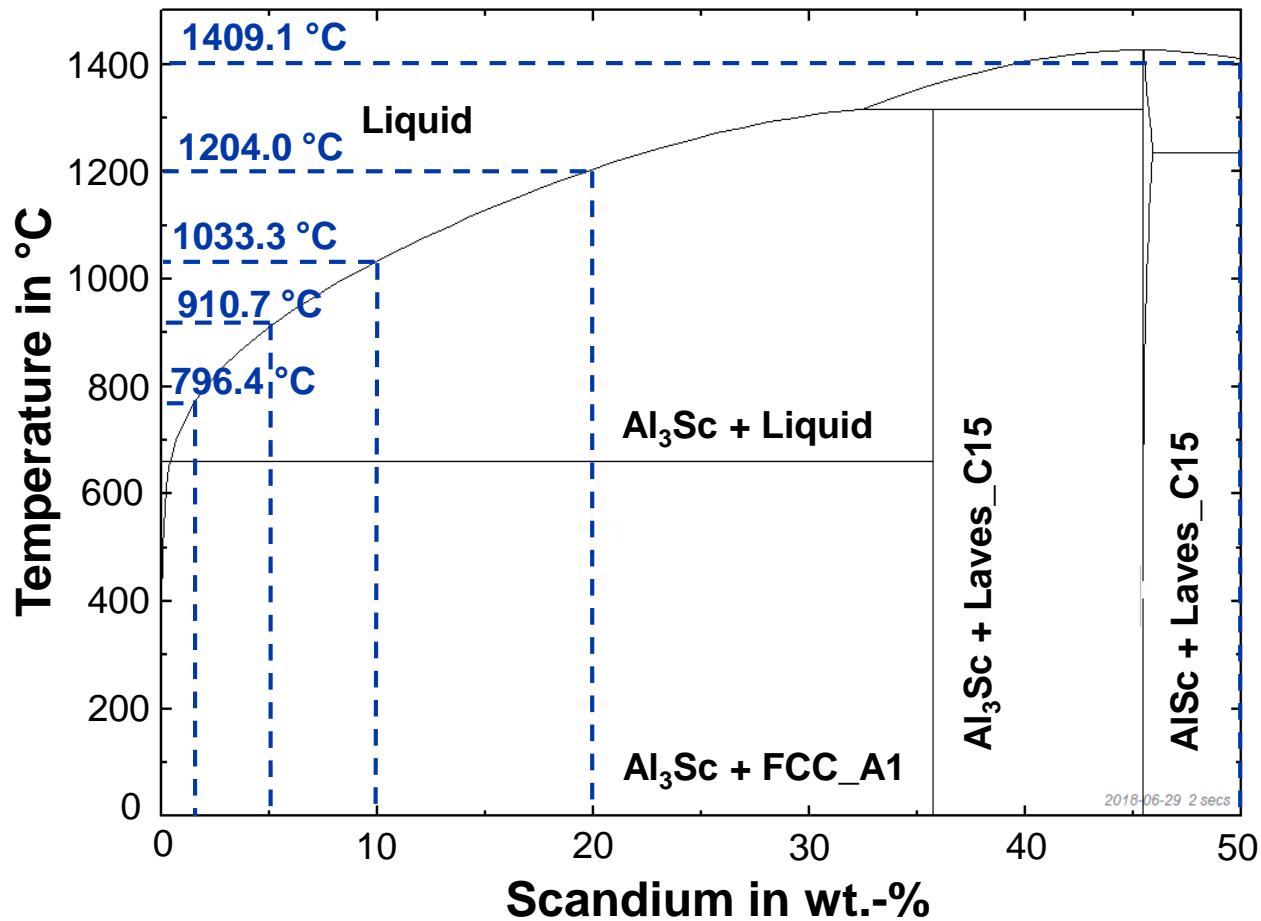


# Modeling Metallothermic Reduction of Aluminium-Scandium Alloys in FactSage 7.2

Frederic Brinkmann, Carolin Mazurek

# Melting Point of Aluminium-Scandium Alloys



# Calculations in FactSage 7.2

Equilib - Reactants

File Edit Table Units Data Search Help

T(C) P(atm) Energy(J) Mass(g) Vol(litre)

1-2

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
20	Sc				1	
+ 80	Al				1	

**Example for 20 wt.-% Al-Sc alloy**

Initial Conditions

Next >>

FactSage 7.2 Compound: 2/20 databases Solution: 1/19 databases

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Mass(g) Vol(litre)

Reactants (2)

(gram) 20 Sc + 80 Al

Products

Compound species

- gas  ideal  real 4
- aqueous 0
- pure liquids 0
- \* pure solids 17
- \* - custom selection species: 21

Solution phases

*	+	Base-Phase	Full Name
	l	FTlite-Liqu	Liquid
	l	FTlite-FCC	FCC_A1
	l	FTlite-BCC	BCC_A2
	l	FTlite-HCP	HCP_A3
	+	FTlite-B2	BCC_B2
	l	FTlite-C15	Laves_C15
	+	FTlite-L12	Prototype_AuCu3-L12
	+	FTlite-L12b	Prototype_AuCu3-L12b

Transitions - temperature

Number of transitions: All

Legend

- l - immiscible 5
- + - selected 4

Show  all  selected

species: 28 solutions: 14 Select

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		0 2000	1	

10 steps  Table 2+ calculations

Equilibrium

- normal
- normal + transitions
- transitions only
- open

Calculate >>>

FactSage 7.2

Equilib - Results 1204.04 C (page 3/3)

Output Edit Show Pages

T(C) P(atm) Energy(J) Mass(g) Vol(litre)

660.15 C | 660.16 C - 1204.04 C -

Species	Amount/mol	Mass fraction
Al	0.44488	0.20000
Sc	2.9650	0.80000

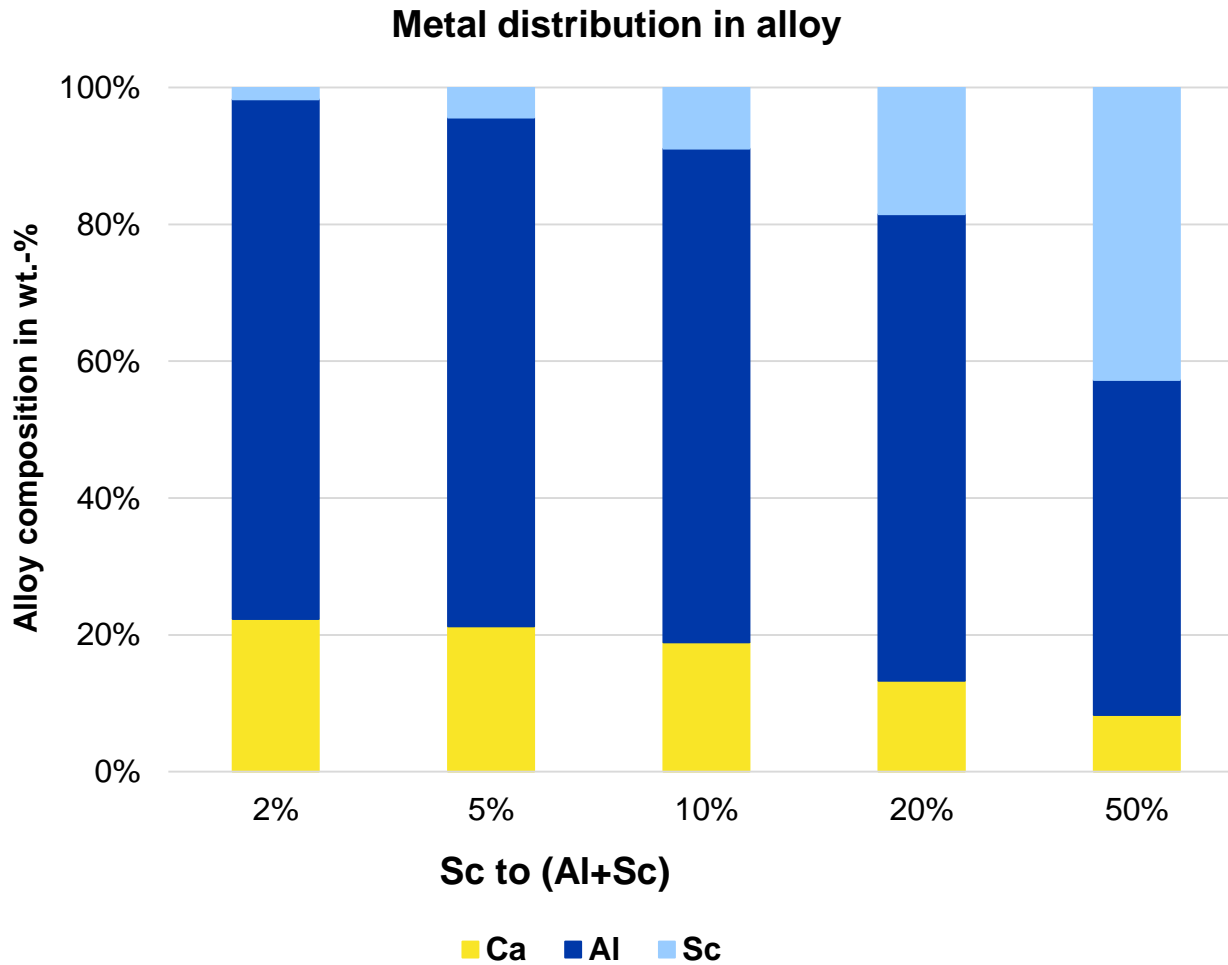
**One liquid phase at 1204.04 °C**

Phase	Species	Amount/mol	Mass fraction	Activity
PHASE: Liquid#1;#2	Al	8.0000E+01	8.0000E-01	7.5835E-01
	Sc	2.0000E+01	2.0000E-01	5.6763E-05
	TOTAL:	1.0000E+02	1.0000E+00	1.0000E+00
PHASE: Prototype_AuCu3-L12	Al3Sc	0.0000E+00	1.0000E+00	1.0000E+00
	TOTAL:	0.0000E+00	1.0000E+00	1.0000E+00
	Sys			
PHASE: BCC_A2#1;#2	Al	0.0000E+00	7.3292E-01	3.6105E-01
	Sc	0.0000E+00	2.6708E-01	7.0240E-05
	TOTAL:	0.0000E+00	1.0000E+00	7.8853E-01
PHASE: FCC_A1#1;#2	Al	0.0000E+00	8.2511E-01	4.5994E-01
	Sc	0.0000E+00	1.7489E-01	5.3897E-05
	TOTAL:	0.0000E+00	1.0000E+00	5.8162E-01
PHASE: Laves C15#1;#2	Al	0.0000E+00	0.86953	0.86953
	Sc	0.0000E+00	0.13047	0.20000
	TOTAL:	0.0000E+00	1.0000E+00	1.0000E+00

## Equilib-Mode

- Database: FactPS, FTlite

# Modeling Aluminium-Scandium Alloys



# Calculations in FactSage 7.2

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
1	ScF3				1	
+ 15.82	Al2O3				1	
+ 19.245	Ca				1	

## Equilib-Mode

- Database: FactPS, FToxid, FTsalt and FTlite
- Results at 1400 °C and 1 atm
- Varying the amount of feed material to get Al-Sc alloys with different Sc-quantities (always starting with 1 g of Al)

Calculation of the composition of various Al-Sc alloys by using ScF3, Al2O3 and Ca as feed material

Example here for 5 wt.-% Al-Sc alloy

Databases - 4/20 compound databases, 3/19 solution databases

**Fact**  FactPS  FToxid  FTsalt  FTmisc  FTall  FT0xCN  FTfritz  FTHelg  FTpulp  FTlite

**FactSage**  FSopp  FSlead  FSstel  FSupsi  ELEM  FTdemo  FTnucl

**SGTE**  BINS  SGPS  SGTE  SGsold  SGnucl

**Private Databases**  SGTEa

Information -  
In Options it is recommended that the 'Minimum solution components' be set to '2'

Compound: C:\FactSage7.2\FACTDATA\Fslead54base.cdb  
- FSlead - FactSage lead intermetallic compounds (2015)

Solution: C:\FactSage7.2\FACTDATA\Fslead54soln.sdc  
- FSlead - FactSage lead alloy solutions (2015)

Options - search for product species

Include compounds:  
 gaseous ions (plasmas)  
 aqueous species

Limits:  
Organic species CxHy..., X(max) = 2  
Minimum solution components: 1 2 3 cpts

# Calculations in FactSage 7.2

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Mass(g) Vol(litre)

Reactants (3)

(gram) ScF3 + 15.82 Al2O3 + 19.245 Ca

Products

Compound species: gas ideal real 34, aqueous 0, pure liquids 0, pure solids 28, custom selection species: 62

Target: none, Estimate T(K): 1000, Mass(g): 0

Final Conditions: T(C) 1400, P(atm) 1, Product H(J)

Equilibrium: normal, transitions only, open

Solution phases table:

*	+	Base-Phase	Full Name
	+	FToxid-CaAl	CaAl2O4
	+	FToxid-MeA2	(Ca,Sr)Al4O7
	+	FToxid-MeA6	(Ca,Sr,Ba)Al12O19
	+	FToxid-CaFh	CaF2-HT
	+	FToxid-CaFl	CaF2-LT
	+	FTsalt-CaFH	CaF2-HT
	+	FTsalt-CaFL	CaF2-LT
		FTsalt-SALTA	A-Salt-liquid

Legend: - immiscible 9, + selected 26, species: 102, solutions: 44

Equilib - Results 1400 C

Output Edit Show Pages

T(C) P(atm) Energy(J) Mass(g) Vol(litre)

```

+ 3.0142E-46 O3
+ 1.4420E-54 O2F(g)
+ 3.3360E-61 F2O2)

+ 20.531 gram Monoxide#1
(20.531 gram, 0.36542 mol)
+ 0 gram Monoxide#2
(1400 C, 1 atm, a=1.0000)
( 99.577 wt.% CaO
+ 0.42345 wt.% Al2O3)

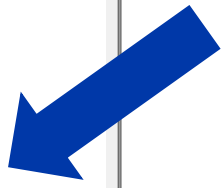
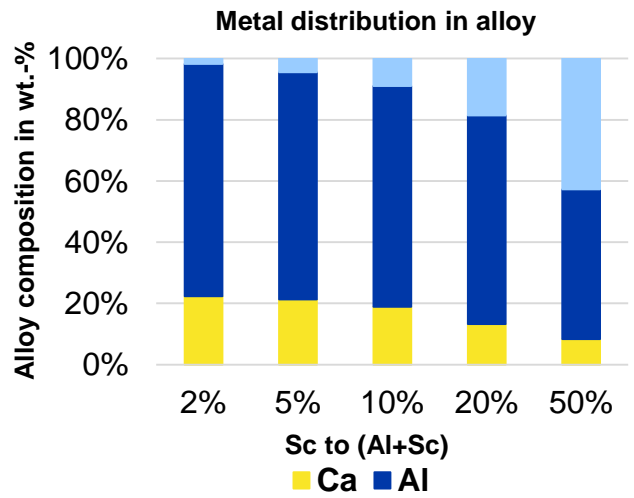
System component      Amount/mol      Amount/gram      Mole fraction      Mass fraction
Ca                     0.36457         14.611           0.49709            0.71166
Al                     1.7053E-03      4.6012E-02       2.3252E-03         2.2411E-03
O                      0.36713         5.8738           0.50058            0.28605

+ 9.9837 gram Liquid#1
(9.9837 gram, 0.33778 mol)
+ 0 gram Liquid#2
(1400 C, 1 atm, a=1.0000)
( 74.326 wt.% Al
+ 21.257 wt.% Ca
+ 2.8554E-15 wt.% F
+ 6.0954E-04 wt.% O
+ 4.4168 wt.% Sc)

System component      Amount/mol      Amount/gram      Mole fraction      Mass fraction
Sc                    9.8086E-03      0.44096          2.9038E-02         4.4168E-02
Ca                    5.2953E-02      2.1222           0.15677            0.21257
Al                    0.27502         7.4204           0.81419            0.74326
F                     1.5005E-17      2.8507E-16      4.4422E-17         2.8554E-17
O                     3.8035E-06      6.0854E-05      1.1260E-05         6.0954E-06

+ 5.5504 gram Liq-Oxyfluoride#1
(5.5504 gram, 8.1649E-02 mol)
+ 0 gram Liq-Oxyfluoride#2
(1400 C, 1 atm, a=1.0000)

```

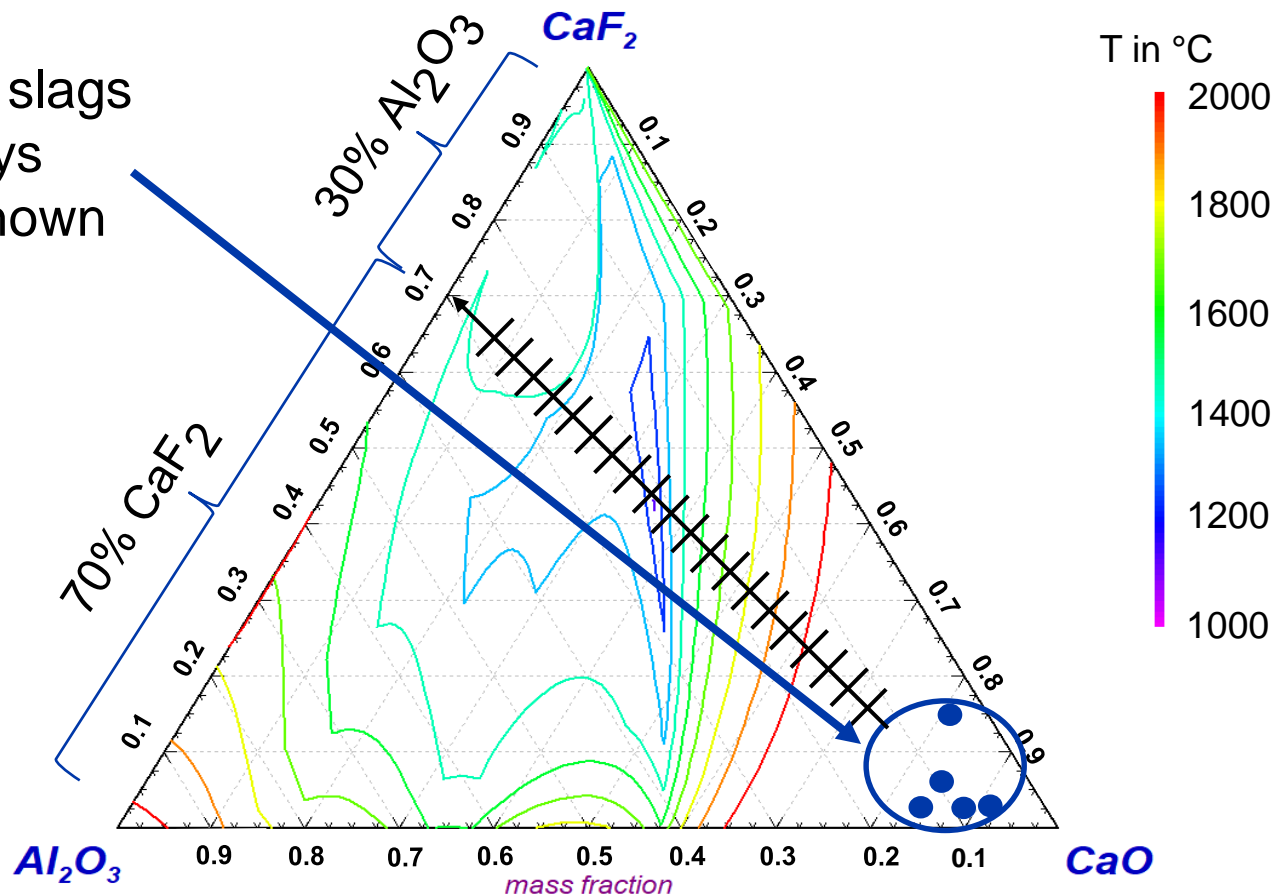


# Modeling of the Slag

## System for 20 % Al-Sc Alloy:

1 g  $\text{ScF}_3$  + 3,33 g  $\text{Al}_2\text{O}_3$  + 4,52 g Ca

Here are the slags  
from the alloys  
previously shown



# Modeling of the Slag

## Target System:

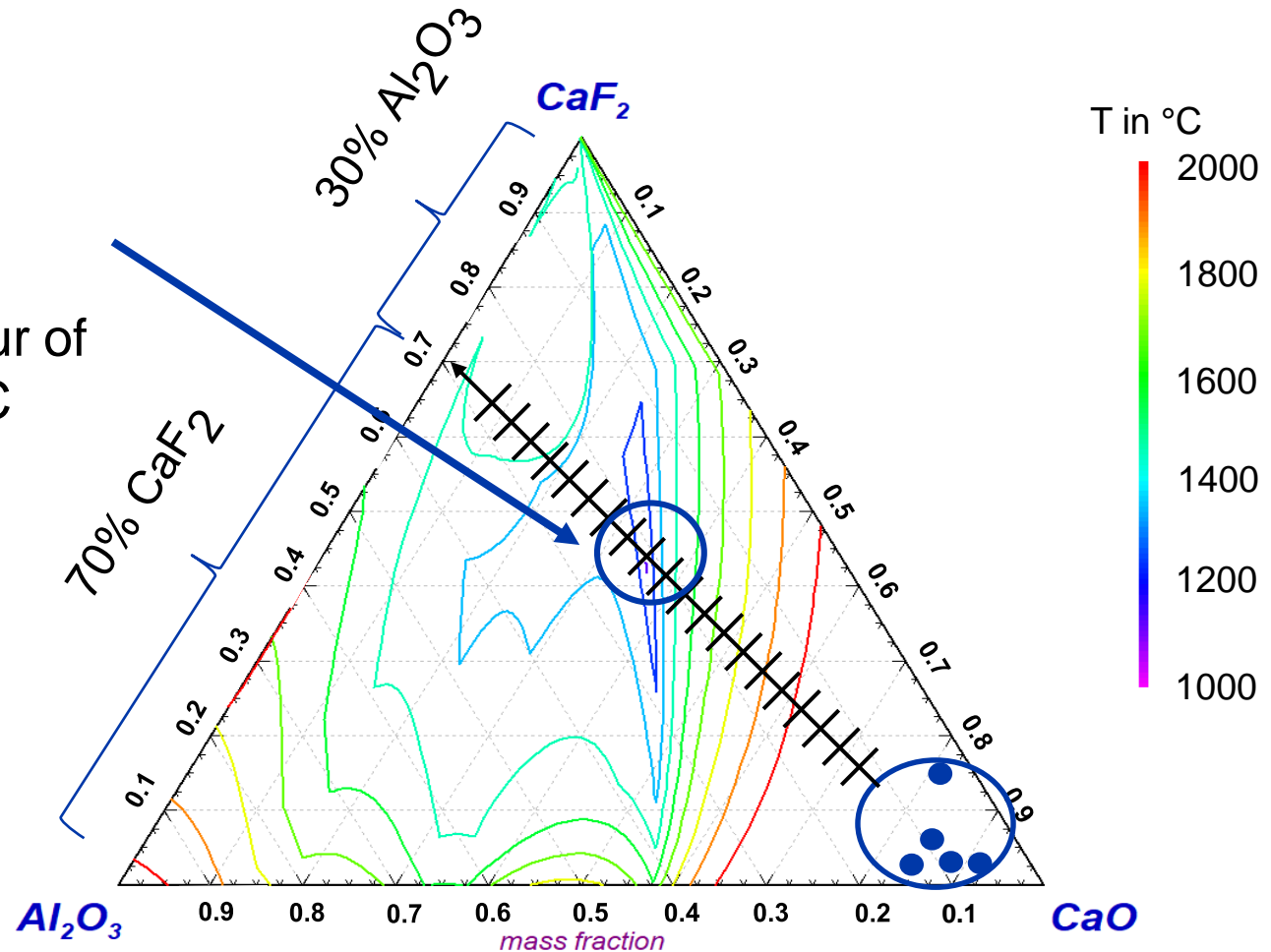
1 g  $\text{ScF}_3$  + (3.33 + 0.3·x) g  $\text{Al}_2\text{O}_3$  + (0.7·x) g  $\text{CaF}_2$  + 4.52 g Ca

x: Coefficient on line

Coefficient **x = 10**  
shows best results



Liquidus temperatur of  
the slag: 1247.5 °C





# Calculations in FactSage 7.2

## Calculated systems:

Coefficient	CaF2	Al2O3	ScF3	Al2O3	Ca
0	0	0	1	3,332	4,5188499
1	0,7	0,3	1	3,332	4,5188499
2	1,4	0,6	1	3,332	4,5188499
3	2,1	0,9	1	3,332	4,5188499
4	2,8	1,2	1	3,332	4,5188499
5	3,5	1,5	1	3,332	4,5188499
6	4,2	1,8	1	3,332	4,5188499
7	4,9	2,1	1	3,332	4,5188499
8	5,6	2,4	1	3,332	4,5188499
9	6,3	2,7	1	3,332	4,5188499
10	7	3	1	3,332	4,5188499
11	7,7	3,3	1	3,332	4,5188499
12	8,4	3,6	1	3,332	4,5188499
13	9,1	3,9	1	3,332	4,5188499
14	9,8	4,2	1	3,332	4,5188499
15	10,5	4,5	1	3,332	4,5188499
16	11,2	4,8	1	3,332	4,5188499
17	11,9	5,1	1	3,332	4,5188499
18	12,6	5,4	1	3,332	4,5188499
19	13,3	5,7	1	3,332	4,5188499
20	14	6	1	3,332	4,5188499



The screenshot shows the 'Equilib - Reactants' window in FactSage 7.2. The 'Reactants' list contains four entries:

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
1	ScF3				1	
+ 3.632	Al2O3				1	
+ 4.5188499	Ca				1	
+ 0.7	CaF2				1	

Below this, the 'Equilib - Menu: last system' window is visible, showing the 'Reactants (4)' list: (gram) ScF3 + 3.632 Al2O3 + 4.5188499 Ca + 0.7 CaF2. The 'Products' section shows a list of solution phases, with 'FTlite-Liqu' (Liquid) selected. The 'Final Conditions' are set to T(C) = 1400 and P(atm) = 1. The 'Equilibrium' options are set to 'normal'.

## Equilib-Mode

- Databases also FactPS, FToxid, FTsalt and FTlite
- Results at 1400 °C and 1 atm
- Varying the amount of feed material to get 20 wt.-% Al-Sc alloy with different slags

# Calculations in FactSage 7.2

Coefficient	Slag to metal ratio	slag composition					melting temperature [°C]	metal composition				
		CaO	Al <sub>2</sub> O <sub>3</sub>	CaF <sub>2</sub>	AlF <sub>3</sub>	Sc <sub>2</sub> O <sub>3</sub>		Ca	Al	Sc	Al	Sc
0	2,72	81,1%	2,4%	13,6%	2,9%		2304,9	13,3%	68,2%	18,5%	78,6%	21,4%
1	3,15	72,6%	4,6%	18,1%	4,7%		2155,24	12,9%	68,5%	18,6%	78,7%	21,3%
2	3,58	65,9%	6,4%	21,6%	6,1%	0,00279	2017,19	12,8%	68,7%	18,5%	78,8%	21,2%
3	4,00	60,7%	7,8%	24,3%	7,1%	0,00649	1897,11	12,8%	68,8%	18,4%	78,9%	21,1%
4	4,43	56,4%	9,0%	26,6%	8,0%	0,00883	1781,93	12,7%	68,9%	18,4%	78,9%	21,1%
5	4,85	52,9%	10,0%	28,4%	8,7%	0,01043	1679,03	12,7%	68,9%	18,3%	79,0%	21,0%
6	5,27	50,0%	10,8%	30,0%	9,2%	0,01160	1586,74	12,7%	69,0%	18,3%	79,0%	21,0%
7	5,70	47,4%	11,5%	31,3%	9,7%	0,01249	1489,57	12,7%	69,0%	18,3%	79,0%	21,0%
8	6,14	45,4%	12,0%	32,4%	10,2%	0,01236	1389,53	12,3%	69,3%	18,3%	79,1%	20,9%
9	6,67	44,1%	12,1%	33,1%	10,7%	0,01760	1299,14	10,0%	71,6%	18,5%	79,5%	20,5%
10	7,21	43,0%	12,1%	33,7%	11,2%	0,03523	1247,54	8,0%	73,8%	18,2%	80,2%	19,8%
11	7,74	41,9%	12,2%	34,1%	11,7%	0,05748	1279,13	6,6%	75,7%	17,8%	81,0%	19,0%
12	8,26	41,0%	12,3%	34,5%	12,2%	0,07844	1330,49	5,5%	77,2%	17,3%	81,7%	18,3%
13	8,77	40,1%	12,4%	34,8%	12,7%	0,09568	1353,81	4,7%	78,4%	16,9%	82,2%	17,8%
14	9,26	39,3%	12,5%	35,0%	13,1%	0,10916	1361,94	4,1%	79,3%	16,6%	82,7%	17,3%
15	9,75	38,6%	12,6%	35,2%	13,6%	0,11966	1363,04	3,7%	80,0%	16,4%	83,0%	17,0%
16	10,24	38,0%	12,7%	35,4%	14,0%	0,12806	1359,91	3,3%	80,5%	16,2%	83,3%	16,7%
17	10,72	37,4%	12,8%	35,5%	14,4%	0,13504	1354,24	3,1%	80,9%	16,0%	83,5%	16,5%
18	11,19	36,8%	12,9%	35,6%	14,7%	0,14109	1361,16	2,8%	81,3%	15,8%	83,7%	16,3%
19	11,67	36,3%	13,0%	35,6%	15,1%	0,14655	1370,68	2,6%	81,7%	15,7%	83,9%	16,1%
20	12,15	35,9%	13,1%	35,7%	15,4%	0,15164	1376,86	2,4%	82,0%	15,6%	84,0%	16,0%

Coefficient of **x = 10** shows best results

- Melting temperature of slag is 1247.54 °C
- Alloy composition is nearly targeted value with 19.8 wt.-% Sc in Al-Sc alloy (after distillation step for Ca-removal)
- Slag to metal ratio is high but acceptable



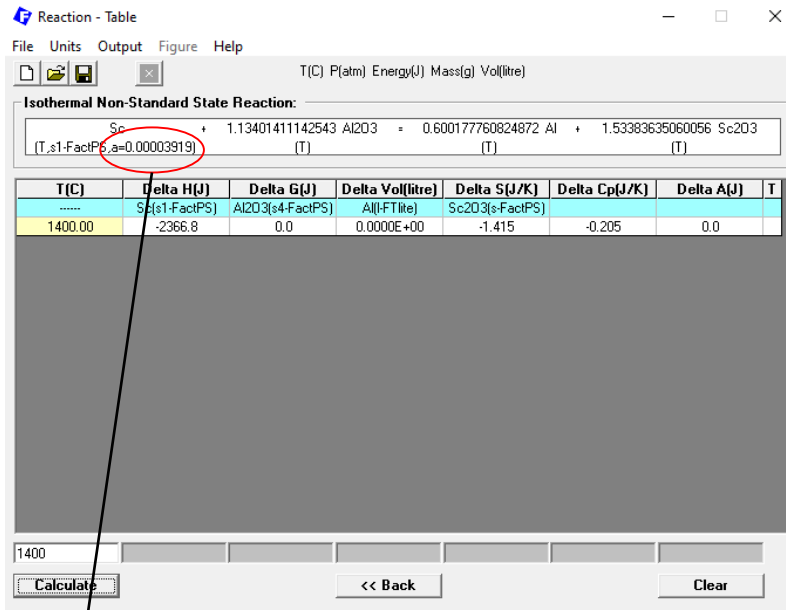
## Feed material

ScF <sub>3</sub>	1 g
Al <sub>2</sub> O <sub>3</sub>	6.332 g
CaF <sub>2</sub>	7 g
Ca	4.52 g

# Calculations in FactSage 7.2

## Sc in Ca/Al: Reaction/Equilib module

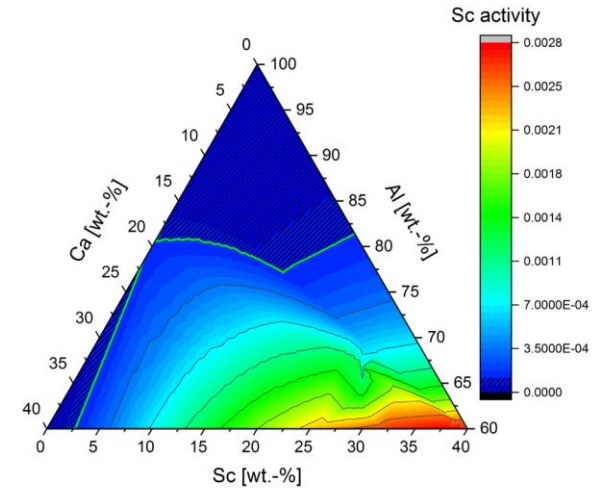
1.



### Reaction module

- Derive equilibrium activity of Sc in contact  $\text{Al}_2\text{O}_3$  (most unstable substance in system)
- Threshold for maximum content attainable in Al-Sc-Ca alloy

2.



### Equilib module

- Calculate Sc activity in the Al-rich corner of the ternary Al-Sc-Ca system with multiple binary cuts
- Indicate the regions where Sc activity is below the derived threshold