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JÜLICH FORSCHUNGSZENTRUM

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Thermodynamic Assessment of the System

Al_2O_3-K_2O-Na_2O-SiO_2-CaO-MgO

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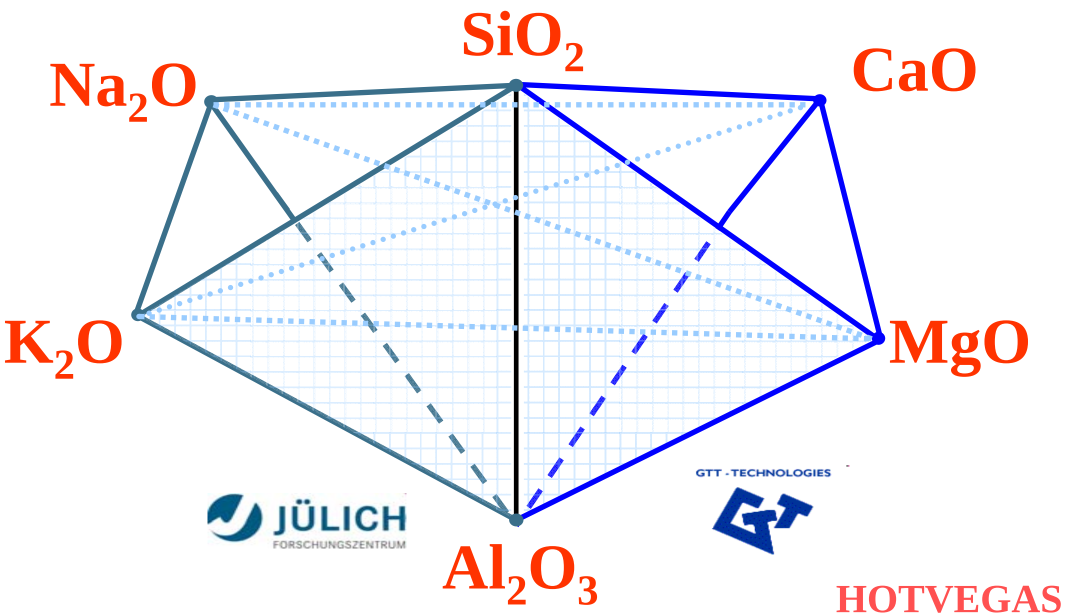
Contents

Motivation and aims

Thermodynamic calculation/prediction for slag relevant oxide systems, which are difficult from the point of view of experimental measurements

Calculation requires:

- ➢Reliable database, based on the experimental data
- ➢Software



Available databases are not sufficient to model the complete coal ash (slag) system

Purpose of out work - development of a new data base, which is:

✓ applicable for the slag relevant system containing alumina, silica, alkali, alkali-earth oxides

✓suitable for the calculations and/or predictions of the phase equilibria and other thermodynamic properties by variation of temperature and composition

Modelling of liquid and solid solutions

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*Applied and **chosen** model for the phases under consideration*

Phase name	**Associate species model**	**Multi-sublattice model**
Liquid	**Liquid pure oxides, binary and ternary liquid species**	**-**
Mullite	$Al_6Si_2O_{13}$: $Al_6Si_2O_{13}$·1/4, Al_2O_3, SiO_2·2	**$(Al^{3+})_1(Al^{3+})_1(Al^{3+}, Si^{4+})_1(O^{2-}, Va)_5$ (Mao et al., 2005)**
Na disilicate	**$(Na_{1-x}K_x)_2Si_2O_5$: $Na_2Si_2O_5$, $K_2Si_2O_5$**	**$(Na^{1+}, K^{1+})_2(Si^{4+})_2(0^{2-})_5$**
K or Na aluminate		**$AlkAlO_2$ - low T, high T** **$(Al^{3+}, Si^{4+})_1(K^{1+}, Na^{1+} Va^0)_1(O^{2-})_2$**
Nepheline, carnegieite		**Nepheline (low T), carnegieite (high T)** **$(Al^{3+}, Si^{4+})_2Va^0{}_1(Na^{1+}, Va^0)_1(O^{2-})_4$**
Natrium aluminate		**$NaAlO_2$ - low T, high T** **$(Al^{3+}, Si^{4+})_1(Na^{1+}, Va^0)_1(O^{2-})_2$ (Fe is by GTT considered)**
K_2MgSiO_4-SiO_2		**Reciprocal: $(Mg^{2+},Si^{4+})_1(Si^{4+})_1(K^{1+},Va^0)_2(O^{2-})_4$**
Beta alumina		**$(Na^{1+},K^{1+})_1(Al^{3+})_9(O^{2-})_{14}$**
Beta`` alumina		**$(Na^{1+},K^{1+})_1(Al^{3+})_{12}(O^{2-})_{19}$ (Mg is by GTT considered)**
Feldspar		**$(Na^{1+},K^{1+})_1 (Al^{3+})_1(Si^{4+})_3(O^{2-})_8$**

Database development

Experimental data:
phase diagram data,
activity data (if they are available)

Choice of the suitable model

Initial data for pure solid and liquid substances, liquid and solid solution components

OptiSage in FactSage™

Adjustable parameters:

ΔH_f^{298} **and** S^{298} **for the liquid and solid solution species**

ΔH_f^{298} **and** S^{298} **for the pure solid compounds (part.)**

interaction parameters between species

optimisation

Comparison of the results with exp. data

disagreement

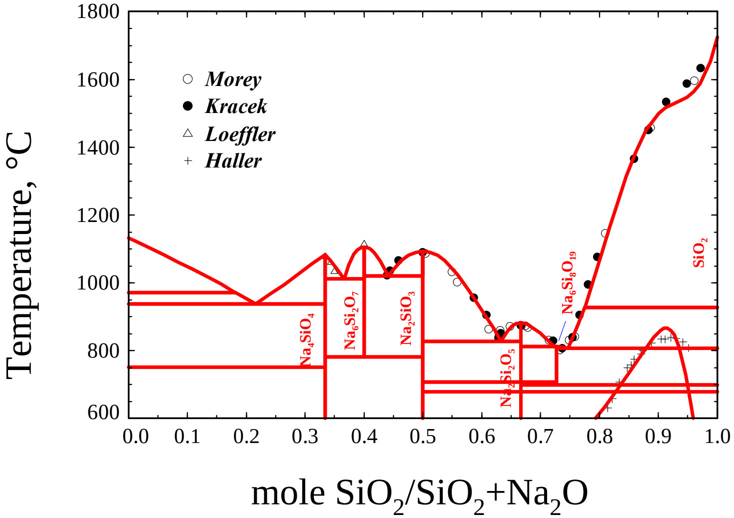
agreement

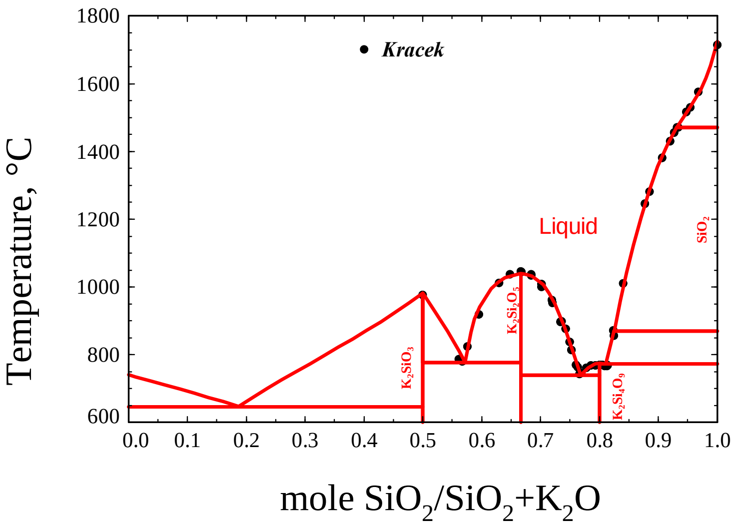
New dataset

✓Re-assessment:
Gibbs energy for pure oxides were changed from FACT to SGTE Pure Substance database

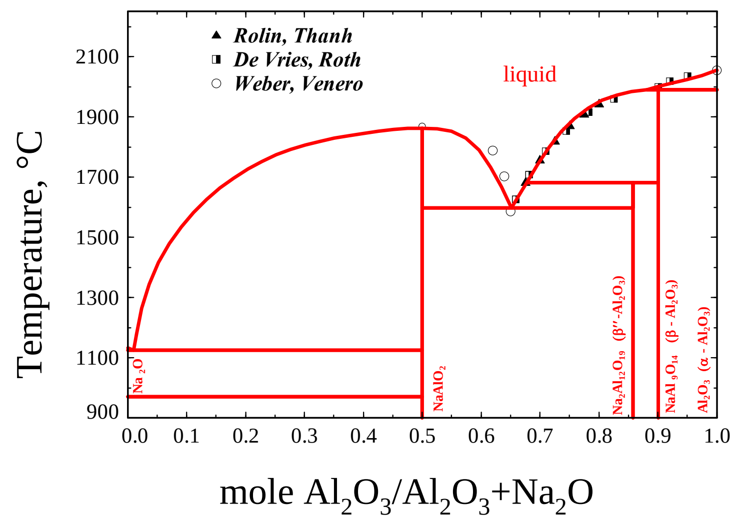
Results of re-assessment for binary systems-1

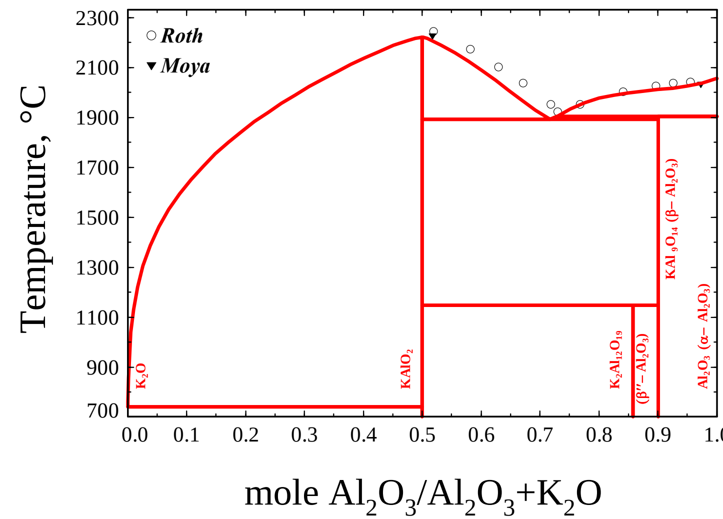
Alk_2O-SiO_2, Alk=Na, K





Alk_2O-Al_2O_3, Alk=Na, K



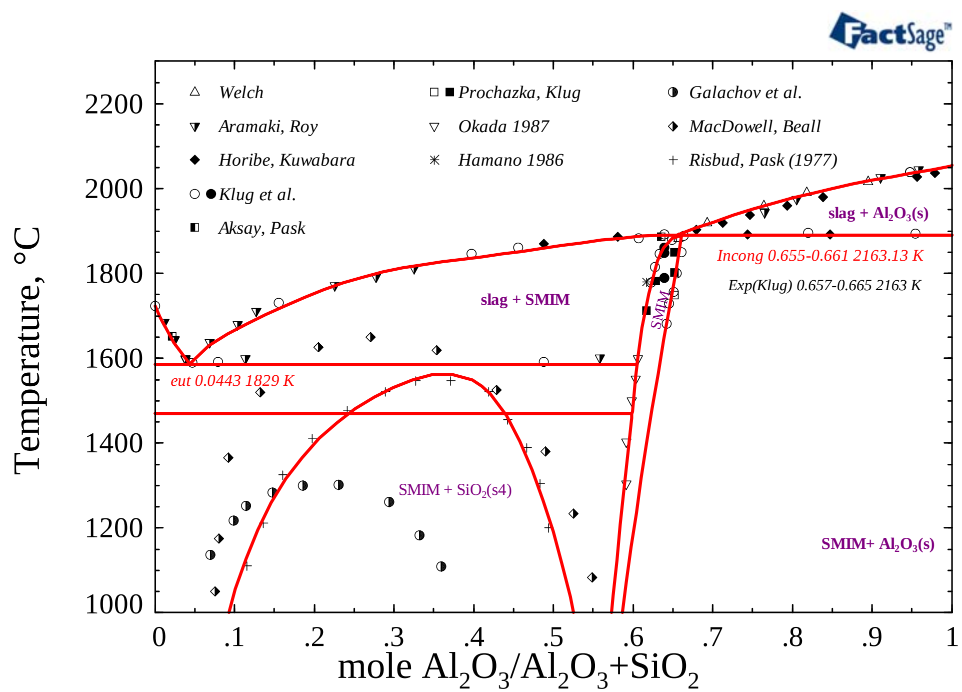


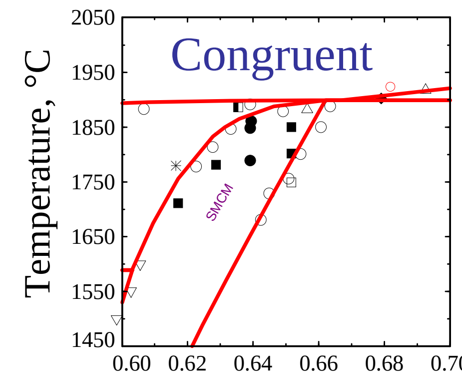
Results of re-assessment for binary systems-2

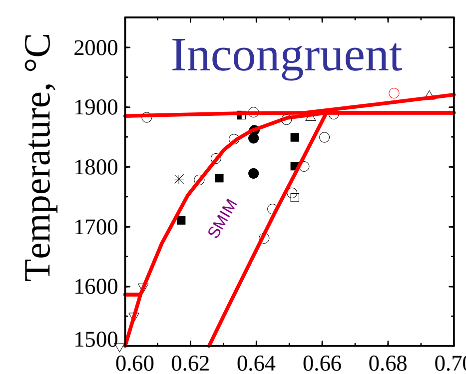
Mullite

Associate species model (introduced by Spear at al. in 2002):
$Al_6Si_2O_{13} \cdot 1/4$, Al_2O_3, $SiO_2 \cdot 2$

4 sublattice model (introduced by Mao et al. in 2005):
$(Al^{3+})_1(Al^{3+})_1(Al^{3+}, Si^{4+})_1(O^{2-}, Va)_5$

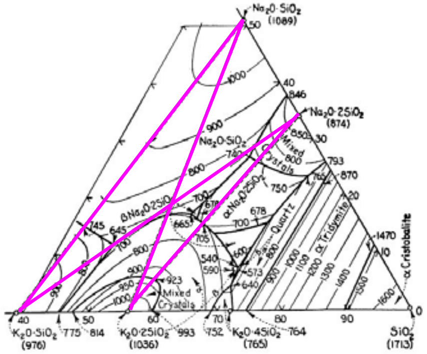






✓*Model parameters are optimised for both melting behaviour of mullite*

Assessment for ternary system Na_2O-K_2O-SiO_2



F.C. Kracek, The ternary system K_2SiO_3-Na_2SiO_3-SiO_2, J. Phys. Chem., ***36*** *[10], (1932), 2529-2542*

Interacting components:

Na_2SiO_3*2/3 - K_2SiO_3*2/3

$Na_2Si_2O_5$*1/2 - $K_2Si_2O_5$*1/2

Na_2SiO_3*2/3 - $K_2Si_2O_5$*1/2

$Na_2Si_2O_5$*1/2 - K_2SiO_3*2/3

Predicted phase fields and ternary points

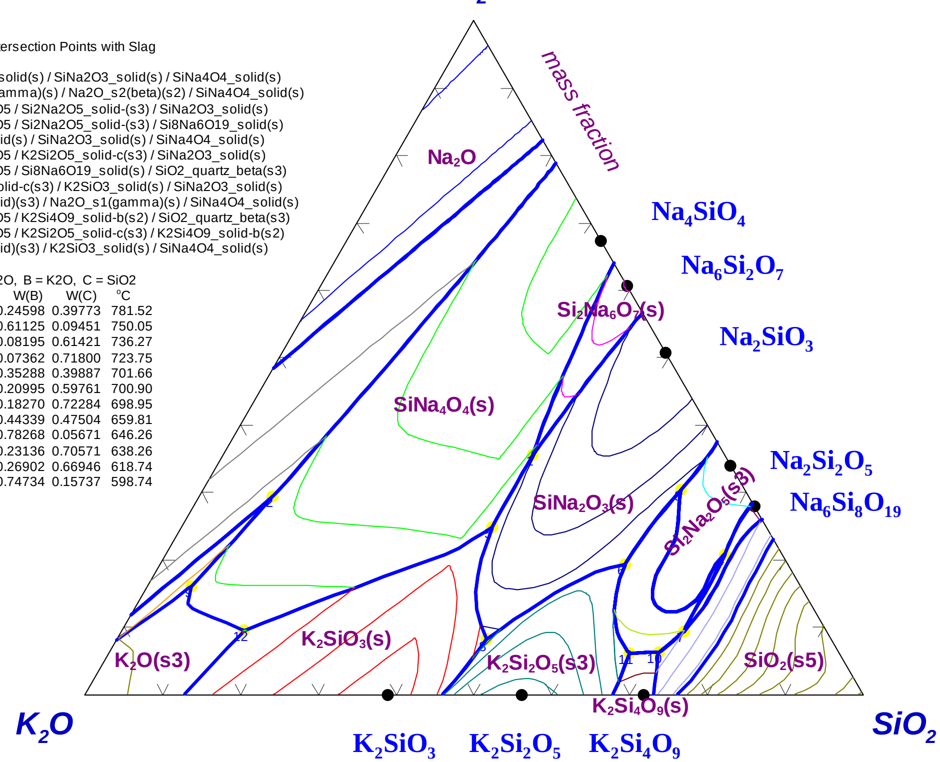
K_2O - Na_2O - SiO_2

Four-Phase Intersection Points with Slag

1: Si2Na6O7_solid(s) / SiNa2O3_solid(s) / SiNa4O4_solid(s)
2: Na2O_s1(gamma)(s) / Na2O_s2(beta)(s2) / SiNa4O4_solid(s)
3: (Na,K)2Si2O5 / Si2Na2O5_solid-(s3) / SiNa2O3_solid(s)
4: (Na,K)2Si2O5 / Si2Na2O5_solid-(s3) / Si8Na6O19_solid(s)
5: K2SiO3_solid(s) / SiNa2O3_solid(s) / SiNa4O4_solid(s)
6: (Na,K)2Si2O5 / K2Si2O5_solid-c(s3) / SiNa2O3_solid(s)
7: (Na,K)2Si2O5 / Si8Na6O19_solid(s) / SiO2_quartz_beta(s3)
8: K2Si2O5_solid-c(s3) / K2SiO3_solid(s) / SiNa2O3_solid(s)
9: K2O_s3(solid)(s3) / Na2O_s1(gamma)(s) / SiNa4O4_solid(s)
10: (Na,K)2Si2O5 / K2Si4O9_solid-b(s2) / SiO2_quartz_beta(s3)
11: (Na,K)2Si2O5 / K2Si2O5_solid-c(s3) / K2Si4O9_solid-b(s2)
12: K2O_s3(solid)(s3) / K2SiO3_solid(s) / SiNa4O4_solid(s)

A = Na2O, B = K2O, C = SiO2

	W(A)	W(B)	W(C)	°C
1:	0.35628	0.24598	0.39773	781.52
2:	0.29424	0.61125	0.09451	750.05
3:	0.30385	0.08195	0.61421	736.27
4:	0.20838	0.07362	0.71800	723.75
5:	0.24826	0.35288	0.39887	701.66
6:	0.19244	0.20995	0.59761	700.90
7:	0.09446	0.18270	0.72284	698.95
8:	0.08157	0.44339	0.47504	659.81
9:	0.16061	0.78268	0.05671	646.26
10:	0.06293	0.23136	0.70571	638.26
11:	0.06152	0.26902	0.66946	618.74
12:	0.09529	0.74734	0.15737	598.74



Quasi binary section in the Na_2O-K_2O-SiO_2 system

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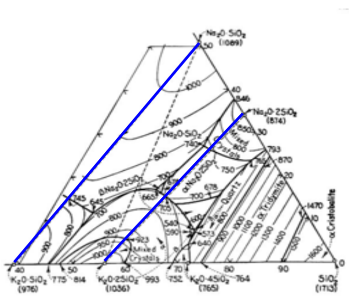
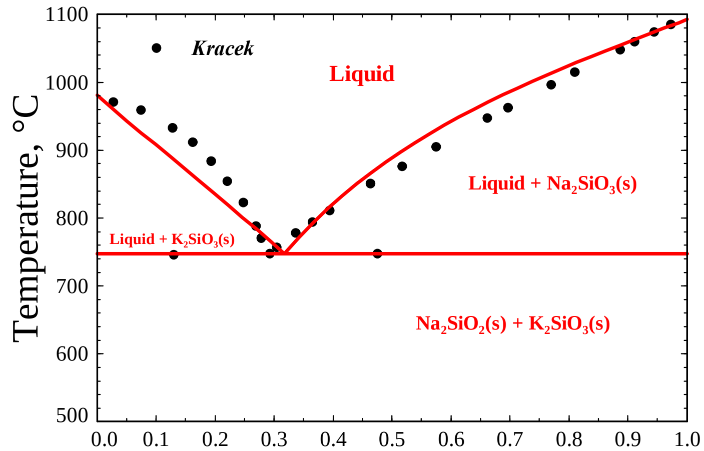
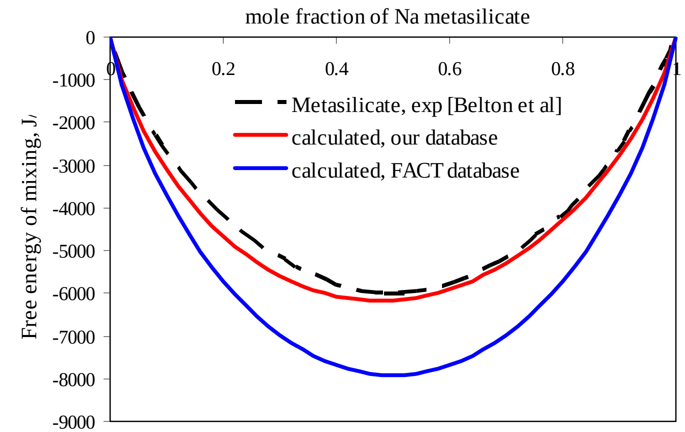
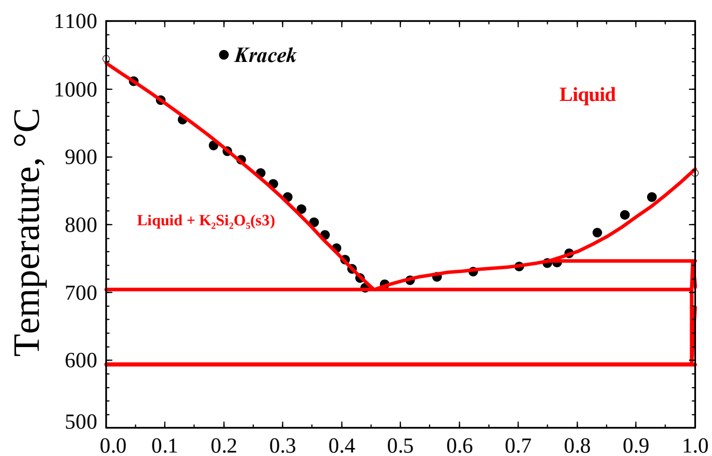
K_2SiO_3-Na_2SiO_3

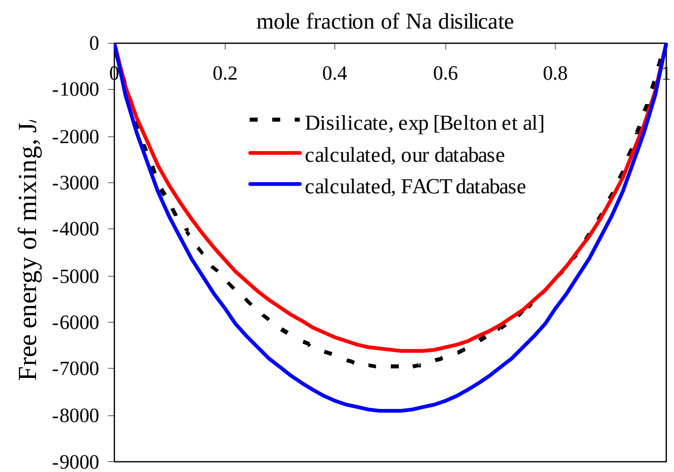






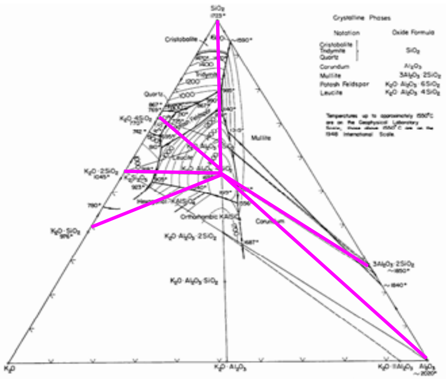
$K_2Si_2O_5$-$Na_2Si_2O_5$



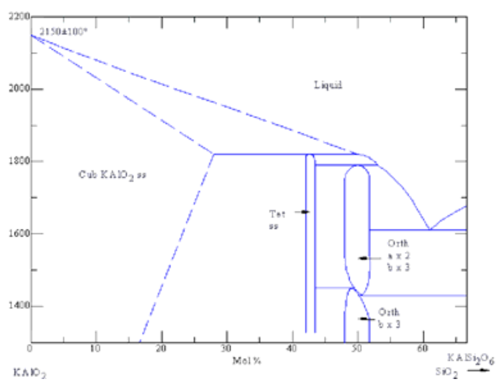


[Belton et al.] *G.R. Belton, U.V. Choudary, D.R. Gaskell, Thermodynamics of mixing in molten sodium-potassium silicates, Phys. Chem.Process. Metall., Richardson Conf., (1974), 247-253*

Assessment for ternary system K_2O-Al_2O_3-SiO_2



J.F. Schairer, N.L. Bowen, The system K_2O-Al_2O_3-SiO_2, *Am. J. Sci.* **253** (1955) 681-746.



R.S. Roth, Phase equilibrium research in portions of the potassium oxide-magnesium oxide-iron (III) oxide-aluminium oxide-silicon dioxide system, Adv. Chem. ***186*** *(1980) 391-408*

Interacting components

Al_2O_3 – $KAlSi_2O_6$*1/2

$K_2Si_2O_5$*1/2 - $KAlSi_2O_6$*1/2

Si_2O_4*1/2 - $KAlSi_2O_6$*1/2

$Al_6Si_2O_{13}$*1/4 - $KAlSi_2O_6$*1/2

K_2SiO_3*2/3 - $KAlSi_2O_6$*1/2

$K_2Si_4O_9$*1/3 - $KAlSi_2O_6$*1/2

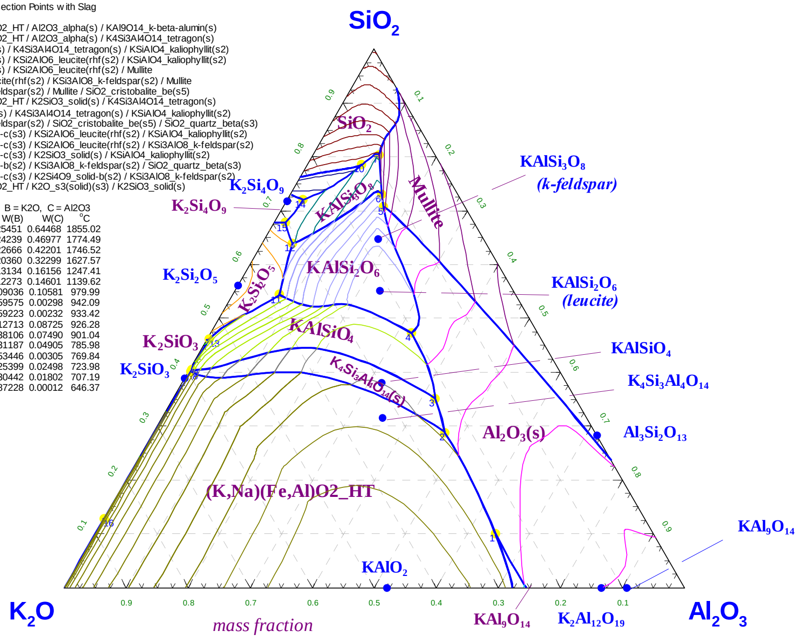
SiO_2 - Al_2O_3 - K_2O

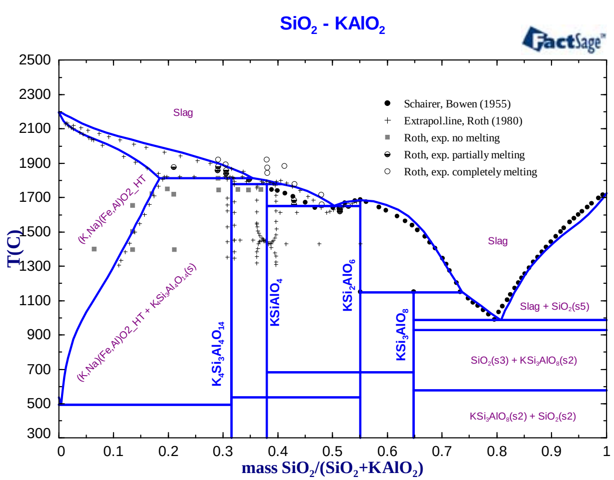
Four-Phase Intersection Points with Slag

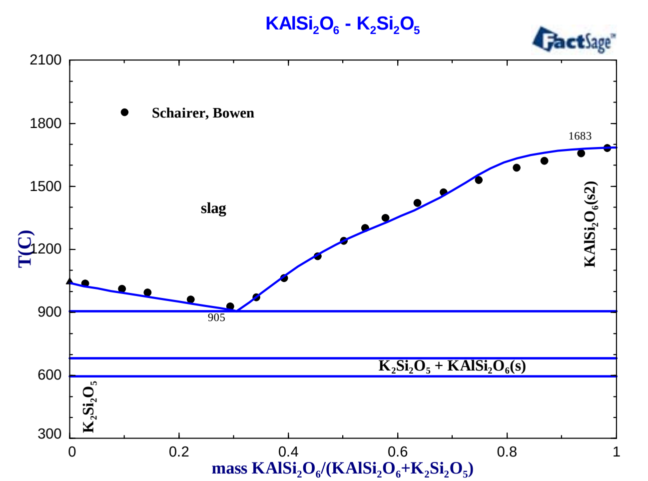
1: (K,Na)(Fe,Al)O2_HT / Al2O3_alpha(s) / KAl9O14_k-beta-alumin(s)
2: (K,Na)(Fe,Al)O2_HT / Al2O3_alpha(s) / K4Si3Al4O14_tetragon(s)
3: Al2O3_alpha(s) / K4Si3Al4O14_tetragon(s) / KSiAlO4_kaliophyllit(s2)
4: Al2O3_alpha(s) / KSi2AlO6_leucite(rhf(s2) / KSiAlO4_kaliophyllit(s2)
5: Al2O3_alpha(s) / KSi2AlO6_leucite(rhf(s2) / Mullite
6: KSi2AlO6_leucite(rhf(s2) / KSi3AlO8_k-feldspar(s2) / Mullite
7: KSi3AlO8_k-feldspar(s2) / Mullite / SiO2_cristobalite_be(s5)
8: (K,Na)(Fe,Al)O2_HT / K2SiO3_solid(s) / K4Si3Al4O14_tetragon(s)
9: K2SiO3_solid(s) / K4Si3Al4O14_tetragon(s) / KSiAlO4_kaliophyllit(s2)
10: KSi3AlO8_k-feldspar(s2) / SiO2_cristobalite_be(s5) / SiO2_quartz_beta(s3)
11: K2Si2O5_solid-c(s3) / KSi2AlO6_leucite(rhf(s2) / KSiAlO4_kaliophyllit(s2)
12: K2Si2O5_solid-c(s3) / KSi2AlO6_leucite(rhf(s2) / KSi3AlO8_k-feldspar(s2)
13: K2Si2O5_solid-c(s3) / K2SiO3_solid(s) / KSiAlO4_kaliophyllit(s2)
14: K2Si4O9_solid-b(s2) / KSi3AlO8_k-feldspar(s2) / SiO2_quartz_beta(s3)
15: K2Si2O5_solid-c(s3) / K2Si4O9_solid-b(s2) / KSi3AlO8_k-feldspar(s2)
16: (K,Na)(Fe,Al)O2_HT / K2O_s3(solid)(s3) / K2SiO3_solid(s)

A = SiO2, B = K2O, C = Al2O3

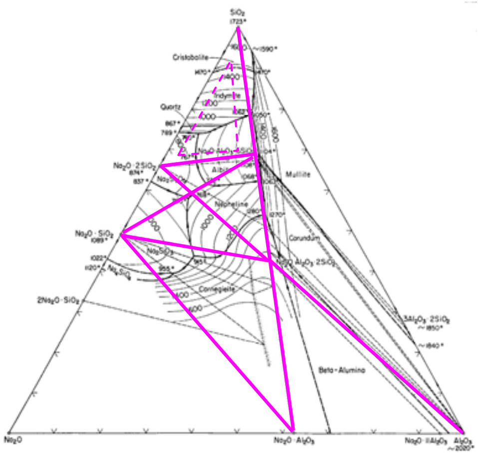
	W(A)	W(B)	W(C)	°C
1:	0.10081	0.25451	0.64468	1855.02
2:	0.28784	0.24239	0.46977	1774.49
3:	0.35133	0.22666	0.42201	1746.52
4:	0.47342	0.20360	0.32299	1627.57
5:	0.70709	0.13134	0.16156	1247.41
6:	0.73126	0.12273	0.14601	1139.62
7:	0.80383	0.09036	0.10581	979.99
8:	0.40127	0.59575	0.00298	942.09
9:	0.40545	0.59223	0.00232	933.42
10:	0.78562	0.12713	0.08725	926.28
11:	0.54404	0.38106	0.07490	901.04
12:	0.63908	0.31187	0.04905	785.98
13:	0.46250	0.53446	0.00305	769.84
14:	0.72103	0.25399	0.02498	723.98
15:	0.67756	0.30442	0.01802	707.19
16:	0.12761	0.87228	0.00012	646.37







Assessment for ternary system Na_2O-Al_2O_3-SiO_2



J.F. Schairer, N.L. Bowen, The system Na_2O-Al_2O_3-SiO_2, Am. J. Sci. 254(2) (1956) 129-195.

Interacting components

Al_2O_3 – $NaAlSi_3O_8$*2/5

$Na_2Si_2O_5$*1/2 – $NaAlSi_3O_8$*2/5

$Na_2Si_2O_5$*1/2 – $NaAlSiO_4$*2/3

Si_2O_4*1/2 – $NaAlSi_3O_8$*2/5

Si_2O_4*1/2 – $NaAlSiO_4$*2/3

Na_2SiO_3*2/3 – $NaAlSi_3O_8$*2/5

Na_2SiO_3*2/3 – $NaAlSiO_4$*2/3

Na_2SiO_3*2/3 – $NaAlO_2$

$NaAlSi_3O_8$*2/5-$NaAlSiO_4$*2/3

$NaAlO_2$ - $NaAlSiO_4$*2/3

Si_2O_4*1/2 – $Na_2Si_2O_5$/1/2 - $NaAlSi_3O_8$*2/5

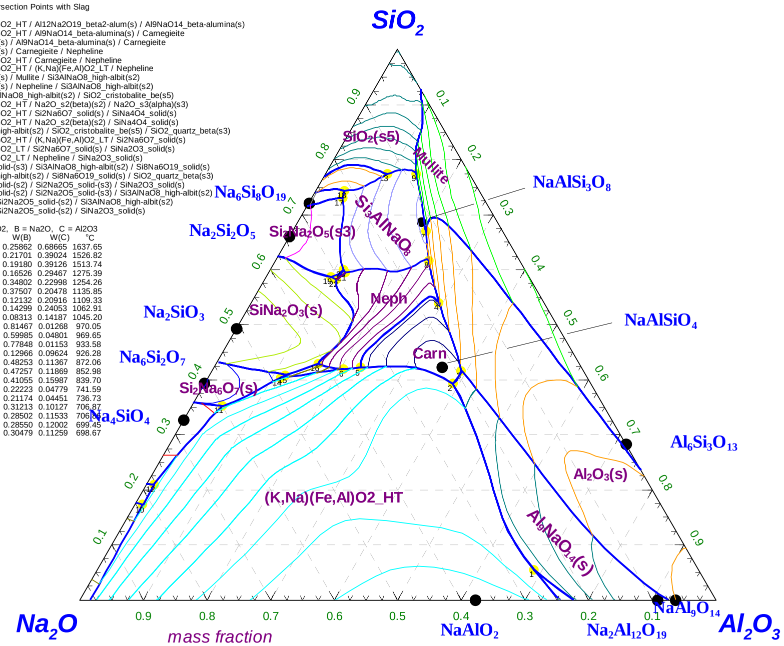
SiO_2 - Al_2O_3 - Na_2O

Four-Phase Intersection Points with Slag

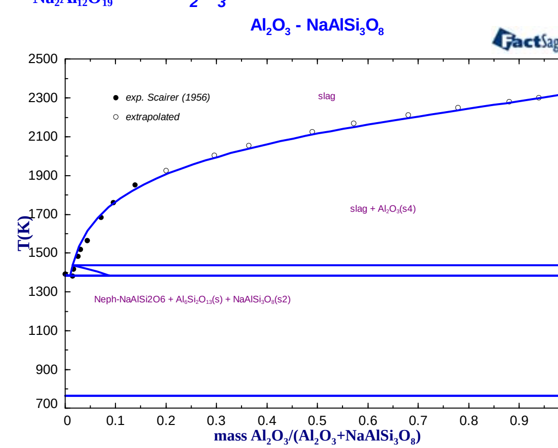
1: (K,Na)(Fe,Al)O2_HT / Al12Na2O19_beta2-alum(s) / Al9NaO14_beta-alumina(s)
2: (K,Na)(Fe,Al)O2_HT / Al9NaO14_beta-alumina(s) / Carnegieite
3: Al2O3_alpha(s) / Al9NaO14_beta-alumina(s) / Carnegieite
4: Al2O3_alpha(s) / Carnegieite / Nepheline
5: (K,Na)(Fe,Al)O2_HT / Carnegieite / Nepheline
6: (K,Na)(Fe,Al)O2_HT / (K,Na)(Fe,Al)O2_LT / Nepheline
7: Al2O3_alpha(s) / Mullite / Si3AlNaO8_high-albit(s2)
8: Al2O3_alpha(s) / Nepheline / Si3AlNaO8_high-albit(s2)
9: Mullite / Si3AlNaO8_high-albit(s2) / SiO2_cristobalite_be(s5)
10: (K,Na)(Fe,Al)O2_HT / Na2O_s2(beta)(s2) / Na2O_s3(alpha)(s3)
11: (K,Na)(Fe,Al)O2_HT / Si2Na6O7_solid(s) / SiNa4O4_solid(s)
12: (K,Na)(Fe,Al)O2_HT / Na2O_s2(beta)(s2) / SiNa4O4_solid(s)
13: Si3AlNaO8_high-albit(s2) / SiO2_cristobalite_be(s5) / SiO2_quartz_beta(s3)
14: (K,Na)(Fe,Al)O2_HT / (K,Na)(Fe,Al)O2_LT / Si2Na6O7_solid(s)
15: (K,Na)(Fe,Al)O2_LT / Si2Na6O7_solid(s) / SiNa2O3_solid(s)
16: (K,Na)(Fe,Al)O2_LT / Nepheline / SiNa2O3_solid(s)
17: Si2Na2O5_solid-(s3) / Si3AlNaO8_high-albit(s2) / Si8Na6O19_solid(s)
18: Si3AlNaO8_high-albit(s2) / Si8Na6O19_solid(s) / SiO2_quartz_beta(s3)
19: Si2Na2O5_solid-(s2) / Si2Na2O5_solid-(s3) / SiNa2O3_solid(s)
20: Si2Na2O5_solid-(s2) / Si2Na2O5_solid-(s3) / Si3AlNaO8_high-albit(s2)
21: Nepheline / Si2Na2O5_solid-(s2) / Si3AlNaO8_high-albit(s2)
22: Nepheline / Si2Na2O5_solid-(s2) / SiNa2O3_solid(s)

A = SiO2, B = Na2O, C = Al2O3

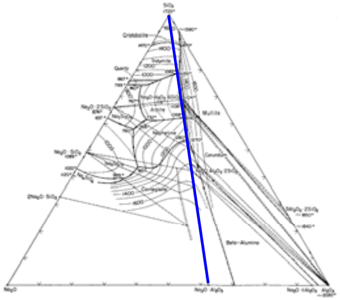
	W(A)	W(B)	W(C)	°C
1:	0.05473	0.25862	0.68665	1637.65
2:	0.39275	0.21701	0.39024	1526.82
3:	0.41694	0.19180	0.39126	1513.74
4:	0.54007	0.16526	0.29467	1275.39
5:	0.42200	0.34802	0.22998	1254.26
6:	0.42014	0.37507	0.20478	1135.85
7:	0.66951	0.12132	0.20916	1109.33
8:	0.61648	0.14299	0.24053	1062.91
9:	0.77500	0.08313	0.14187	1045.20
10:	0.17265	0.81467	0.01268	970.05
11:	0.35214	0.59985	0.04801	969.65
12:	0.20999	0.77848	0.01153	933.58
13:	0.77409	0.12966	0.09624	926.28
14:	0.40379	0.48253	0.11367	872.06
15:	0.40874	0.47257	0.11869	852.98
16:	0.42958	0.41055	0.15987	839.70
17:	0.72998	0.22223	0.04779	741.59
18:	0.74374	0.21174	0.04451	736.73
19:	0.58660	0.31213	0.10127	706.87
20:	0.59965	0.28502	0.11533	706.86
21:	0.59447	0.28550	0.12002	699.45
22:	0.58262	0.30479	0.11259	698.67



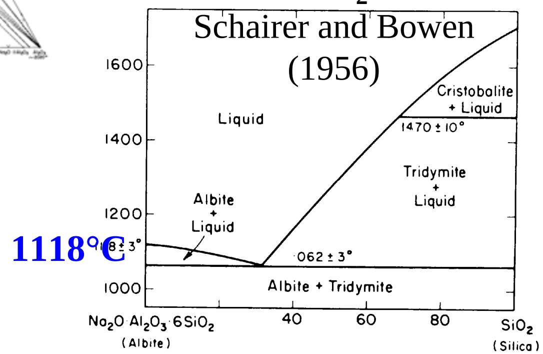
Predicted phase fields and ternary points



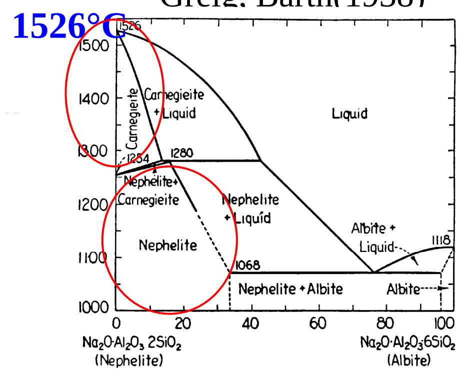
Results of the assessment for the system $NaAlO_2$-SiO_2

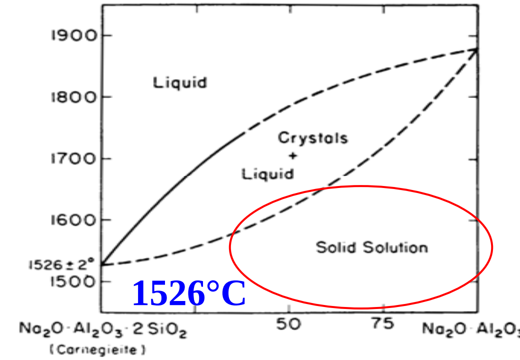


$NaAlSi_3O_8$ (Albite) - SiO_2
Schairer and Bowen (1956)



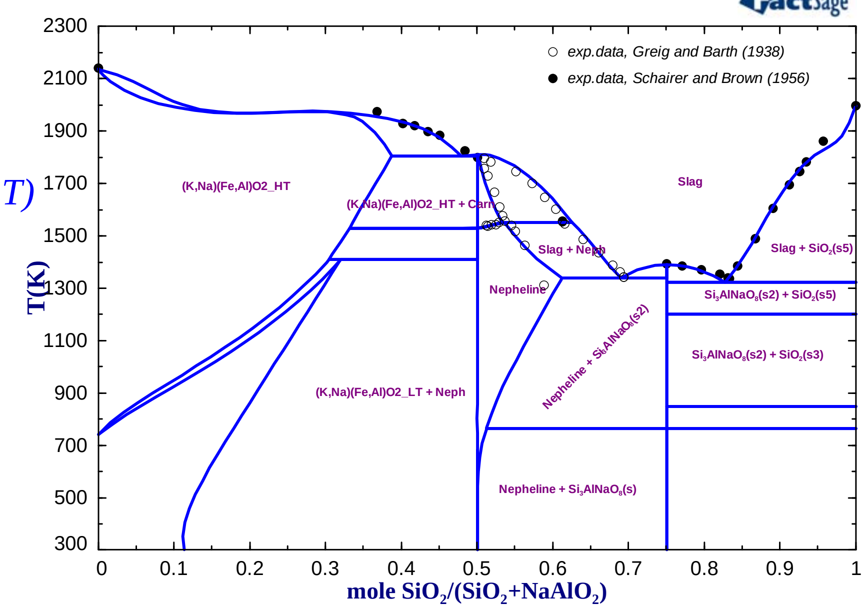
$NaAlSiO_4$ – $NaAlSi_3O_8$
Greig, Barth(1938)





$NaAlSiO_4$ - $NaAlO_2$
Schairer and Bowen (1956)

SiO_2 - $NaAlO_2$



Sublattice solutions are added:

$(Al^{3+}, Si^{4+}, Fe^{3+})_1(Na^{1+}, K^{1+}, Va^0)_1(O^{2-})_2$ *for $NaAlO_2$ (low T, high T)*

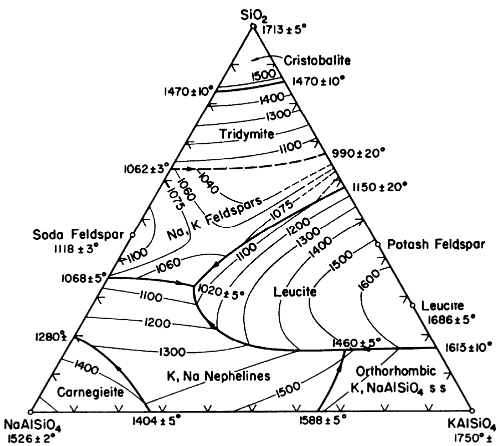
$(Al^{3+}, Si^{4+})_2(Va^0)_1(Na^{1+}, Va^0)_1(O^{2-})_4$ *for $NaAlSiO_4$ (Neph, Carn)*

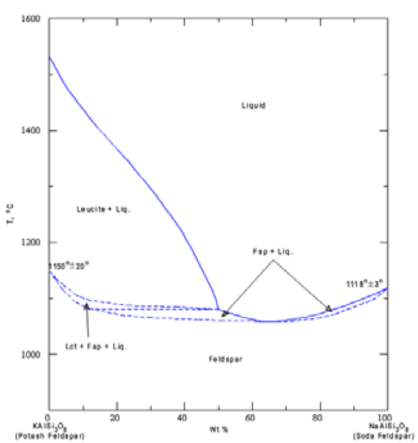
Problems:

✓ *Unknown solubility boundaries for $NaAlO_2$ (low T, high T) solutions*

Feldspar section in the quaternary system
Na_2O-K_2O-Al_2O_3-SiO_2

SiO_2 – $KAlSiO_4$ - $NaAlSiO_4$



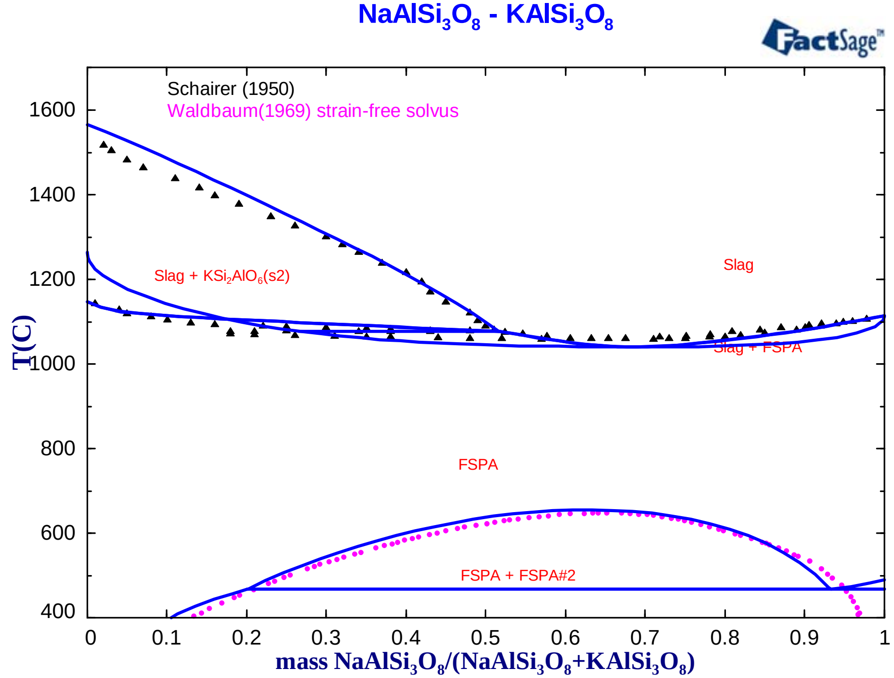


Schairer, J.F., The alkali-feldspar join in the system $NaAlSiO_4$-$KAlSiO_4$-SiO_2, J. Geol. ***58*** *(5) (1950)512-517*

Interacting components in liquid

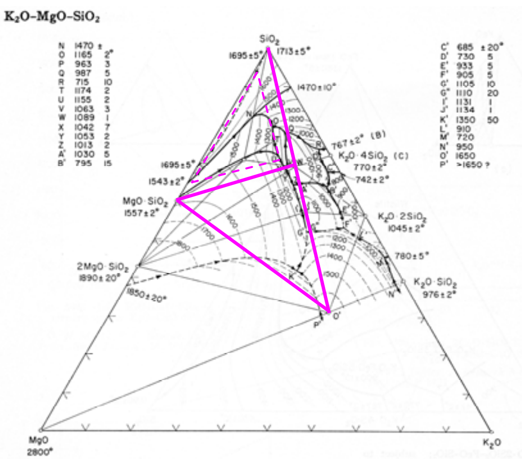
$NaAlSi_3O_8$*2/5 - $KAlSi_2O_6$*1/2

$NaAlSi_3O_8$ - $KAlSi_3O_8$



Sublattice solution $(Al^{3+})_1(Na^{1+}, K^{1+})_1(Si^{4+})_3(O^{2-})_8$ *for feldspar is added.*

Ternary system K_2O-MgO-SiO_2



*E.W. Roedder, The system K_2O-MgO-SiO_2, Am. J. Sci. **249**(2) (1951) 81-130.*

Liquid

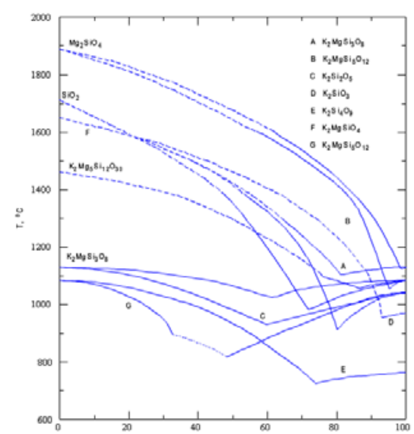
- binary associate species K_2O-SiO_2, MgO-K_2O, MgO-SiO_2 are kept
- new ternary species are introduced: $(K_2MgSiO_4)/2$, $(K_2MgSi_5O_{12})/4$
- new interaction parameters between binary and ternary species are added

Solids

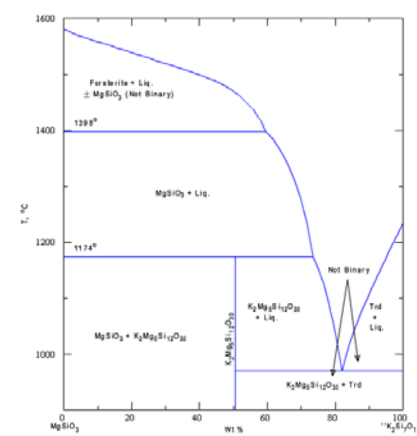
- binary compounds from K_2O-SiO_2, MgO-K_2O, MgO-SiO_2 are kept
- new ternary compounds (K_2MgSiO_4, $K_2MgSi_3O_8$, $K_2MgSi_5O_{12}$, $K_2Mg_5Si_{12}O_{30}$, $K_4Mg_2Si_5O_{14}$, $K_{10}Mg_5Si_{11}O_{32}$) are introduced
- reciprocal solid solution $(Mg^{2+},Si^{4+})_1(Si^{4+})_1(K^{1+},Va^0)_2(O^{2-})_4$ is added

Interacting components in liquid

Si_2O_4*1/2 – $K_2MgSi_5O_{12}$*1/4
$MgSiO_3$ - K_2MgSiO_4*1/2
$MgSiO_3$ - $K_2MgSi_5O_{12}$*1/4
K_2MgSiO_4*1/2 - $K_2MgSi_5O_{12}$*1/4
Si_2O_4*1/2 – $MgSiO_3$ - $K_2MgSi_5O_{12}$*1/4

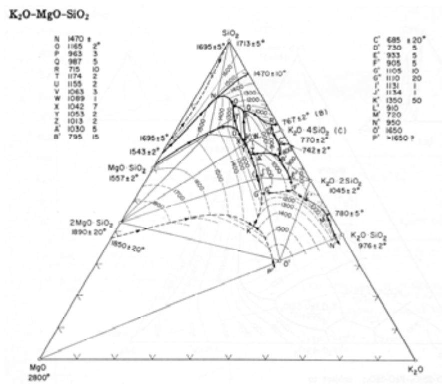


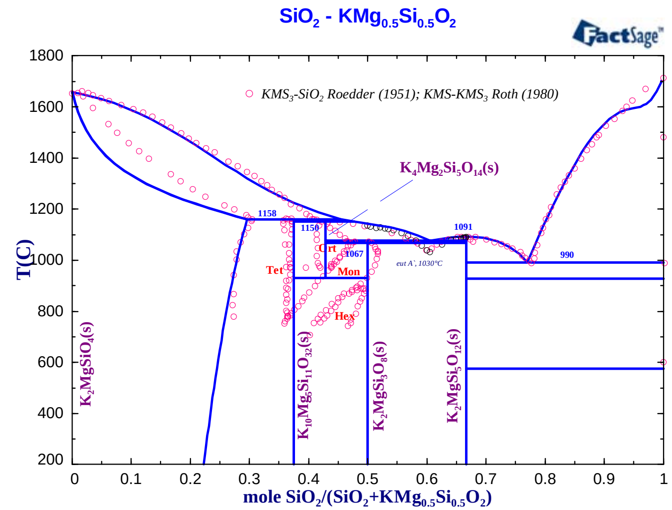
System K_2O-MgO-SiO_2; various binary sub-systems



System MgO·SiO2-K_2O·5MgO·12SiO_2; partially binary; K_2O·7SiO_2 not a compound

Assessment for ternary system K_2O-MgO-SiO_2





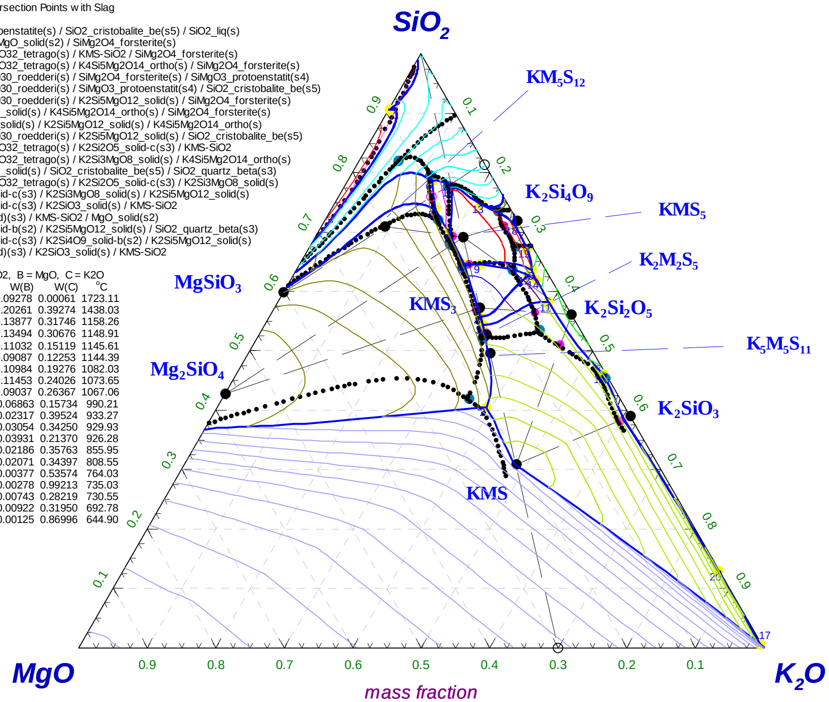
SiO_2 - K_2O - MgO

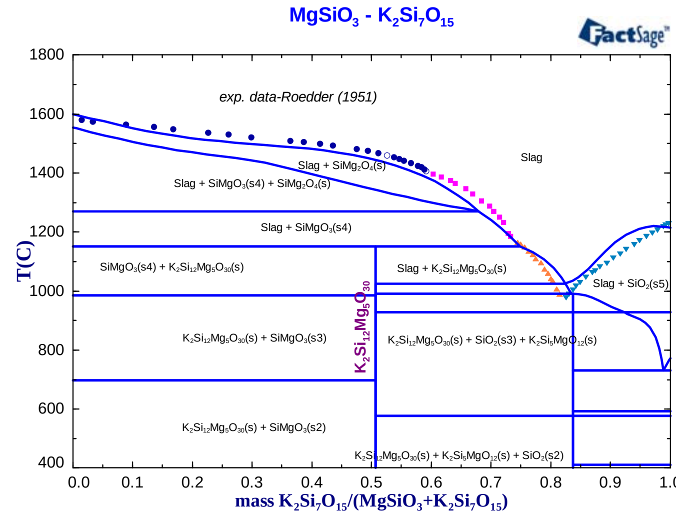
Four-Phase Intersection Points with Slag

1: SiMgO3_clinoenstatite(s) / SiO2_cristobalite_be(s5) / SiO2_liq(s)
2: KMS-SiO2 / MgO_solid(s2) / SiMg2O4_forsterite(s)
3: K10Si11Mg5O32_tetrago(s) / KMS-SiO2 / SiMg2O4_forsterite(s)
4: K10Si11Mg5O32_tetrago(s) / K4Si5Mg2O14_ortho(s) / SiMg2O4_forsterite(s)
5: K2Si12Mg5O30_roedderi(s) / SiMg2O4_forsterite(s) / SiMgO3_protoenstatit(s4)
6: K2Si12Mg5O30_roedderi(s) / SiMgO3_protoenstatit(s4) / SiO2_cristobalite_be(s5)
7: K2Si12Mg5O30_roedderi(s) / K2Si5MgO12_solid(s) / SiMg2O4_forsterite(s)
8: K2Si5MgO12_solid(s) / K4Si5Mg2O14_ortho(s) / SiMg2O4_forsterite(s)
9: K2Si3MgO8_solid(s) / K2Si5MgO12_solid(s) / K4Si5Mg2O14_ortho(s)
10: K2Si12Mg5O30_roedderi(s) / K2Si5MgO12_solid(s) / SiO2_cristobalite_be(s5)
11: K10Si11Mg5O32_tetrago(s) / K2Si2O5_solid-c(s3) / KMS-SiO2
12: K10Si11Mg5O32_tetrago(s) / K2Si3MgO8_solid(s) / K4Si5Mg2O14_ortho(s)
13: K2Si5MgO12_solid(s) / SiO2_cristobalite_be(s5) / SiO2_quartz_beta(s3)
14: K10Si11Mg5O32_tetrago(s) / K2Si2O5_solid-c(s3) / K2Si3MgO8_solid(s)
15: K2Si2O5_solid-c(s3) / K2Si3MgO8_solid(s) / K2Si5MgO12_solid(s)
16: K2Si2O5_solid-c(s3) / K2SiO3_solid(s) / KMS-SiO2
17: K2O_s3(solid)(s3) / KMS-SiO2 / MgO_solid(s2)
18: K2Si4O9_solid-b(s2) / K2Si5MgO12_solid(s) / SiO2_quartz_beta(s3)
19: K2Si2O5_solid-c(s3) / K2Si4O9_solid-b(s2) / K2Si5MgO12_solid(s)
20: K2O_s3(solid)(s3) / K2SiO3_solid(s) / KMS-SiO2

A = SiO2, B = MgO, C = K2O

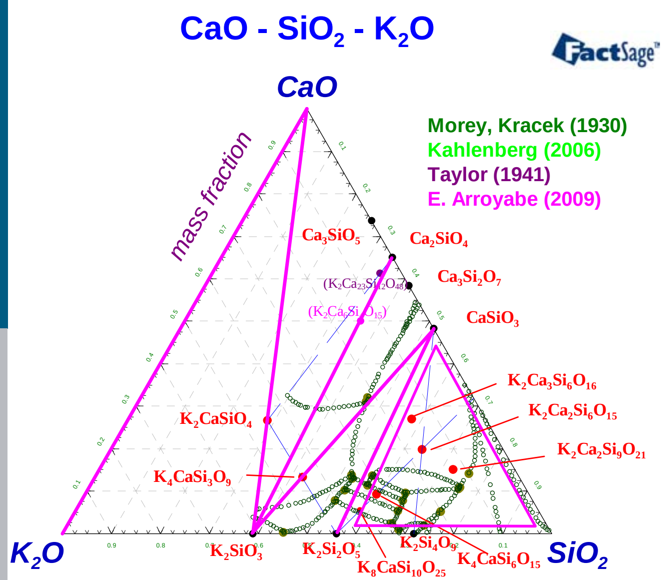
	W(A)	W(B)	W(C)	°C
1:	0.90661	0.09278	0.00061	1723.11
2:	0.40465	0.20261	0.39274	1438.03
3:	0.54377	0.13877	0.31746	1158.26
4:	0.55830	0.13494	0.30676	1148.91
5:	0.73849	0.11032	0.15119	1145.61
6:	0.78660	0.09087	0.12253	1144.39
7:	0.69740	0.10984	0.19276	1082.03
8:	0.64521	0.11453	0.24026	1073.65
9:	0.64596	0.09037	0.26367	1067.06
10:	0.77403	0.06863	0.15734	990.21
11:	0.58160	0.02317	0.39524	933.27
12:	0.62696	0.03054	0.34250	929.93
13:	0.74699	0.03931	0.21370	926.28
14:	0.62051	0.02186	0.35763	855.95
15:	0.63532	0.02071	0.34397	808.55
16:	0.46050	0.00377	0.53574	764.03
17:	0.00509	0.00278	0.99213	735.03
18:	0.71038	0.00743	0.28219	730.55
19:	0.67128	0.00922	0.31950	692.78
20:	0.12879	0.00125	0.86996	644.90





Ternary system K_2O-CaO-SiO_2

JÜLICH FORSCHUNGSZENTRUM



*G.W. Morey, F.C. Kracek, N.L. Bowen, The ternary system K_2O-CaO-SiO_2,J. Soc. Glass Technol. **14** (1930) 149-187.*

Liquid

- **binary associate species K_2O-SiO_2, CaO-K_2O, CaO-SiO_2 are kept**
- **new ternary species are introduced: $(K_2CaSiO_4)/2$**
- **new interaction parameters between binary and ternary species are added**

Solids

- **binary compounds from K_2O-SiO_2, CaO-K_2O, CaO-SiO_2 are kept**
- **new ternary compounds (K_2CaSiO_4, $K_4CaSi_3O_9$, $K_2Ca_2Si_9O_{21}$, $K_8CaSi_{10}O_{25}$, $K_4CaSi_6O_{15}$, $K_2Ca_2Si_6O_{15}$, $K_2Ca_3Si_6O_{16}$) are introduced**

Interacting components in liquid

K_2SiO_3*2/3 – $CaSiO_3$

K_2SiO_3*2/3 – CaO

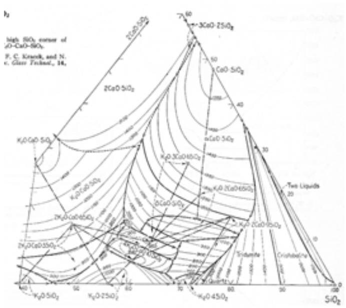
K_2O – Ca_2O_2

$K_2Si_2O_5$*1/2 – $CaSiO_3$

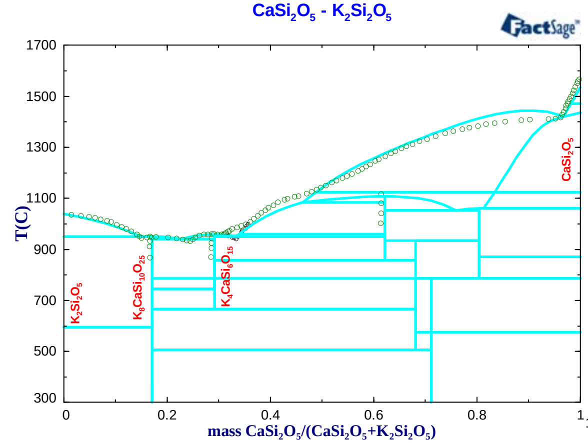
K_2SiO_3*2/3 – Ca_2SiO_4*2/3

$K_2Si_2O_5$*1/2 – Si_2O_4*1/2 - $CaSiO_3$

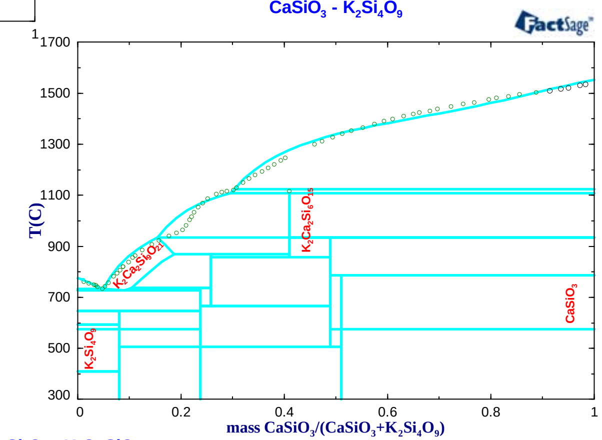
Current results for ternary system K_2O-CaO-SiO_2



$CaSi_2O_5$ - $K_2Si_2O_5$



$CaSiO_3$ - $K_2Si_4O_9$



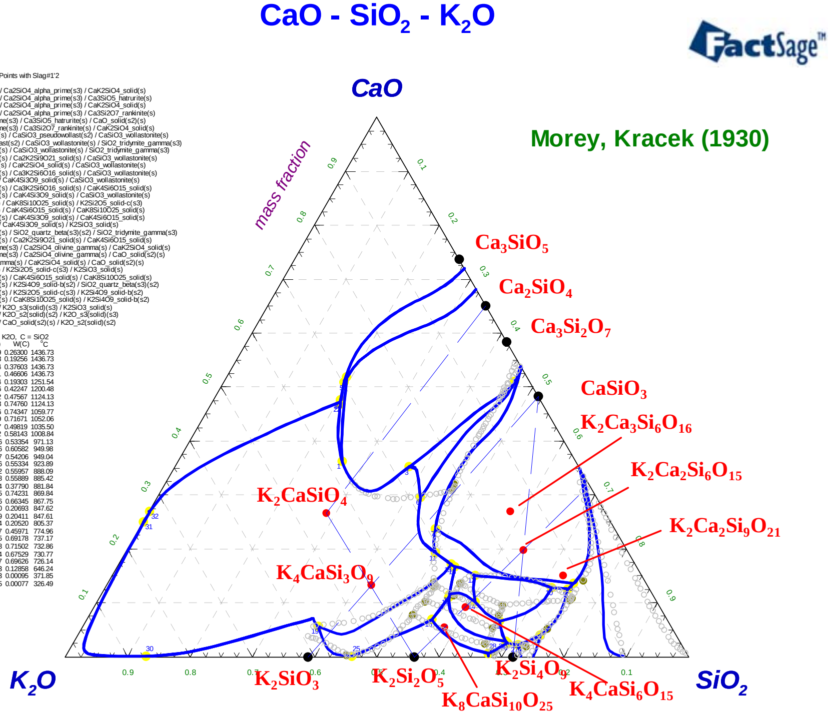
CaO - SiO_2 - K_2O

Four-Phase Intersection Points with Slag#1'2

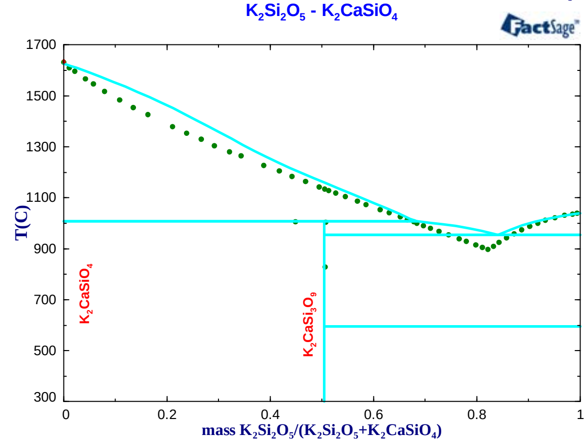
1: Ca2SiO4_alpha(s2) / Ca2SiO4_alpha_prime(s3) / CaK2SiO4_solid(s)
2: Ca2SiO4_alpha(s2) / Ca2SiO4_alpha_prime(s3) / Ca3SiO5_hatrurite(s)
3: Ca2SiO4_alpha(s2) / Ca2SiO4_alpha_prime(s3) / CaK2SiO4_solid(s)
4: Ca2SiO4_alpha(s2) / Ca2SiO4_alpha_prime(s3) / Ca3Si2O7_rankinite(s)
5: Ca2SiO4_alpha_prime(s3) / Ca3SiO5_hatrurite(s) / CaO_solid(s2)(s)
6: Ca2SiO4_alpha_prime(s3) / Ca3Si2O7_rankinite(s) / CaK2SiO4_solid(s)
7: Ca3Si2O7_rankinite(s) / CaSiO3_pseudowollast(s2) / CaSiO3_wollastonite(s)
8: CaSiO3_pseudowollast(s2) / CaSiO3_wollastonite(s) / SiO2_tridymite_gamma(s3)
9: Ca2K2Si9O21_solid(s) / CaSiO3_wollastonite(s) / SiO2_tridymite_gamma(s3)
10: Ca2K2Si6O15_solid(s) / Ca2K2Si9O21_solid(s) / CaSiO3_wollastonite(s)
11: Ca3Si2O7_rankinite(s) / CaK2SiO4_solid(s) / CaSiO3_wollastonite(s)
12: Ca2K2Si6O15_solid(s) / Ca3K2Si6O16_solid(s) / CaSiO3_wollastonite(s)
13: CaK2SiO4_solid(s) / CaK4Si3O9_solid(s) / CaSiO3_wollastonite(s)
14: Ca2K2Si6O15_solid(s) / Ca3K2Si6O16_solid(s) / CaK4Si6O15_solid(s)
15: Ca3K2Si6O16_solid(s) / CaK4Si3O9_solid(s) / CaSiO3_wollastonite(s)
16: CaK4Si3O9_solid(s) / CaK8Si10O25_solid(s) / K2Si2O5_solid-c(s3)
17: CaK4Si3O9_solid(s) / CaK4Si6O15_solid(s) / CaK8Si10O25_solid(s)
18: Ca3K2Si6O16_solid(s) / CaK4Si3O9_solid(s) / CaK4Si6O15_solid(s)
19: CaK2SiO4_solid(s) / CaK4Si3O9_solid(s) / K2SiO3_solid(s)
20: Ca2K2Si9O21_solid(s) / SiO2_quartz_beta(s3)(s2) / SiO2_tridymite_gamma(s3)
21: Ca2K2Si6O15_solid(s) / Ca2K2Si9O21_solid(s) / CaK4Si6O15_solid(s)
22: Ca2SiO4_alpha_prime(s3) / Ca2SiO4_olivine_gamma(s) / CaK2SiO4_solid(s)
23: Ca2SiO4_alpha_prime(s3) / Ca2SiO4_olivine_gamma(s) / CaO_solid(s2)(s)
24: Ca2SiO4_olivine_gamma(s) / CaK2SiO4_solid(s) / CaO_solid(s2)(s)
25: CaK4Si3O9_solid(s) / K2Si2O5_solid-c(s3) / K2SiO3_solid(s)
26: Ca2K2Si9O21_solid(s) / CaK4Si6O15_solid(s) / CaK8Si10O25_solid(s)
27: Ca2K2Si9O21_solid(s) / K2Si4O9_solid-b(s2) / SiO2_quartz_beta(s3)(s2)
28: CaK8Si10O25_solid(s) / K2Si2O5_solid-c(s3) / K2Si4O9_solid-b(s2)
29: Ca2K2Si9O21_solid(s) / CaK8Si10O25_solid(s) / K2Si4O9_solid-b(s2)
30: CaK2SiO4_solid(s) / K2O_s3(solid)(s3) / K2SiO3_solid(s)
31: CaK2SiO4_solid(s) / K2O_s2(solid)(s2) / K2O_s3(solid)(s3)
32: CaK2SiO4_solid(s) / CaO_solid(s2)(s) / K2O_s2(solid)(s2)

A = CaO, B = K2O, C = SiO2

	W(A)	W(B)	W(C)	°C
1:	0.36231	0.37469	0.26300	1436.73
2:	0.51836	0.28908	0.19256	1436.73
3:	0.35193	0.27204	0.37603	1436.73
4:	0.51013	0.02381	0.46606	1436.73
5:	0.50834	0.29864	0.19303	1251.54
6:	0.29507	0.28246	0.42247	1200.48
7:	0.23770	0.28662	0.47567	1124.13
8:	0.13592	0.11648	0.74760	1124.13
9:	0.12517	0.13136	0.74347	1059.77
10:	0.12780	0.15549	0.71671	1052.06
11:	0.19234	0.30947	0.49819	1035.50
12:	0.15056	0.26802	0.58143	1008.84
13:	0.17119	0.29526	0.53354	971.13
14:	0.10253	0.29166	0.60582	949.98
15:	0.16638	0.29157	0.54206	949.04
16:	0.06870	0.37796	0.55334	923.89
17:	0.10980	0.33062	0.55957	888.09
18:	0.11524	0.32588	0.55889	885.42
19:	0.05566	0.56644	0.37790	881.84
20:	0.03914	0.21855	0.74231	869.84
21:	0.06559	0.27096	0.66345	867.75
22:	0.46877	0.32430	0.20693	847.62
23:	0.47600	0.31989	0.20411	847.61
24:	0.47316	0.32164	0.20520	805.37
25:	0.00053	0.53977	0.45971	774.96
26:	0.02857	0.27965	0.69178	737.17
27:	0.02240	0.26258	0.71502	732.86
28:	0.00637	0.31834	0.67529	730.77
29:	0.02597	0.27777	0.69626	726.14
30:	0.00079	0.87063	0.12858	646.24
31:	0.24981	0.74923	0.00095	371.85
32:	0.26949	0.72975	0.00077	326.49



$K_2Si_2O_5$ - K_2CaSiO_4

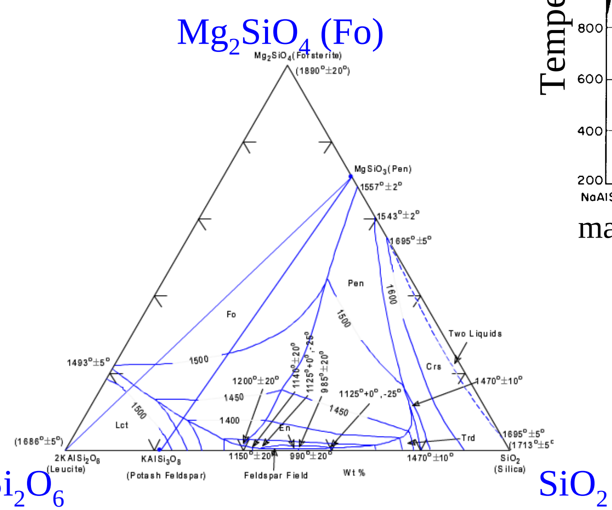


Conclusions

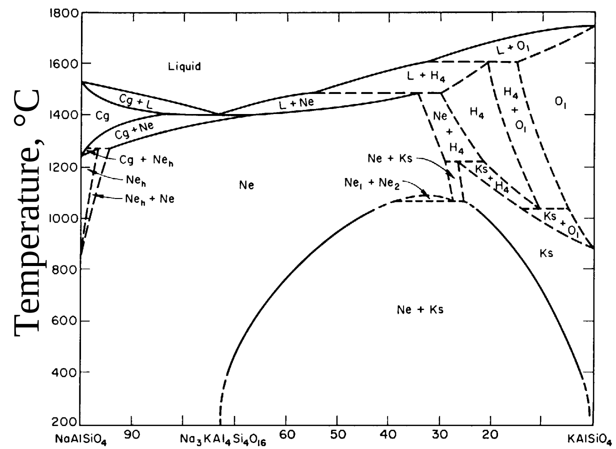
- The solution data for the binary systems Alk_2O-SiO_2, Alk_2O-Al_2O_3 (Alk=Na, K) and Al_2O_3-SiO_2 were re-optimised to accurate description of the phase diagrams taking into account the changes concerning the data on the pure liquid oxides
- Solid and liquid solutions in the ternary systems Na_2O-K_2O-SiO_2, Alk_2O-Al_2O_3-SiO_2 (Alk=Na, K) and quaternary Na_2O-K_2O-Al_2O_3-SiO_2 as well were described using the new database
- Sublattice model was successfully applied for the solid solutions in the many-component systems
- The ternary systems concerning earth alkali oxides are considered. The corresponding thermodynamic data on the new ternary compounds and the liquid and solid solutions are added in order to calculate the ternary phase diagrams

Outlook

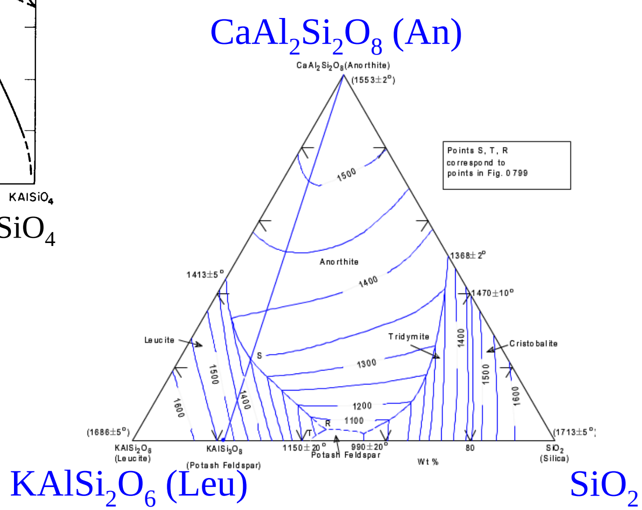
- Assessment of the system $NaAlSiO_4$-$KAlSiO_4$-SiO_2 system
- Creation of the database for quaternary solutions with the compositions (Na, K)(Al, Si)O_4 and different structures
- Alk_2O-MgO-SiO_2 (Alk=Na, K) systems should be finished
- Further “fusion” of the thermodynamic data on earth alkali- and alkali-containing parts of the slag relevant system

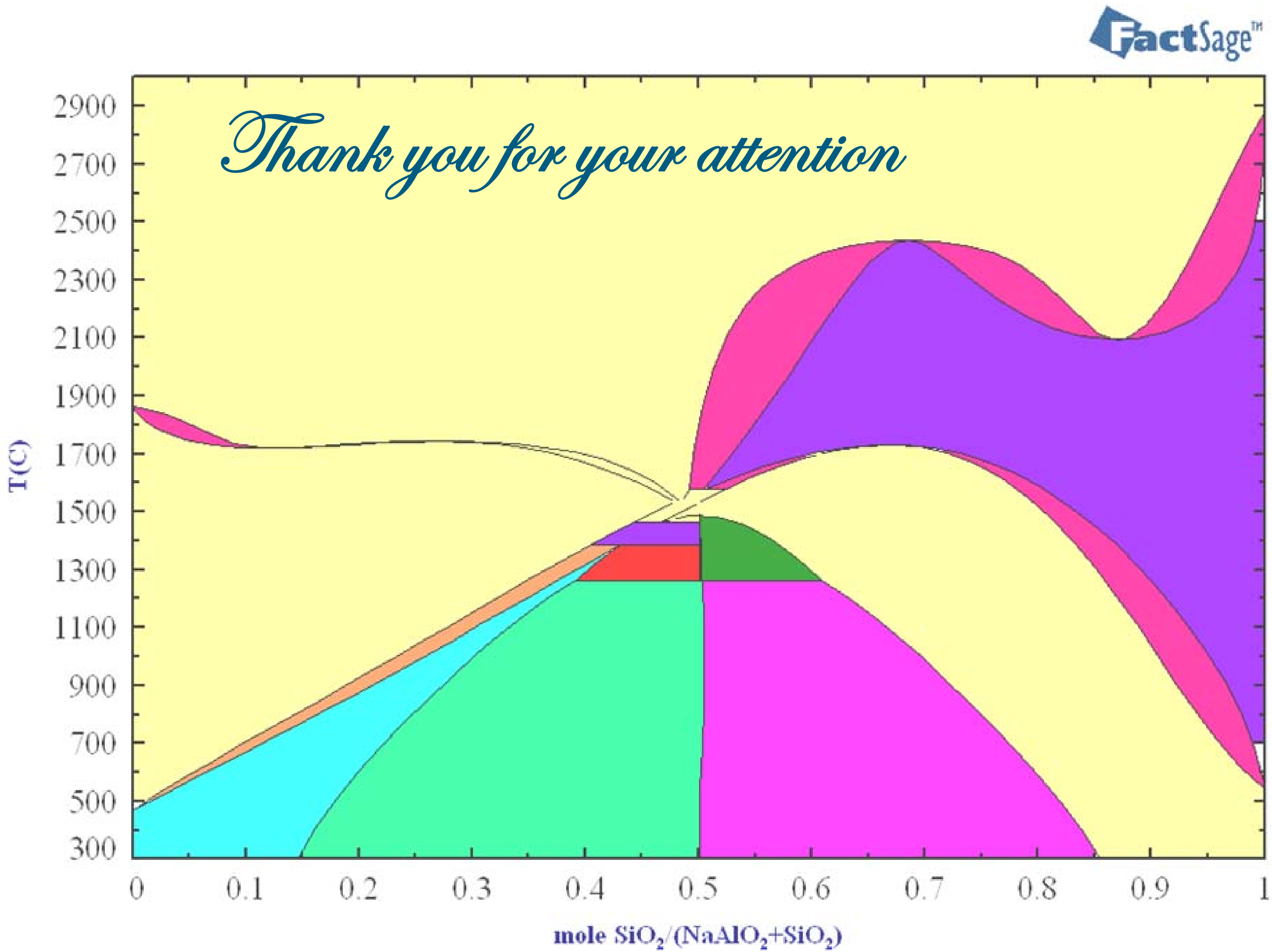


$NaAlSiO_4$ – $KAlSiO_4$



mass percent $KAlSiO_4$/$NaAlSiO_4$+$KAlSiO_4$





FactSage™
Thank you for your attention
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
300
T(C)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
mole $SiO_2/(NaAlO_2+SiO_2)$