and peritectic ($e_{LiF\text{-}KF}$, $e_{KF\text{-}LaF3}$, $e_{LiF\text{-}LaF3}$, $p_{KF\text{-}LaF3}$) and compounds (R_1≡ KF·LaF_3 and R_2≡3KF·LaF_3) are used as initial data at PD simulation. The form of binary curves (i.e. curve convex downwards or upwards) are taken into consideration while liquidus simulation. The coordinates of ternary eutectic (E), peritectic (P) and two quasi-peritectics (Q_1 and Q_2) [3] also was given as initial data.

As solid phase solubility in this system are not present, the solidus and solvus surfaces are absent. As a result the given PD includes five surfaces of primary crystallization (with contours Q_{LiF}: $LiFe_{LiF\text{-}KF}EQ_2Q_1e_{LiF\text{-}LaF3}$; Q_{KF}: $KFe_{LiF\text{-}KF}EPe_{KF\text{-}LaF3}$; Q_{LaF3}: $LaF_3e_{LiF\text{-}LaF3}Q_1p_{KF\text{-}LaF3}$; $Q_{KF\text{-}LaF3}$: $e_{KF\text{-}LaF3}PQ_2Q_1p_{KF\text{-}LaF3}$; Q_R: EPQ_2) and sixteen ruled surfaces (Q^r_{AC}: $e_{LiF\text{-}LaF3}Q_1A_{Q1}A_{eLiF\text{-}LaF3}$, Q^r_{CA}: $e_{LiF\text{-}LaF3}Q_1C_{Q1}C_{eLiF\text{-}LaF3}$, Q^r_{AB}: $e_{LiF\text{-}KF}EA_EA_{eLiF\text{-}KF}$, Q^r_{BA}: $e_{LiF\text{-}KF}EB_EB_{eLiF\text{-}KF}$, Q^r_{CR1}: $p_{KF\text{-}LaF3}Q_1C_{Q1}C_{R1}$, Q^r_{R1C}: $p_{KF\text{-}LaF3}Q_1R1_{Q1}R_1$, Q^r_{R1B}: $e_{KF\text{-}LaF3}PR1_PR1_{eKF\text{-}LaF3}$, Q^r_{BR1}: $e_{KF\text{-}LaF3}PB_PB_{eKF\text{-}LaF3}$, Q^r_{AR1}: $Q_1Q_2A_{Q2}A_{Q1}$, Q^r_{R1A}: $Q_1Q_2R1_{Q2}R1_{Q1}$, Q^r_{R2A}: $EQ_2R2_{Q2}R2_E$, Q^r_{AR2}: $EQ_2A_{Q2}A_E$, Q^r_{R1R2}: $PQ_2R1_{Q2}R1_P$, Q^r_{R2R1}: $PQ_2R2_{Q2}R2_P$, Q^r_{BR2}: PEB_EB_P, Q^r_{R2B}: $PER2_ER2_P$), four horizontal complexes at the temperature of invariant points (H_E: $A_EB_ER2_EE$; H_P: $B_PR2_PR1_PP$; H_{Q1}: $A_{Q1}C_{Q1}R1_{Q1}Q_1$; H_{Q2}: $A_{Q2}R1_{Q2}R2_{Q2}Q_2$) and two vertical planes of triangulation (V_{R1}: $A_{Q1}A^0R^0{}_1R1_{Q1}$; V_{R2}: $A_{Q2}A^0R^0{}_2R2_{Q2}$) (Fig. 1). The surfaces curvature can be corrected according to the experimental data or thermodynamic calculation results.

Considered phase diagram of LiF-KF-LaF_3 system [16, 17] includes a one-phase region L, seven two-phase regions and eleven three-phase regions (Table 1).

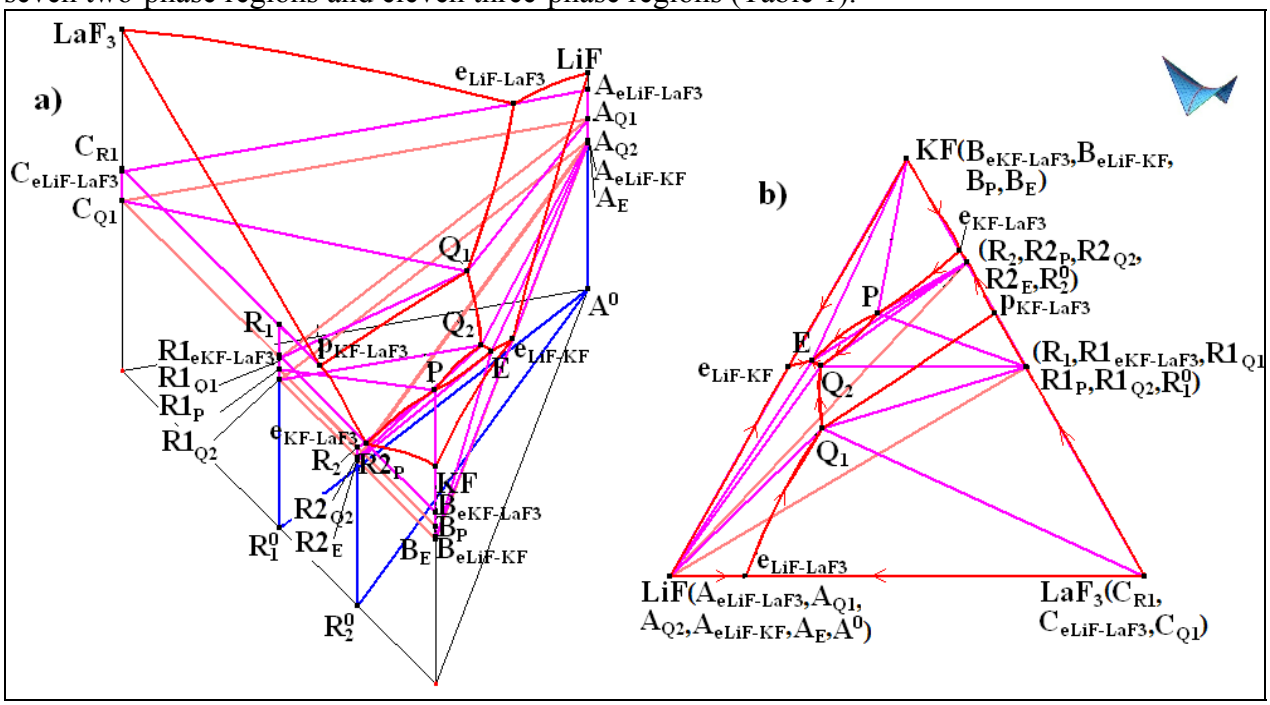

Fig. 1 Computer model of LiF-KF-LaF_3 system in prizm (a) and its XY projection (b)

Table 1 Phase Regions Structure

Symbol	Bounding Sufaces	Symbol	Bounding Sufaces	Symbol	Bounding Surfaces
L+A	Q_{LiF}, Q^r_{AB}, Q^r_{AC}, Q^r_{AR1}, Q^r_{AR2}	A+R2	V_{R2}	L+B+R2	Q^r_{BR2}, Q^r_{R2B}, H_E, H_P
L+B	Q_{KF}, Q^r_{BA}, Q^r_{BR1}, Q^r_{BR2}	L+A+B	Q^r_{AB}, Q^r_{BA}, H_E	L+C+R1	Q^r_{CR1}, Q^r_{R1C}, H_{Q1}
L+C	Q_{LaF3}, Q^r_{CA}, Q^r_{CR1}	L+A+C	Q^r_{AC}, Q^r_{CA}, H_{Q1}	L+R1+R2	Q^r_{R1R2}, Q^r_{R2R1}, H_P, H_{Q2}
L+R1	$Q_{KF-LaF3}$, Q^r_{R1R2}, Q^r_{R1A},Q^r_{R1B}, Q^r_{R1C}	L+A+R2	Q^r_{R2A}, Q^r_{AR2}, H_{Q2}, V_{R2}	A+B+R2	H_E, V_{R2}
L+R2	Q_R, Q^r_{R2R1}, Q^r_{R2A}, Q^r_{R2B}	L+A+R1	Q^r_{AR1}, Q^r_{R1A}, H_{Q1}, H_{Q2}, V_{R1}	A+C+R1	H_{Q1}, V_{R1}
A+R1	V_{R1}	L+B+R1	Q^r_{R1B}, Q^r_{BR1}, H_P	A+R1+R2	H_{Q2}, V_{R1}, V_{R2}

Horizontal and Vertical Sections of T-x-y Diagram LiF-KF-LaF_3 System

The arbitrary horizontal and vertical sections can be made for obtained computer model of LiF-KF-LaF_3 system. So horizontal sections at $T_{pKF-LaF3}<T<T_{eKF-LaF3}$ and $T_P<T<T_{Q2}$ are presented on Fig. 2. Vertical sections were constructed parallel to sides of prizm LiF-KF, LiF-LaF and KF-LaF_3 (Fig. 3).

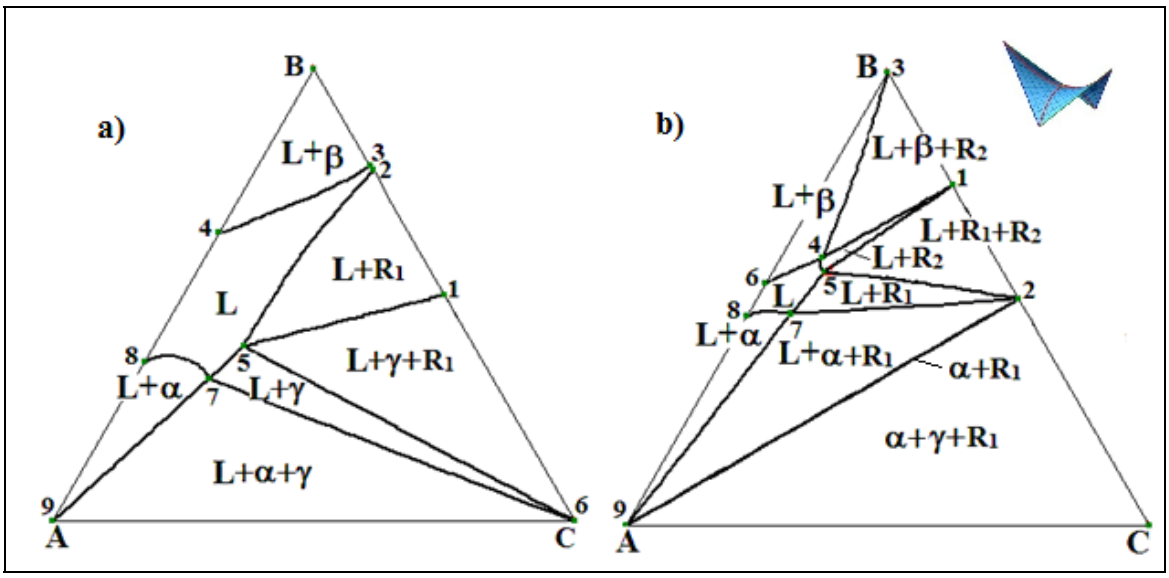

Fig. 2 Horizontal sections at $T_{pKF\text{-}LaF3}>T>T_{eKF\text{-}LaF3}$ (a) and $T_P>T>T_{Q2}$

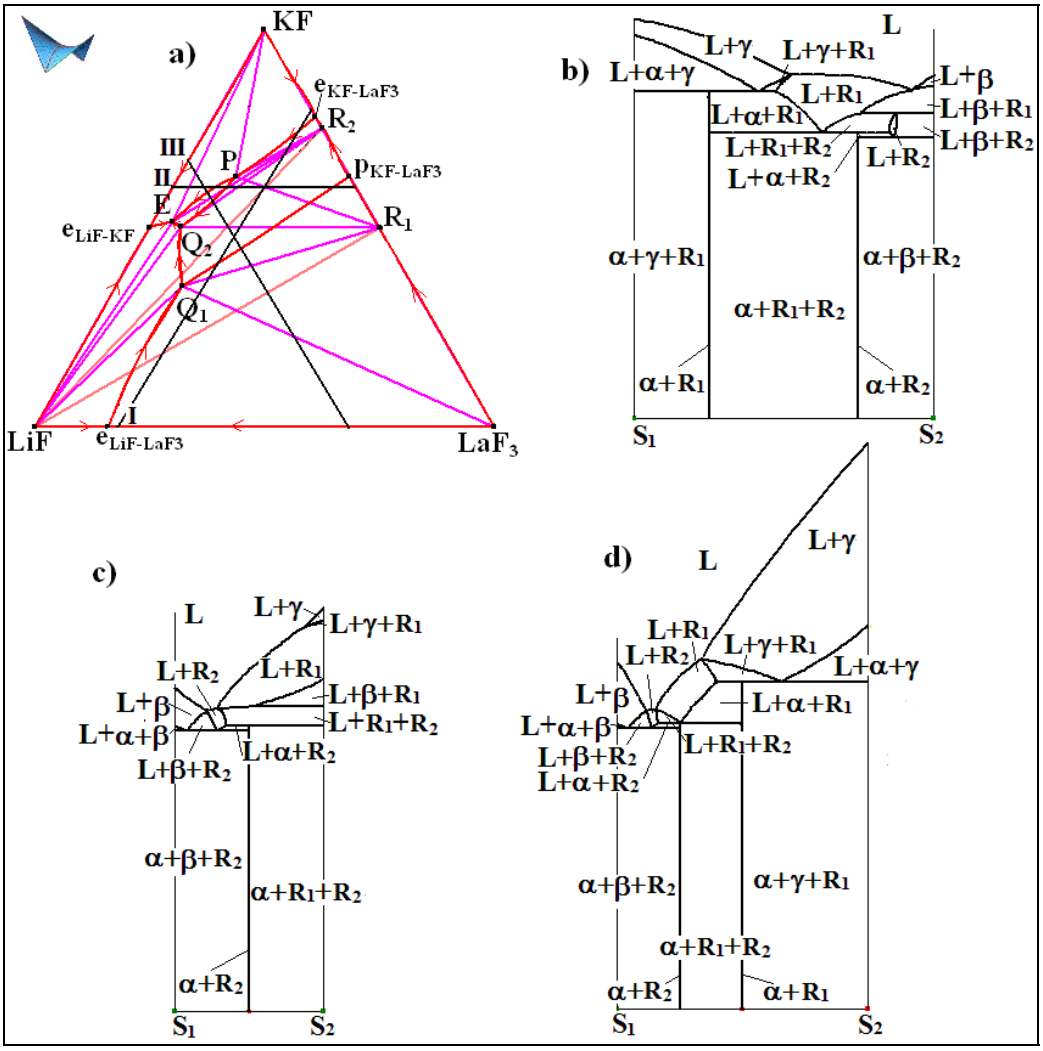

Fig. 3 Arrangment of vertical sections on XY proejction (a); vertical sections || LiF-KF $S_1(0.8; 0; 0.2)$-$S_2(0; 0.8; 0.2)$ (b); || LiF-LaF_3 $S_1(0.4; 0.6; 0)$-$S_2(0; 0.6; 0.4)$ (c); || KF-LaF_3 $S_1(0.33; 0.67; 0)$-$S_2(0.33; 0; 0.67)$ (d)

Summary

The elaborated phase diagrams computer models makes possible to study fluoride and other systems and can be used at the design of materials employing as possible fuel components for molten salt reactor. To ensure reliable exploitation of new generation reactor, exhaustive information are to be used about the chemical processes and equilibria in the fluoride melts of this type. As neither experimental data, nor thermodynamic calculation itself do not guarantee the validity of multidimensional phase diagram for multicomponent system and its isothermal sections and isopleths, then an assemblage of a whole diagram from its geometrical elements should be realized too.

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