Isothermal Evaporation Process Simulation using Pitzer Model for the Quinary System LiCl–NaCl–KCl–$SrCl_2$–H_2O at 298.15 K

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Table S1. Pitzer Binary Parameters of the Quinary System LiCl–NaCl–KCl–$SrCl_2$–H_2O at 298.15 K

species	$\beta^{(0)}$	$\beta^{(1)}$	$C^{(\phi)}$	ref.
LiCl	0.20818	-0.07264	-0.004241	11,23
NaCl	0.0765	0.2664	0.001270	24
KCl	0.04835	0.2122	-0.000840	24
$SrCl_2$	0.2827	1.5625	-0.000225	17
	0.28344	1.6256	-0.000891	19

Table S2. Pitzer Mixing Ion-interaction Parameters o of the Quinary System LiCl–NaCl–KCl–$SrCl_2$–H_2O at 298.15 K

species	θ	Ψ	ref.
Li^+, Na^+	0.02016		11,23
Li^+, K^+	-0.05075		11,23
Li^+, Sr^{2+}	-0.0359		22
Na^+, K^+	-0.01200		11,23
Na^+, Sr^{2+}	0.07885		17
	0.0562		17
K^+, Sr^{2+}	0.0271		18
Li^+, Na^+, Cl^-		-0.007416	11,23
Li^+, K^+, Cl^-		-0.005909	11,23
Li^+, Sr^{2+}, Cl^-		0.001921	22
Na^+, K^+, Cl^-		-0.001800	11,23
Na^+, Sr^{2+}, Cl^-		-0.01230	17
		-0.00705	17
K^+, Sr^{2+}, Cl^-		-0.0251	18

Table S3. μ^0/RT for Species of the Quinary System LiCl–NaCl–KCl–$SrCl_2$–H_2O at 298.15 K

species	μ^0/RT	ref.
H_2O	-95.6635	23
Li^+	-118.0439	23
Na^+	-105.651	23
K^+	-113.957	23
Sr^{2+}	-228.4630	this study
Cl^-	-52.955	23
$LiCl·H_2O$	-254.5962	23
NaCl	-154.99	23
KCl	-164.84	23
$SrCl_2·6H_2O$	-904.0272	24
$SrCl_2·2H_2O$	-517.1011	24

Table S4. Experimental and Predicted compositions (units: mol·kg^{-1}) of Invariant Points for the Systems at 298.15 K

NaCl–$SrCl_2$–H_2O	NaCl	$SrCl_2$	Precipitating solids
Experimental[12]	2.00	2.94	NaCl + $SrCl_2·6H_2O$
Experimental[16]	2.07	2.90	
Calculated[a]	1.97	2.94	
Calculated[b]	2.00	2.93	
Calculated[c]	1.97	2.92	
Calculated[d]	2.00	2.91	

[a]With binary parameters and mixing parameters to the saturated molalities.[17] [b]With binary parameters[19] and mixing parameters to the saturated molalities.[17] [c]With binary parameters and mixing parameters fitted with ionic strengths below 7.0 mol·kg^{-1}.[17] [d]With binary parameters[19] and mixing parameters fitted with ionic strengths below 7.0 mol·kg^{-1}.[17]

KCl–$SrCl_2$–H_2O	KCl	$SrCl_2$	Precipitating solids
Experimental[13]	1.60	3.37	KCl + $SrCl_2·6H_2O$
Experimental[16]	1.41	3.29	
Calculated[e]	1.59	3.35	
Calculated[f]	1.62	3.35	

[e] With binary parameters[17] and mixing parameters.[18] [f] With binary parameters[19] and mixing parameters.[18]

LiCl–$SrCl_2$–H_2O	LiCl	$SrCl_2$	Precipitating solids
Experimental[14]	–	–	LiCl·H_2O + $SrCl_2·2H_2O$
Experimental[15]	18.67	0.10	
Calculated[g]	19.39	0.012	
Calculated[h]	19.39	0.013	
Experimental[14]	–	–	$SrCl_2·2H_2O$ + $SrCl_2·6H_2O$
Experimental[15]	9.61	0.45	
Calculated[g]	10.37	0.72	
Calculated[h]	10.38	0.72	

[g]With binary parameters[17] and mixing parameters fitted with experimental water activities.[22]

[h]With binary parameters[19] and mixing parameters fitted with experimental water activities.[22]

NaCl–KCl–$SrCl_2$–H_2O	NaCl	KCl	$SrCl_2$	Precipitating solids
Experimental[16]	1.79	1.31	2.70	NaCl + KCl + $SrCl_2·6H_2O$
Calculated	1.75	1.44	2.88	

Table S5. Solid Phases during Isothermal Evaporation of the mother liquor for the oilfield brine from Nanyishan district in the Qaidam Basin[a]

No.	NaCl		KCl		$SrCl_2 \cdot 6H_2O$		$SrCl_2 \cdot 2H_2O$	
	m/mol	Precipitation ratio/%	m/mol	Precipitation ratio/%	m/mol	Precipitation ratio/%	m/mol	Precipitation ratio/%
B	0.0000	0.00	0.0000	0.00	0.0000	0.00	0.0000	0.00
C	0.0000	0.00	0.0606	5.69	0.0000	0.00	0.0000	0.00
D	2.2444	98.71	1.0309	96.71	0.0000	0.00	0.0000	0.00
E	2.2702	99.84	1.0568	99.14	0.0466	78.74	0.0000	0.00
F	2.2733	99.98	1.0582	99.28	0.0000	0.00	0.0591	99.83

[a]Calculated using 1 kg water in original brine.

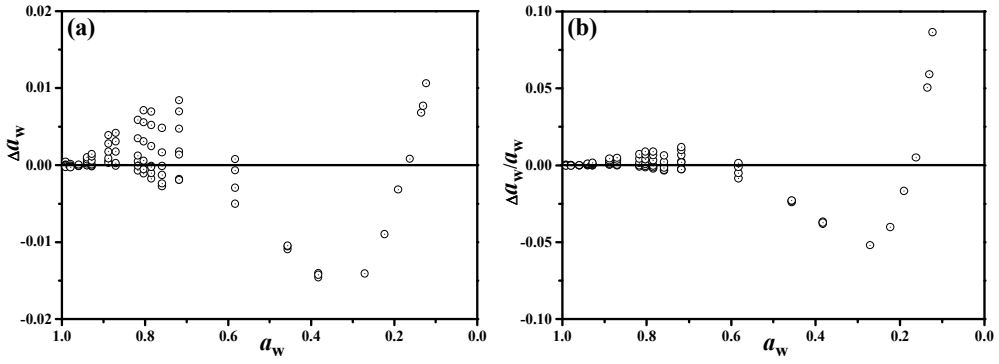

Figure S1. Calculated and experimental water activities of the system $LiCl–SrCl_2–H_2O$ at 298.15 K. (a) $\triangle a_w = a_w(\text{exp}) - a_w(\text{cal})$;

(b) $\triangle a_w / a_w = (a_w(\text{exp}) - a_w(\text{cal}))/ a_w(\text{exp})$.