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

**Frederic Brinkmann, Carolin Mazurek**

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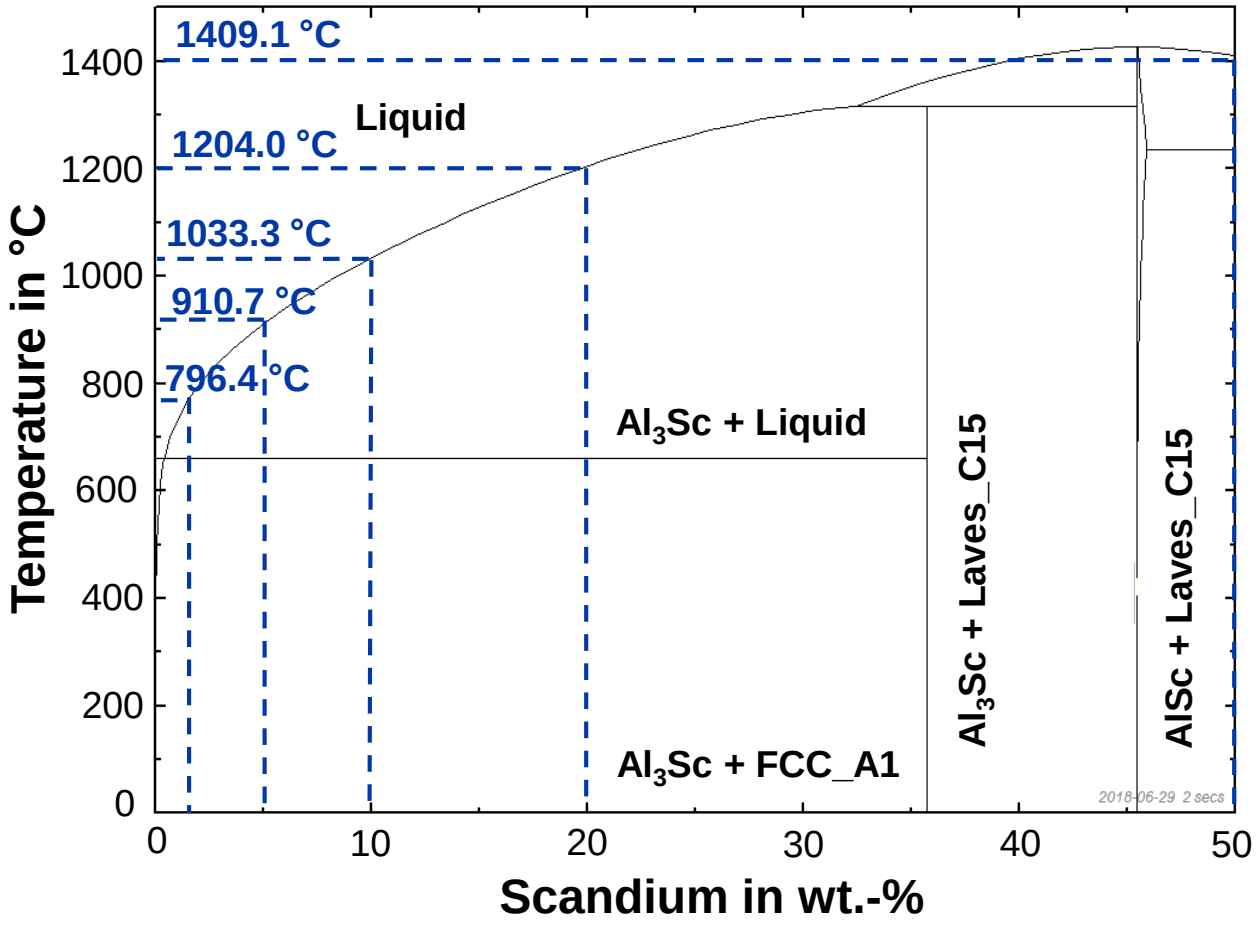
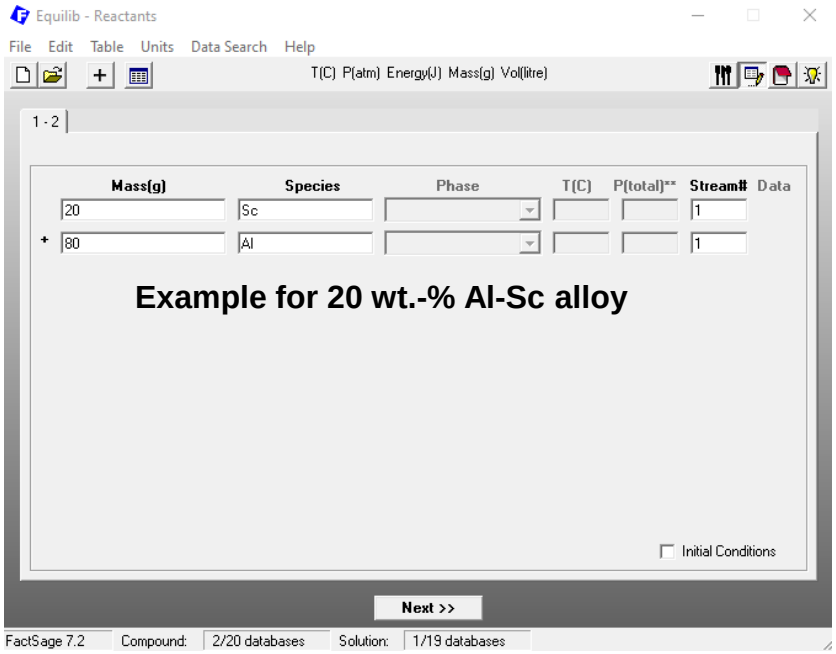
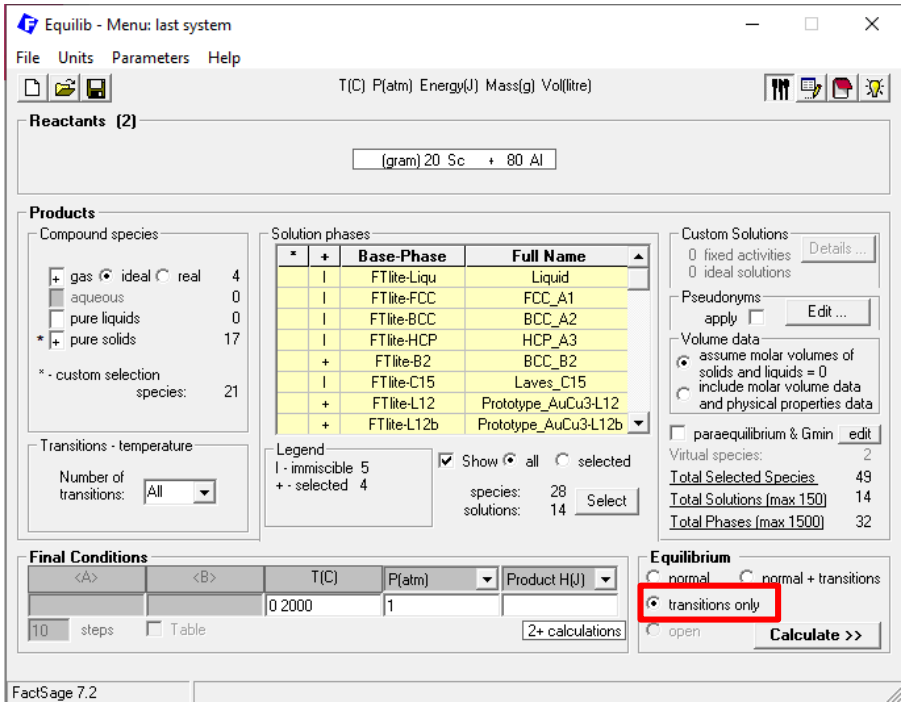
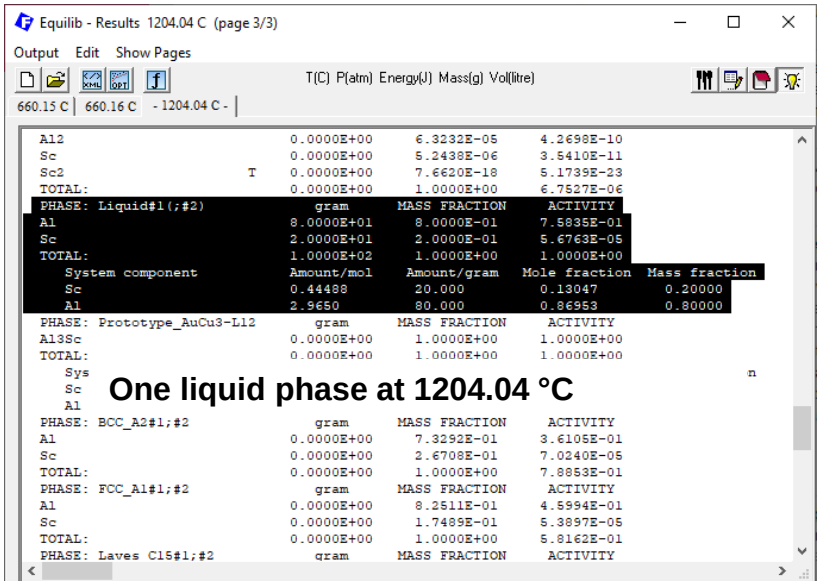
# Melting Point of Aluminium-Scandium Alloys



# Calculations in FactSage 7.2




## Equilib-Mode

- Database: FactPS, FTlite

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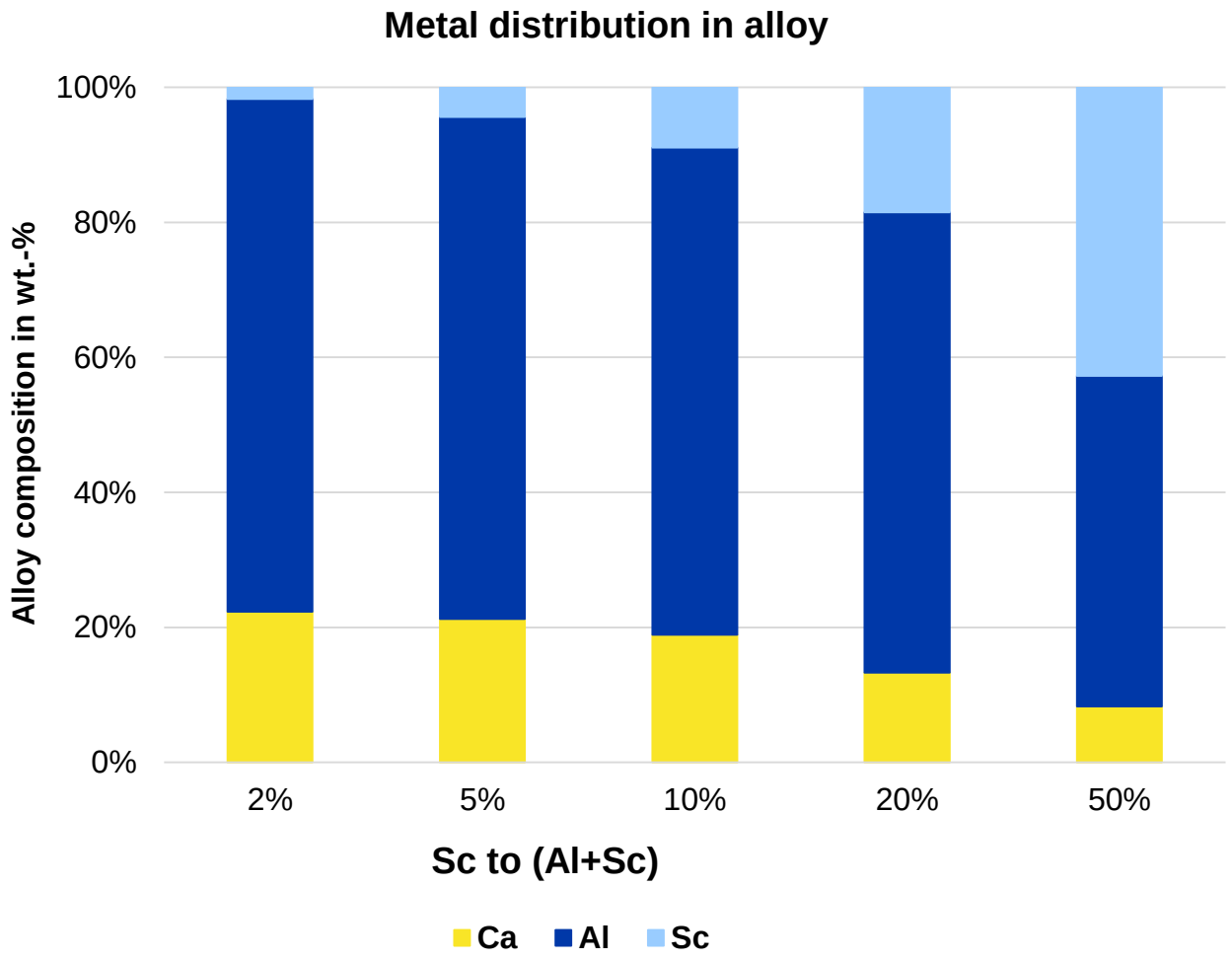
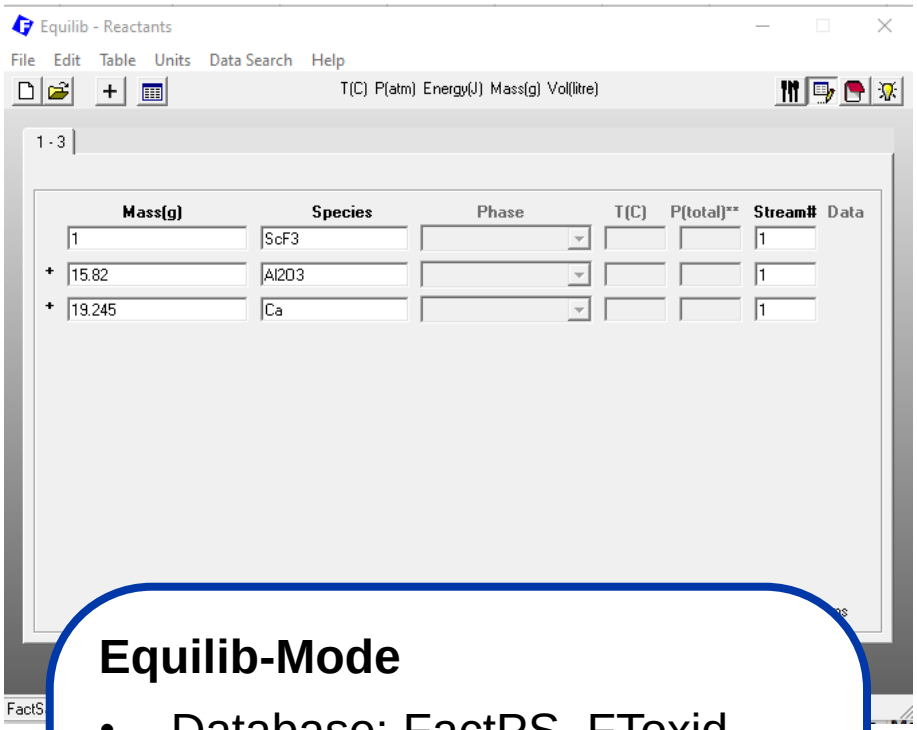
# Modeling Aluminium-Scandium Alloys

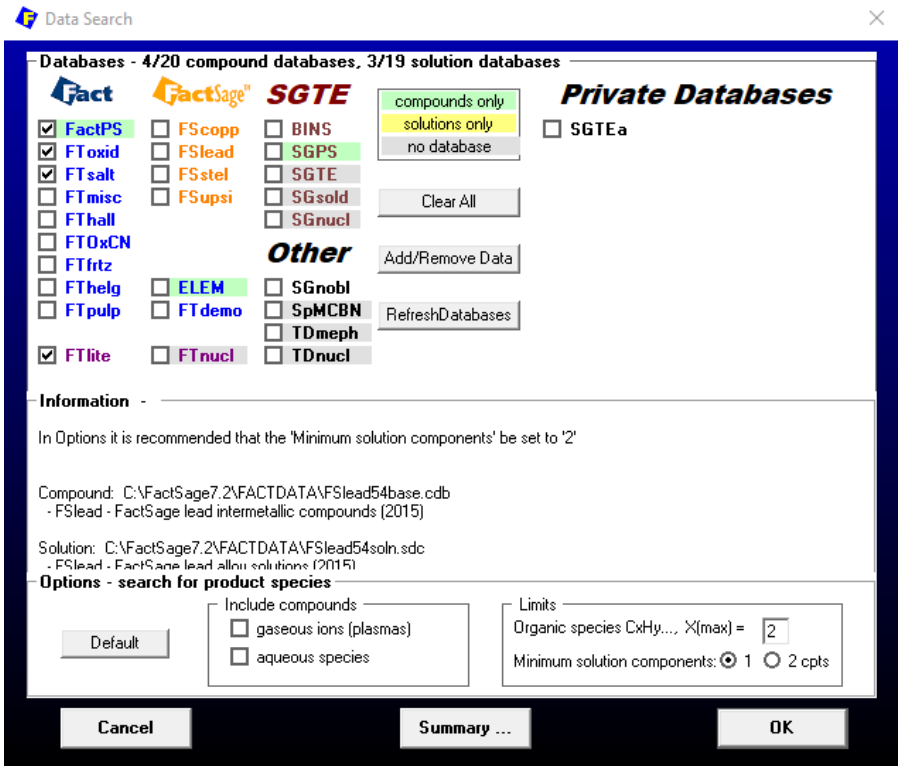


# Calculations in FactSage 7.2




**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**




## 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)

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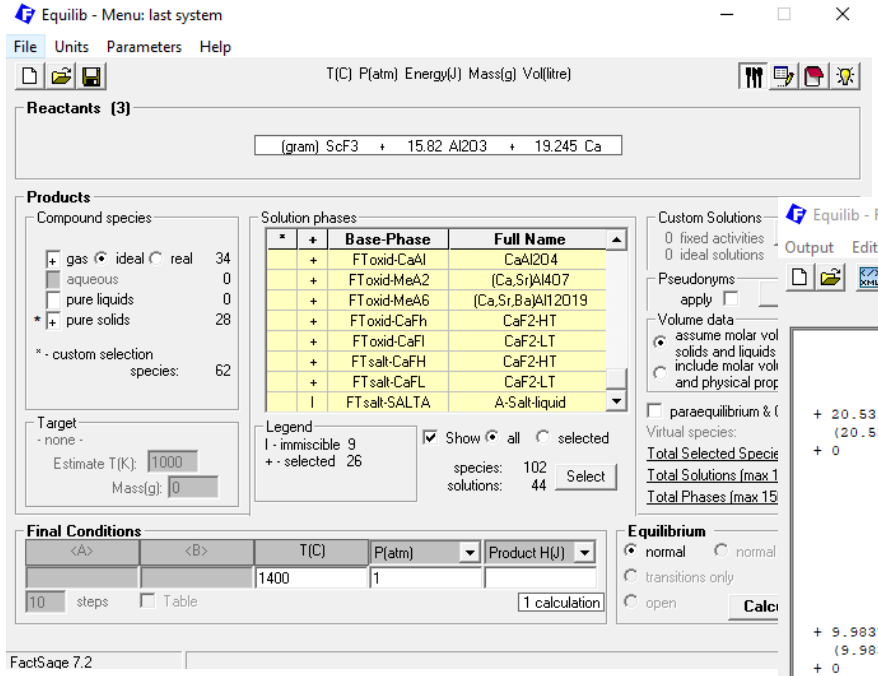
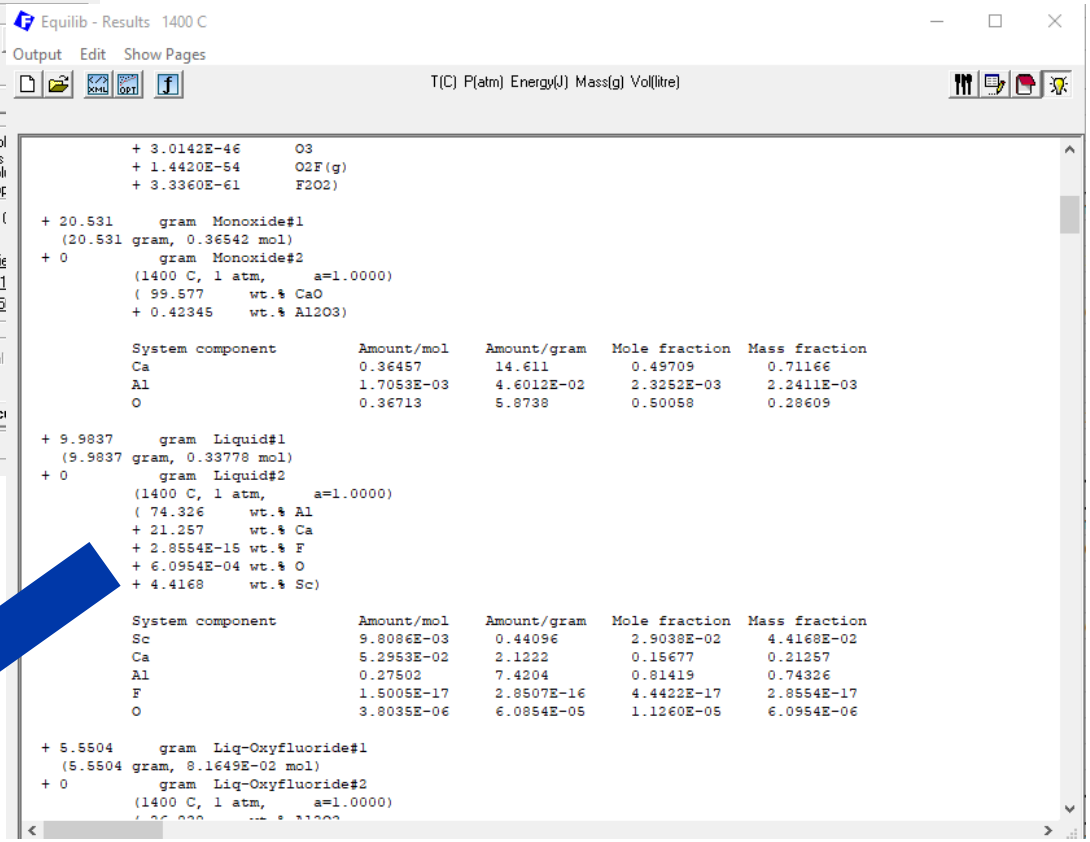
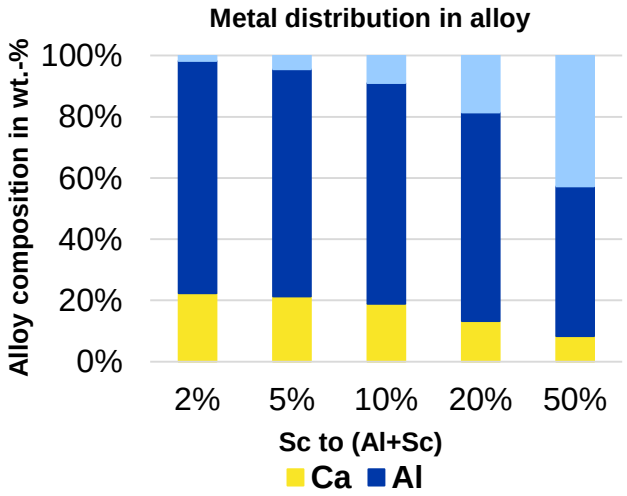
# Calculations in FactSage 7.2

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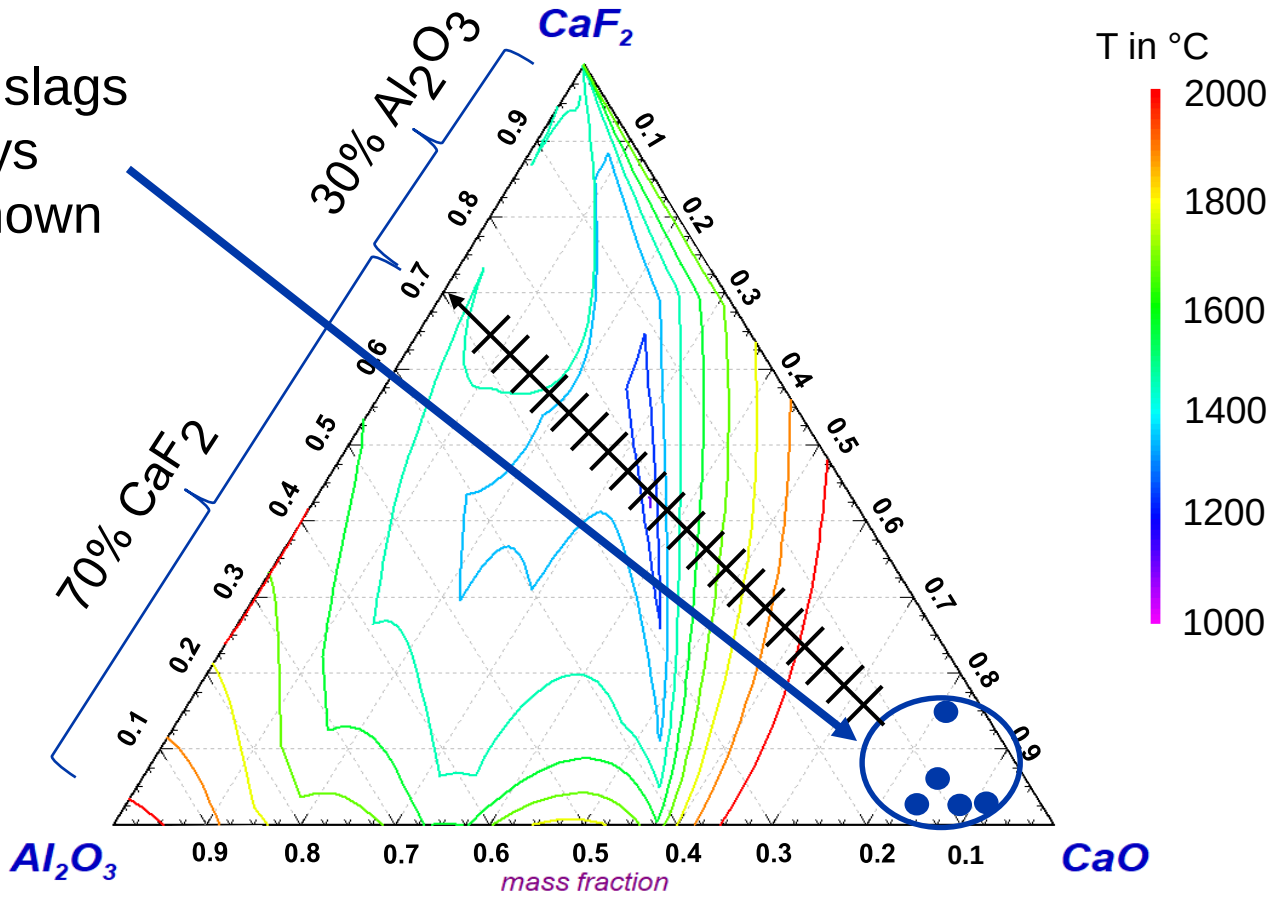
# Modeling of the Slag

**System for 20 % Al-Sc Alloy:**

1 g $ScF_3$ + 3,33 g $Al_2O_3$ + 4,52 g Ca

Here are the slags from the alloys previously shown



# Modeling of the Slag

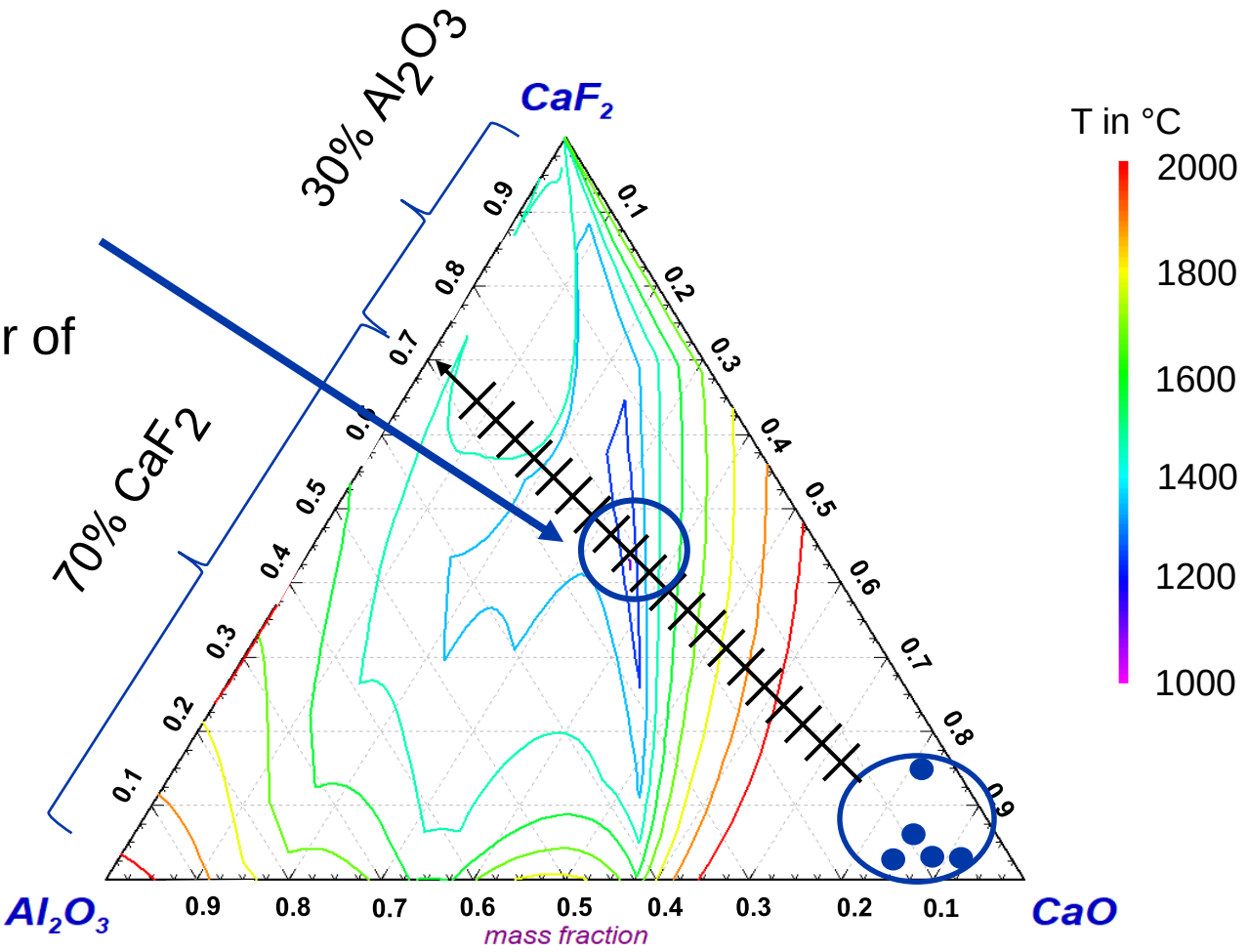
**Target System:**

1 g $ScF_3$+(3.33 + 0.3·x) g $Al_2O_3$+ (0.7·x) g $CaF_2$ + 4.52 g Ca

x: Coefficient on line

Coefficient x = 10
shows best results

Liquidus temperatur of the slag: 1247.5 °C

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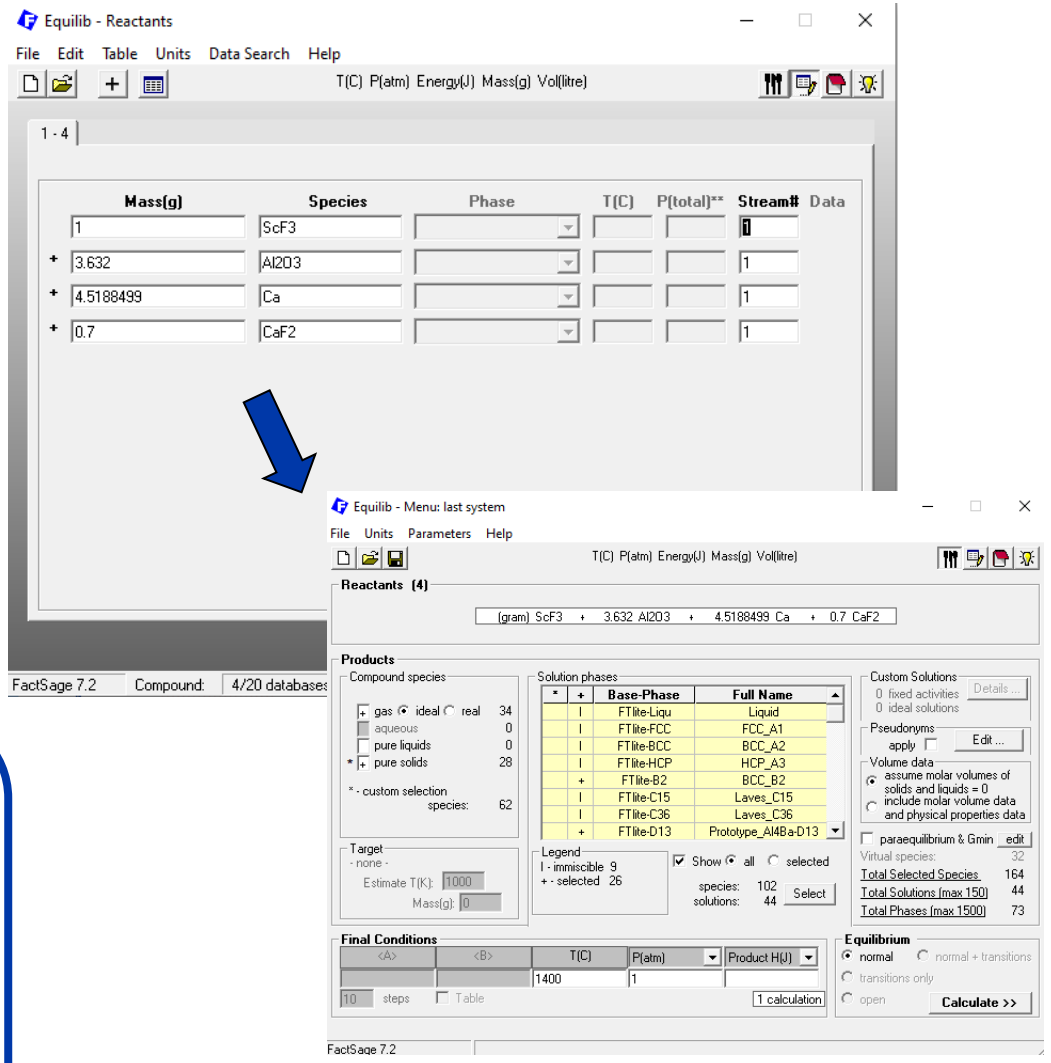
# Calculations in FactSage 7.2

## 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 |




## 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

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# Calculations in FactSage 7.2

| | Slag to metal ratio | slag composition | | | | | | metal composition | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Coefficient | | CaO | Al2O3 | CaF2 | AlF3 | Sc2O3 | melting temperature [°C] | 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 temperatur of slag is 1247.54 °C
- Alloy composition is nearly targeted value with 19.8 wt.-% Sc in Al-Sc alloy (after destillation step for Ca-removal)
- Slag to metal ratio is high but acceptable

**Feed material**

| | |
|---|---|
| $ScF_3$ | 1 g |
| $Al_2O_3$ | 6.332 g |
| $CaF_2$ | 7 g |
| Ca | 4.52 g |

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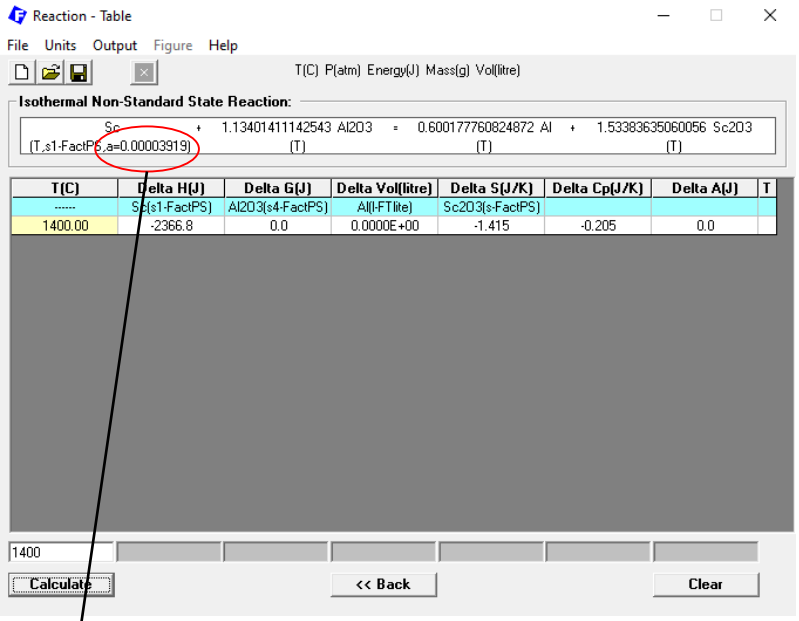
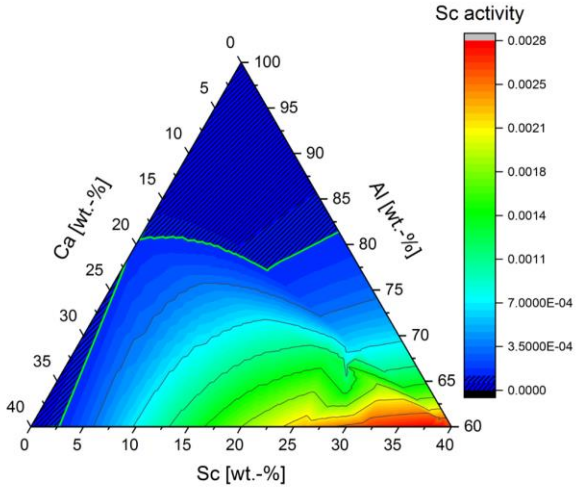
# Calculations in FactSage 7.2

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

**1.**




**2.**




### Reaction module

- Derive equilibrium activity of Sc in contact $Al_2O_3$ (most unstable substance in system)
- Threshold for maximum content attainable in Al-Sc-Ca alloy

### 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