

FactSage Practical

MSE302

Practical 3. Phase Diagram Calculation

Acknowledgements

The teaching team of MSE302 is grateful to:

Professor Mansoor Barati (UofT)

Professor Elmira Moosavi (ETS)

Professor Arthur Pelton (CRCT)

Professors In-Ho Jung and M. -A. Van Ende (Seoul National University)

Dr. Sina Mostaghel (SNC-Lavalin)

Professor Kinnor Chattopadhyay (UofT)

Drs. Daigen Fukayama, Takahiro Sasaki (RCCM)

Drs. Moritz to Baden and Guixuan Wu (GTT Technologies)

Phase Diagram Calculations in FactSage

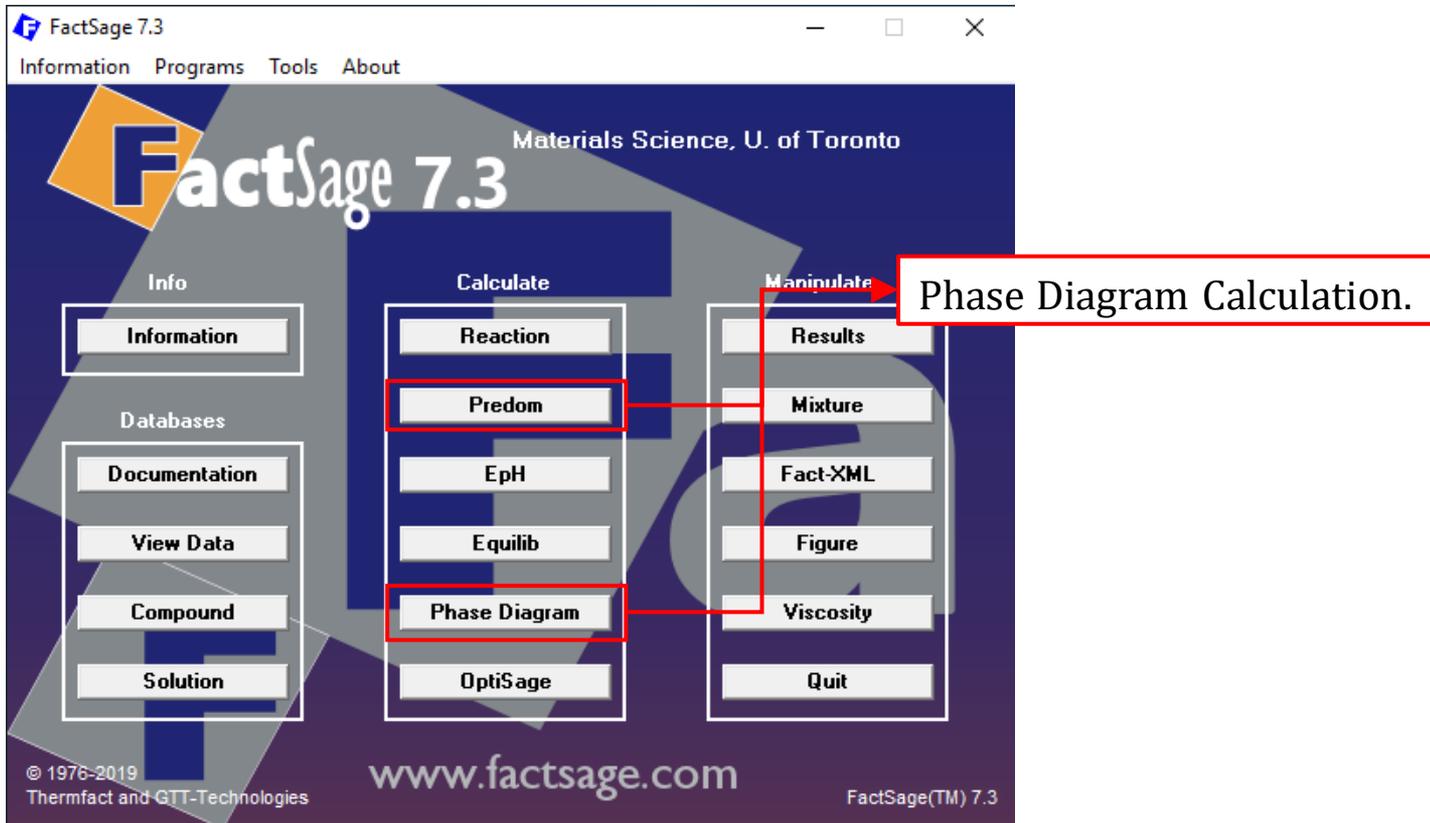
We have already shown in the *FactSage Overview* that there are three modules which are available in FactSage 7.3 for the calculation of phase diagrams:

- ✓ **Predom Module.**
- ✓ **EpH Module.**
- ✓ **Phase Diagram Module.**

In MSE302, since our focus is mainly on the **non-aqueous system**, the EpH module will not be discussed. However, you should be aware that in fields of electrochemistry and hydrometallurgy, the EpH module has found wide applications.

Phase Diagram Calculations in FactSage

Predom Module and Phase Diagram Module



FactSage Practical

MSE302

Practical 3. Phase Diagram Calculation

Predom Module

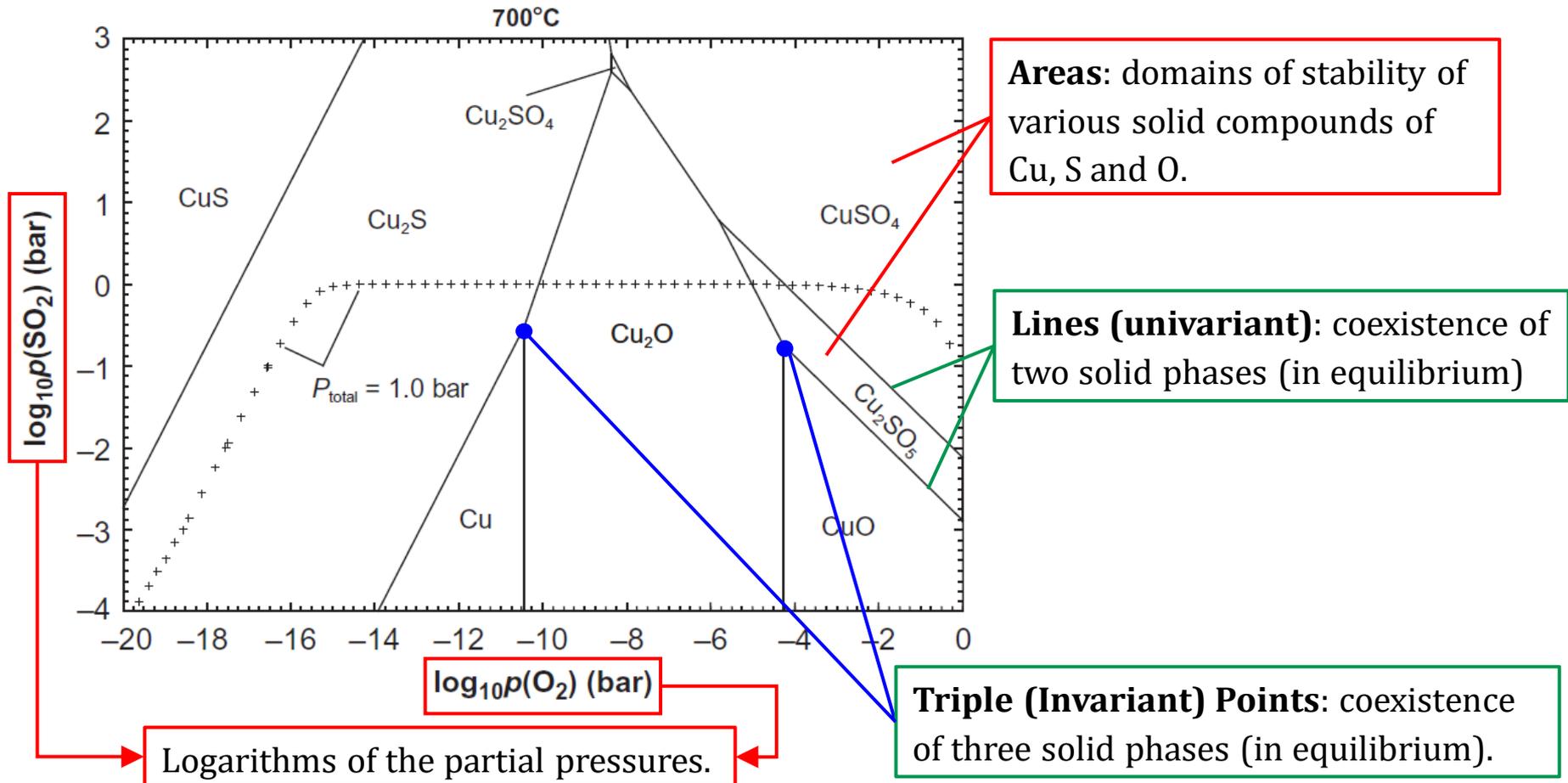
Predominance Diagram

The **predominance diagrams** are a particularly simple type of phase diagram that have many applications in the fields of hot corrosion, chemical vapor deposition, etc.

Let us discuss the construction of a predominance diagram using the Cu-SO₂-O₂ system.

Predominance Diagram: Theoretical Basis

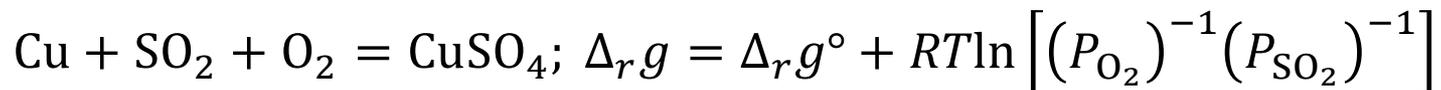
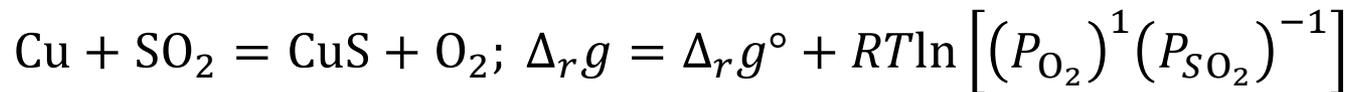
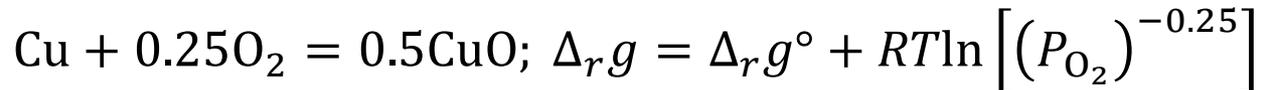
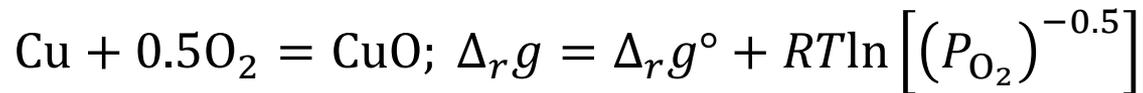
Predominance Diagram of the Cu-SO₂-O₂ System at 700 °C



Predominance Diagram: Theoretical Basis

A **predominance diagram** can be constructed by calculating the lines which indicate the coexistence of two solid compounds. The detailed procedure has been discussed by Bale et al.

We formulate a reaction for the formation of each solid phase, always from 1.0 mol of Cu and involving the gaseous species whose pressures are used as the axes; here, we use SO_2 and O_2 .



At equilibrium, $\Delta_r g = 0$, and $\log(P_{\text{SO}_2}) \sim \log(P_{\text{O}_2})$ can be calculated.

Predominance Diagram: Theoretical Basis

You can repeat the above procedure for the formation of Cu_2S , Cu_2SO_4 , and Cu_2SO_5 .

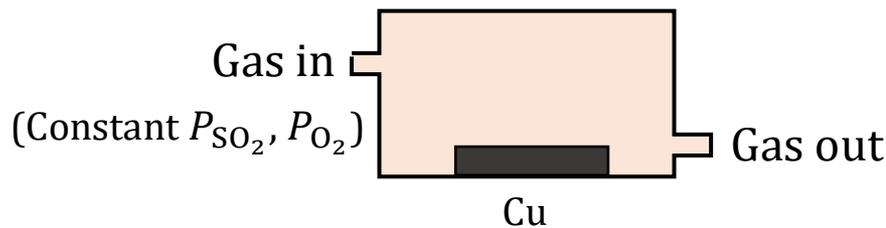
You may note that in some equilibrium equations, there is no P_{O_2} or P_{SO_2} . This means that the equilibrium between two solid compounds are independent of P_{O_2} or P_{SO_2} , and the lines would be horizontal or vertical.

Also, by reformulating the reaction for the formation of each solid phase, in terms of, for example, S_2 and O_2 rather than SO_2 and O_2 , a predominance diagram with logarithms of P_{S_2} and P_{O_2} as axes can be constructed.

Predominance Diagram: Theoretical Basis

Application I of Predominance Diagram

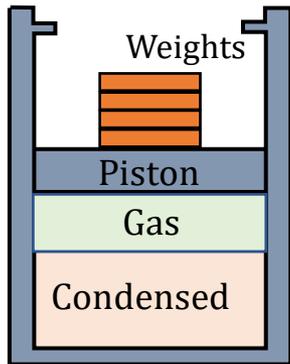
Say we introduce a large amount of SO_2 and O_2 into a system, the gas mixture reacts with a small amount of Cu . Because the amount of Cu is small, the change in the gas composition is negligible. If we adjust P_{SO_2} and P_{O_2} , different products would result. A predominance diagram of $\text{Cu-SO}_2\text{-O}_2$ can be used to study this problem.



Predominance Diagram: Theoretical Basis

Application II of Predominance Diagram

You may notice from the predominance diagram of the Cu-SO₂-O₂ system, there is a curve shown by the crosses. Along this curve, the **total (hydrostatic) pressure** is 1.0 bar.



We can fix a constant **hydrostatic** pressure of 1 bar by placing the system in a cylinder fitted with a piston (left graph). Under this condition, if the gas phase is present, then the gas phase consists not only of SO₂ and O₂, but also of other species such as S₂, S₃, O₃, etc. whose equilibrium partial pressures can be calculated.

It is noted that when the total (hydrostatic) pressure is controlled, P_{SO_2} and P_{O_2} can not be independently varied.

Predominance Diagram: Theoretical Basis

Application II of Predominance Diagram

The cross line is used to study the system's equilibria when we have a closed system and the total (hydrostatic) pressure is controlled. Above the total pressure line, the total pressure is greater than 1.0 bar even though the sum of the partial pressures of SO_2 and O_2 might be less than 1.0 bar. Caution must therefore be exercised using such diagrams. If the total pressure is **no** greater than 1.0 bar, states above the $P_{\text{total}} = 1.0$ bar are inaccessible. In other words, the calculated diagram for a total (hydrostatic) pressure of 1.0 bar terminates at this line.

Predom Module: Cu-S-O System

The Predom Module allows you to calculate predominance diagrams. These diagrams are calculated under quite restrictive conditions.

- ✓ **Only** compound databases are accessed.
- ✓ Temperature is fixed (isothermal calculation).

The partial pressures are permitted to vary for non-metallic species, and the total pressure which is the sum of the partial pressures of all species can also vary.

Again, before you work on your project, check the Directory!!!

Predom Module: Cu-S-O System

Database Selection

Choose FactPS.

This might be the default database for examples.

The maximum number of Metals is 3.

Information - Predom only accesses COMPOUND databases
Predom only accesses COMPOUND databases

Options - search for product species

Include compounds

- gaseous ions (plasmas)
- aqueous species
- limited data compounds (25C)

Limits

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

Predom Module: Cu-S-O System

Define **Elements**: Metals and Non-metals

The maximum number of Metals is 3.

Click on "Next" to activate the calculation.

The maximum number of Non-metals is also 3.

Predom Module: Cu-S-O System

Define List of Species

Click on “List” to see all the species that are going to be considered. You could eliminate species from consideration, but there is no need to do so – the program effectively does that for us since it displays only the stable species.

The screenshot shows the Predom software interface with the 'List' dialog box open. The dialog displays a table of species with the following columns: Code, A, T, Species, Data, A/P/M, Cp range, DG(KJ), and DG(Kcal). The species are grouped into Cu gases, Cu liquids, and Cu solids.

+	Code	A	T	Species	Data	A/P/M	Cp range	DG(KJ)	DG(Kcal)
Cu gases:									
+	1			Cu(g)	FactPS	1.0000E+00	298 - 6000	210.424	50.292
+	2			Cu2(g)	FactPS	1.0000E+00	298 - 6000	321.564	76.856
+	3			CuO(g)	FactPS	1.0000E+00	298 - 6000	213.307	50.982
+	4			CuS(g)	FactPS	1.0000E+00	298 - 2000	145.562	34.790
Cu liquids:									
+	5			Cu(l)	FactPS	1.0000E+00	298 - 4000	3.617	0.865
+	6		T	CuO(l)	FactPS	1.0000E+00	1673 - 3000	-47.939	-11.458
+	7			Cu2O(l)	FactPS	1.0000E+00	298 - 2000	-75.397	-18.020
+	8			Cu2S(l)	FactPS	1.0000E+00	298 - 1500	-113.883	-27.219
Cu solids:									
+	9			Cu(s)	FactPS	1.0000E+00	298 - 2001	0.000	0.000
+	10			CuO(s)	FactPS	1.0000E+00	298 - 3000	-68.340	-16.334
+	11			Cu2O(s)	FactPS	1.0000E+00	298 - 2000	-97.527	-23.310
+	12			CuS(s)	FactPS	1.0000E+00	273 - 1273	-48.886	-11.684
+	13			CuS2(s)	FactPS	1.0000E+00	298 - 1350	-36.167	-8.644
+	14			Cu2S(s)	FactPS	1.0000E+00	298 - 1500	-110.635	-26.442
+	15			Cu2S(s2)	FactPS	1.0000E+00	298 - 1500	-116.747	-27.903
+	16			Cu2S(s3)	FactPS	1.0000E+00	298 - 9999	-117.217	-28.016
+	17		T	Cu7S4(s)	FactPS	1.0000E+00	298 - 298	-358.404	-85.661
+	18		T	Cu9S5(s)	FactPS	1.0000E+00	298 - 298	-432.104	-103.275
+	19			Cu5O4(s)	FactPS	1.0000E+00	298 - 2000	-417.756	-99.846
+	20			Cu2SO4(s)	FactPS	1.0000E+00	298 - 1000	-431.186	-103.056
+	21			(CuO)(Cu5O4)(s)	FactPS	1.0000E+00	298 - 1500	-493.600	-117.973

Predom Module: Cu-S-O System

Define Parameters: Pressures and Temperature

Elements

- 1-Metal Example ..
- 2-Metal Example ..
- 3-Metal Example ..

Metals: Cu
Non-metals: S O optional

Clear Next >>

Metal Mole Fractions

2-Metal Diagram
3-Metal Diagram

Species

<input checked="" type="checkbox"/> gas	19
<input checked="" type="checkbox"/> liquids	6
<input type="checkbox"/> aqueous	0
<input checked="" type="checkbox"/> solids	16

m: 1.0 List

Parameters

Pressure: Isobar: P(atm): 1.0

Constants: Temperature: T(K): 973 Z: log10(Z):

Y-axis: log10(Y) Y: P(SO2) max: 3 min: -4 step: 1

X-axis: log10(X) X: P(O2) max: 0 min: -20 step: 1

Labels and Display: chemical 12 size full screen titles

Calculate

- diagram
- invariant point
- detailed point

Calculate >>

Total hydrostatic pressure.

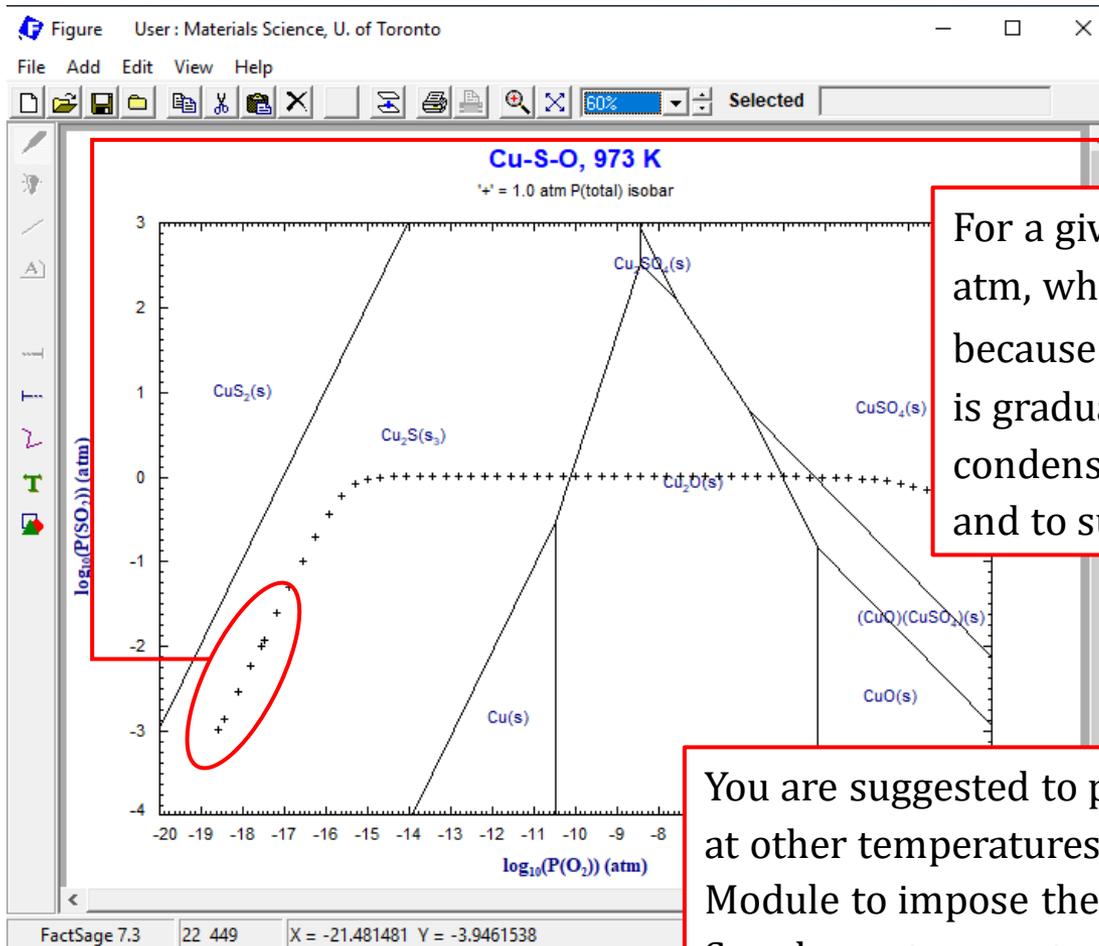
Temperature is 700 °C.

Axes: partial pressures of species.

Choose "diagram". The triple points can be calculated by choosing "invariant point".

Predom Module: Cu-S-O System

Define Parameters: Pressures and Temperature



For a given total hydrostatic pressure of 1 atm, when P_{O_2} is low, P_{SO_2} is also low. This is because that P_{S_2} is high. As P_{O_2} increases, S_2 is gradually converted to SO_2 and the condensed phases go from a sulfide to oxide, and to sulfate.

You are suggested to perform the calculations at other temperatures and use the Figure Module to impose these diagrams (See the Supplementary material).

Predom Module: Cr-C-O System

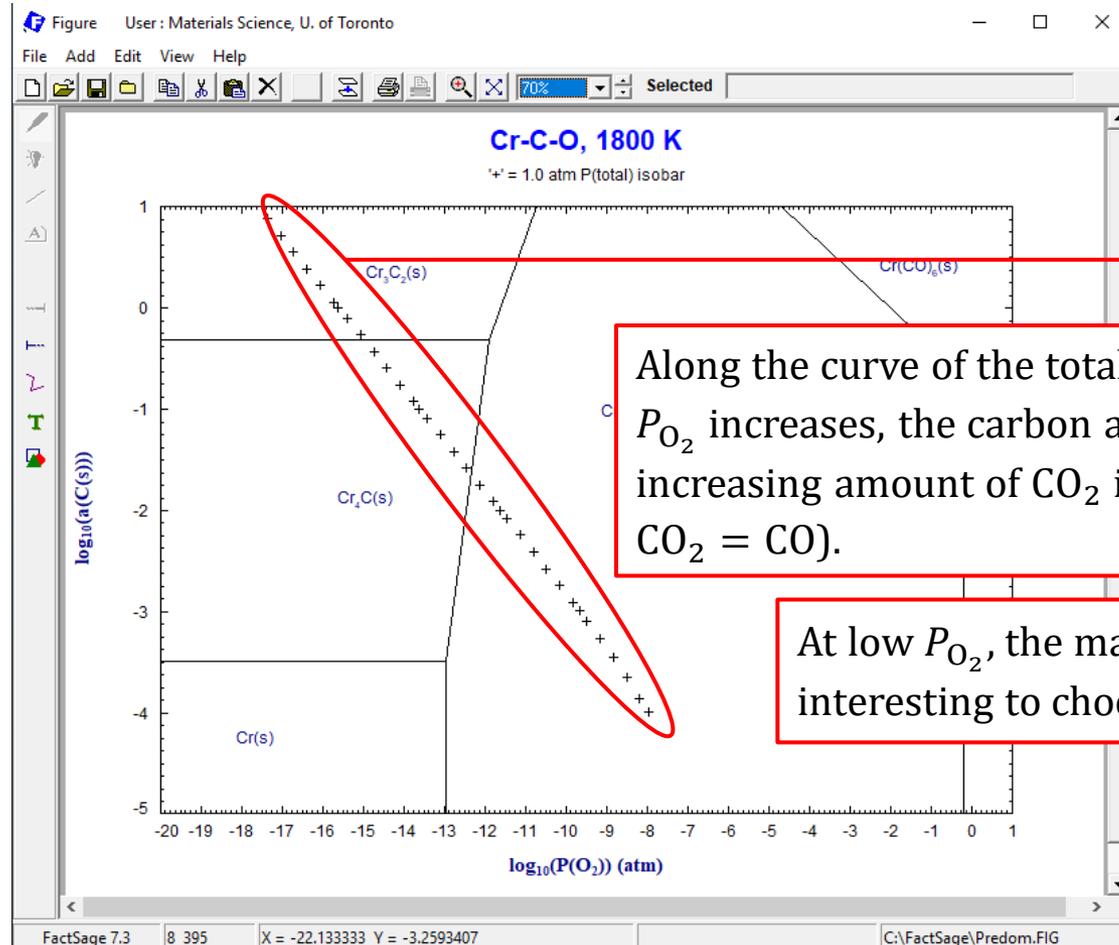
The second example we will look at is the Cr-C-O system at 1800 K.

The screenshot shows the Predom software interface. The 'Elements' section has 'Metals' set to 'Cr' and 'Non-metals' set to 'C' and 'O'. The 'Parameters' section has 'Temperature' set to 1800 K, 'Pressure' set to 1.0 atm, and 'Y-axis' set to $\log_{10}(Y)$ with $a[C(s)]$ selected. The 'X-axis' is set to $\log_{10}(X)$ with $P(O_2)$ selected. The 'max' field for the Y-axis is set to 1. A red arrow points from this field to a text box.

Here, the maximum carbon activity is set as 10. In reality, the carbon activity cannot exceed unity. The program permits one to calculate the diagram under the conditions that cannot be achieved in practice. **However**, we should never use ridiculously high values for activities and partial pressures.

Predom Module: Cr-C-O System

The second example we will look at is the Cr-C-O system at 1800 K.



Along the curve of the total hydrostatic pressure of 1 atm, as P_{O_2} increases, the carbon activity is dropping because of an increasing amount of CO_2 in the gas phase (consider: $\text{C} + \text{CO}_2 = \text{CO}$).

At low P_{O_2} , the main gas species is CO . It is therefore interesting to choose P_{CO} as the Y-axis.

Predom Module: Cr-C-O System

The second example we will look at is the Cr-C-O system at 1800 K.

Elements

1-Metal Example ...
2-Metal Example ...
3-Metal Example ...

Metals:
Non-metals:

Clear optional Next >>

Parameters

Pressure
Isobar: P(atm):

Constants
Temperature
T(K): Z:
log10(Z):

Y-axis log10(Y)
Y:
max:
min:
step:

X-axis log10(X)
X:
max:
min:
step:

Labels and Display
 chemical number none
size: color:
 full screen titles

Calculate
 diagram invariant point detailed point
Calculate >>

Species

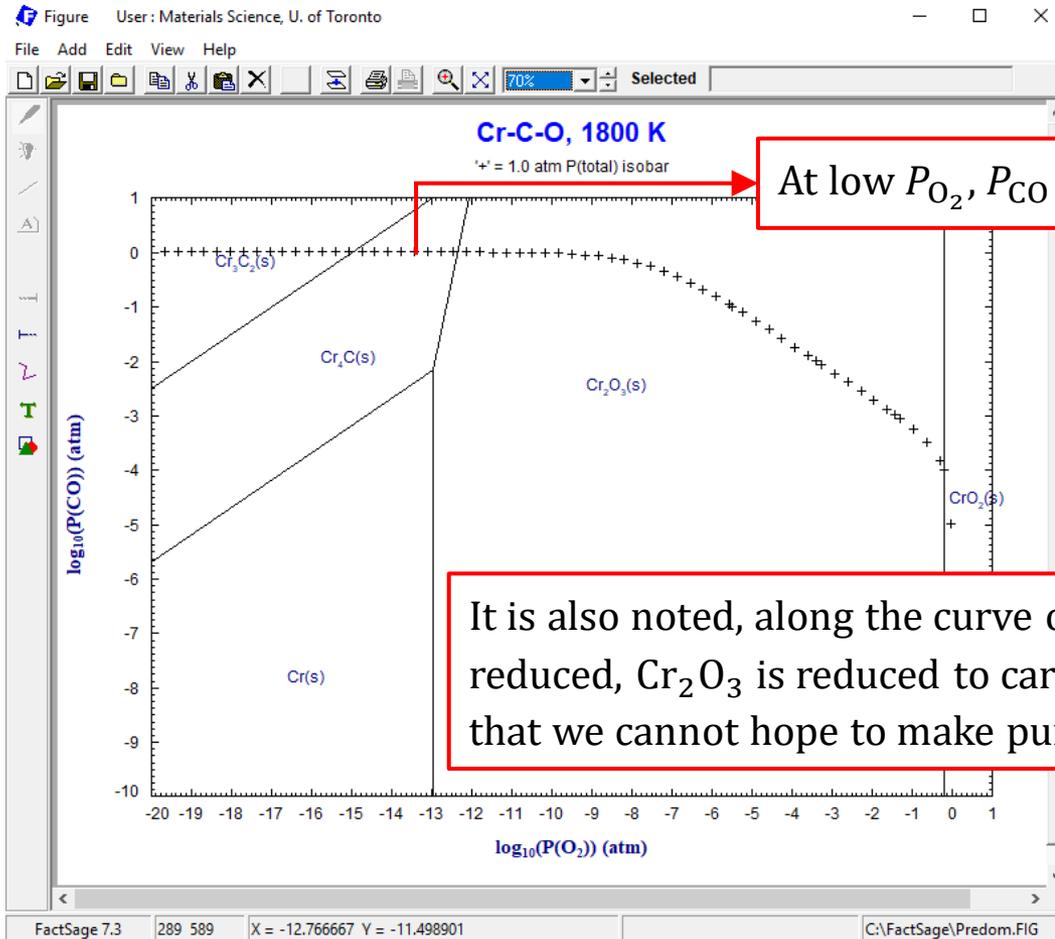
<input checked="" type="checkbox"/>	gas	16
<input checked="" type="checkbox"/>	liquids	6
<input type="checkbox"/>	aqueous	0
<input checked="" type="checkbox"/>	solids	15

m: List

Choose P_{CO} as the Y-axis.

Predom Module: Cr-C-O System

The second example we will look at is the Cr-C-O system at 1800 K.



FactSage Practical

MSE302

Practical 3. Phase Diagram Calculation

**Phase Diagram Module: Unary and Binary
System**

Phase Diagram Module

Phase diagrams are a **graphical representation of phase equilibria**, showing the phases at equilibrium with respect to temperature, pressure, etc. We have already shown various types of phase diagrams for systems containing stoichiometric compounds as well as solution phases in lectures. For binary systems, the most common type is $T \sim X_B$ diagram.

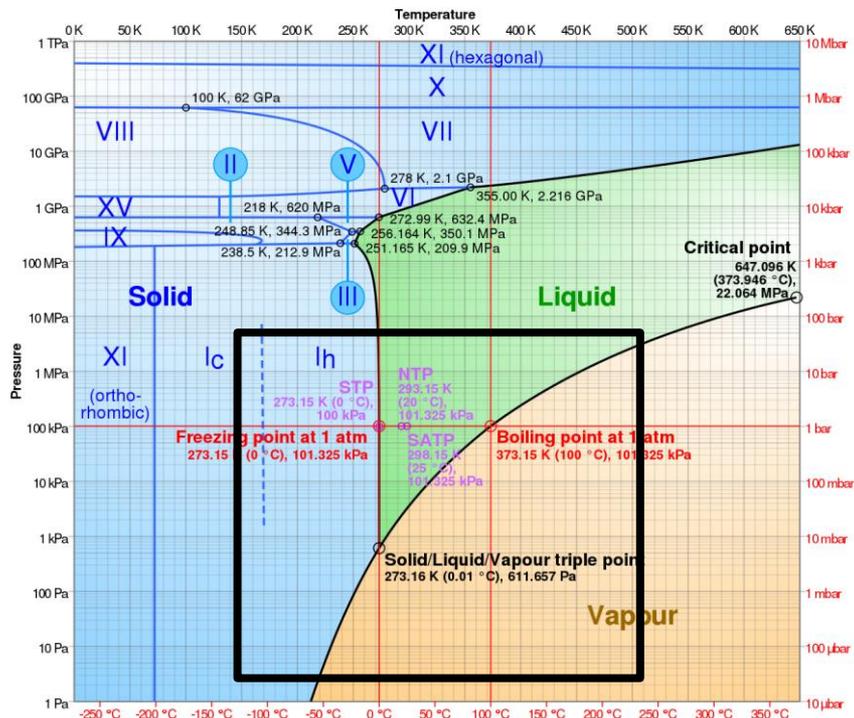
The **Phase Diagram Module** is a very powerful module and is superior to the Predom Module in many ways. However, it takes a lot of care to use it correctly. The general rules of constructing **single-valued** phase diagrams is thoroughly discussed by Pelton.

Like the Equilib Module, selection of databases, especially, solution database, and selection of the phases that may exist at equilibrium are quite challenging for high-order systems. **Always consult the Documentation Module!!!**

Phase Diagram Module: H₂O

Let us start with a simple example: unary phase diagram of H₂O. We would like to know how the equilibrium between **water vapor**, **liquid water** and **ice** is shifted when the system's pressure and temperature are varied.

We would like to plot a diagram that is similar to the graph below.



Phase Diagram Module: H₂O

Components Window: Define Components

Phase Diagram - Components

File Edit Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Qua

Components

H₂O

classical phase diagram (default)
 aqueous diagram with molalities, and iso-Eh & iso-pH lines
 reciprocal diagram with 2 cations and 2 anions
 Scheil-Gulliver constituent diagram

Next >>

FactSage 7.3 Compound: 1/14 databases Solution: 0/15 databases

Don't forget to check your Directory.

We are plotting single-component phase diagram: H₂O

Phase Diagram Module: H₂O

Components Window: Choose Units

The screenshot shows the 'Phase Diagram - Components' window in FactSage 7.3. The 'Units' menu is highlighted with a red box and a red arrow labeled 'Left click'. The 'Units: T(C), P(atm), Energy(J), Quantity(mol), Vol(litre)' dialog box is open, showing the following options:

- Temperature: Kelvin, K; Celsius, °C; Fahrenheit, °F
- Pressure: bar; atm; psi; Pa; GPa
- Energy: J; cal; BTU; kwh
- Quantity: mol; g; lb; kg; tonne
- Volume: litre (dm3); ft3

Below the selection boxes, there is a note: 'Volume units are set by pressure units.' and a table of energy conversions:

Energy:				
1 J	= 1/4.184 cal	= 1/1055.06 BTU	= 1/3.6e6 kwh	
4.184 J	= 1 cal	= 4.184/1055.06 BTU	= 4.184/3.6e6 kwh	
1055.06J	= 1055.06/4.184 cal	= 1 BTU	= 1055.06/3.6e6 kwh	
3.60e6 J	= 3.60e6/4.184 cal	= 3.6e6/1055.06 BTU	= 1 kwh	

Buttons: Cancel, SI, Eng, OK. Below the dialog box, there are checkboxes for diagram types: Classical phase diagram (default), aqueous diagram with molalities, and iso-Eh & iso-pH lines, reciprocal diagram with 2 cations and 2 anions, Scheil-Gulliver constituent diagram. A 'Next >>' button is at the bottom of the dialog box. The status bar at the bottom shows: FactSage 7.3, Compound: 1/14 databases, Solution: 0/15 databases.

Phase Diagram Module: H₂O

Menu Window: Choose Products/Phases (Compounds and Solution Phases)

The screenshot shows the FactSage Phase Diagram Module interface. The main window is titled "Phase Diagram - Menu: last system". It has a menu bar with "File", "Units", "Parameters", and "Variable". Below the menu bar are icons for file operations and a "Components (1)" section. The "Products" section is highlighted with a red box and contains a list of compound species with radio buttons for "gas", "ideal", "real", "aqueous", "pure liquids", and "pure solids". The "Target" section shows "Estimate T(K): 1000". The "Variables" section shows "T(C)" with a range of "-20 300" and "-3".

Three sub-windows are open, each titled "Selection - Phase Diagram - no results -".

- The first sub-window shows "Selected: 1/9" and "GAS". It contains a table with the following data:

+ Code	Species	Data	Phase
1	H(g)	FactPS	gas
2	H2(g)	FactPS	gas
3	O(g)	FactPS	gas
4	O2(g)	FactPS	gas
5	O3(g)	FactPS	gas
6	OH(g)	FactPS	gas
+ 7	H2O(g)	FactPS	Steam
8	HOO(g)	FactPS	gas
9	HOOH(g)	FactPS	gas

- The second sub-window shows "Selected: 1/2" and "LIQUID". It contains a table with the following data:

+ Code	Species	Data	Phase
10	HOOH(liq)	FactPS	liquid
+ 11	H2O(liq)	FactPS	liquid

- The third sub-window shows "Selected: 1/1" and "SOLID". It contains a table with the following data:

+ Code	Species	Data	Phase
+ 12	H2O(s)	FactPS	Ice

A red arrow points from the "Estimate T(K): 1000" field to the "Variables" section.

We need to tell FactSage which phases should be **considered** before performing equilibrium calculations. Then FactSage will only retrieve the models of the selected phases from the chosen database, and then perform the minimization of Gibbs energy under the conditions that will be specified later.
Choose H₂O(*g*), H₂O(*l*) and H₂O(*s*).

Phase Diagram Module: H₂O

Menu Window: Choose Variables

Phase Diagram - Menu: last system

File Units Parameters **Variables** Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (1)

Variables: H₂O log₁₀ P(atm) vs T(C)

Variables

compositions 0

log₁₀(a) 0

Next >>

T and P

Temperature

T(C) X-axis

Max: 300

Min: -20

1/TK

Pressure or Volume

P(atm) Y-axis

log P Max: 2

Min: -3

V(litre)

log V P = 1.0000E-03 to 100

Variables

Variable	Range
T(C)	-20 300
log P	-3 2

log₁₀ P(atm) vs T(C)

Cancel OK

We are calculating $\log(P) \sim T$ phase diagram.

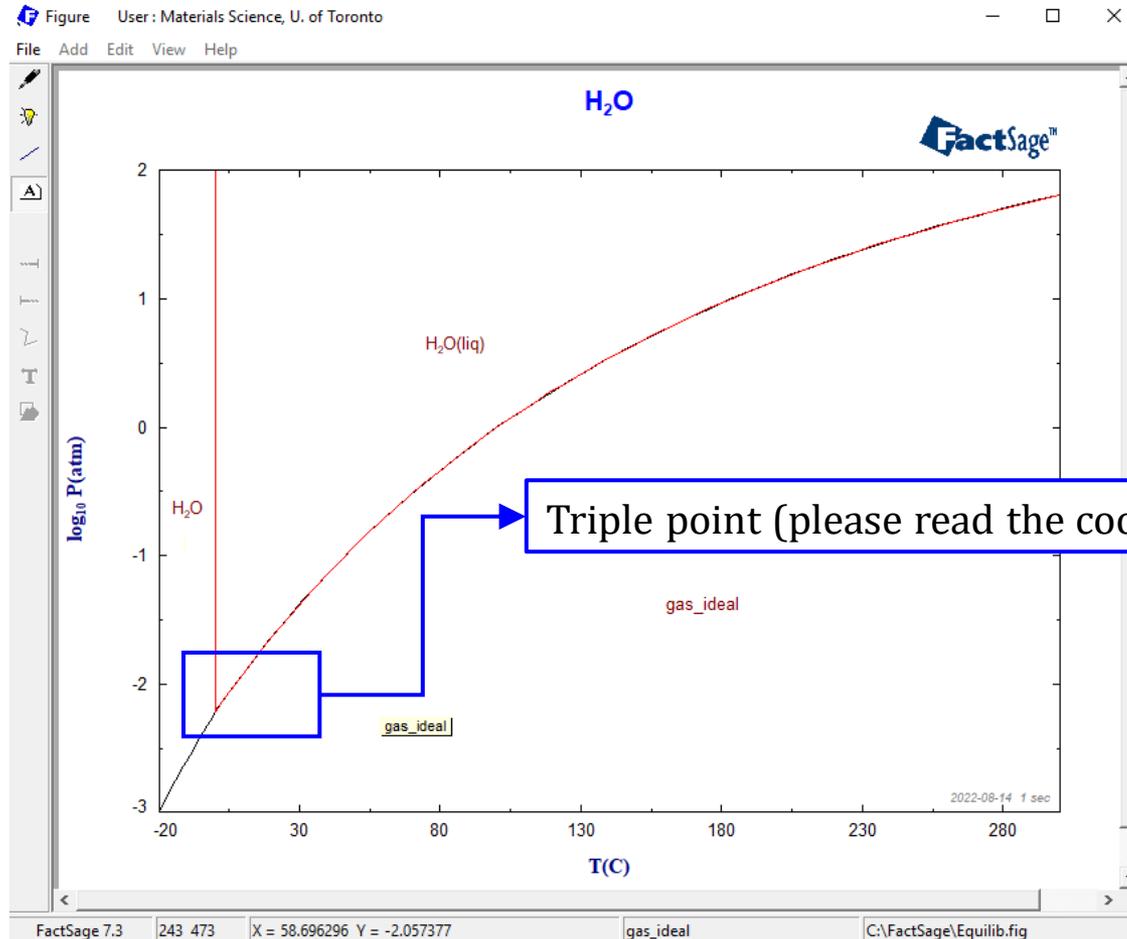
Temperature range.

Pressure range. We are using the logarithm scale.

Left click

Phase Diagram Module: H₂O

Results



Phase Diagram Module: Fe-Cr System

The second example guides you through the calculation of the $T \sim X_B$ diagrams for binary alloy system.

Say we would like to calculate the Fe-Cr phase diagram. We are aware that in this system, both **stoichiometric compounds** and **solution phases** could exist.

Therefore, we need to determine which database(s) should be used. To do this, we could either use the search function in the **Documentation** Module, or use the **View Data** Module.

Phase Diagram Module: Fe-Cr System

View the model quality for the Fe-Cr system in the View Data Module.

View Data

View solutions - enter a list of elements or ALL

Examples:
Ca Al O S - solutions with Ca, Al, O and/or S
H O Fe S - solutions (including aqueous) of H, O, Fe and/or S
ALL - ALL solutions

Pressure: atm bar
Energy: J cal

Data: compound solution
minimum solution components: 1 2 cpts

Solution Databases (16):
Summary ... Add ... Remove ... FTlite
C:\FactSage\FACTDATA\FTlite60soln.sdc
FTlite - FACT Alloy and Mg-alloy solutions (2019)

Elements or ALL: Fe Cr

Exit Assessments ... Information ... OK

Database evaluation

Elements: Fe Cr

FScope (binaries) FSlead (binaries) FSstel (binaries) FTlite (binaries) SGNobl (binaries) SpM...

		26	24
		Fe	Cr
26	Fe	U	
24	Cr	Q	U

Note that these are only for binary evaluations, ternary evaluations may differ from database to database.

- id Ideal Bragg-Williams Treatment
- Q Modified Quasichemical Model
- BW Bragg-Williams Model (liquid sc
- Top quality
- Good quality (maybe a missing |
- Rough estimate, probably missi
- Noble gas system (use FACTPS C
- Computed using pure substance

The above information from the Documentation Module and View Data Module indicates that FTlite could be used to calculate the Fe-Cr system.

Phase Diagram Module: Fe-Cr System

Components Window: Define Components

The screenshot displays the 'Phase Diagram - Components' window in FactSage 7.3. The 'File' menu is open, highlighting 'Add a new Reactant' (Ctrl+R). A red box highlights this menu item, with an arrow pointing to a text box that says '2. Add a new Component.' Another red box highlights the '+' button in the 'Components' list, with an arrow pointing to a text box that says '1. Don't forget to check your Directory.' The 'Components' list shows 'Fe' and 'Cr' as existing components. The 'classical phase diagram (default)' option is checked in the diagram type selection area. The status bar at the bottom shows 'FactSage 7.3', 'Compound: 1/14 databases', and 'Solution: 0/15 databases'.

1. Don't forget to check your Directory.

2. Add a new Component.

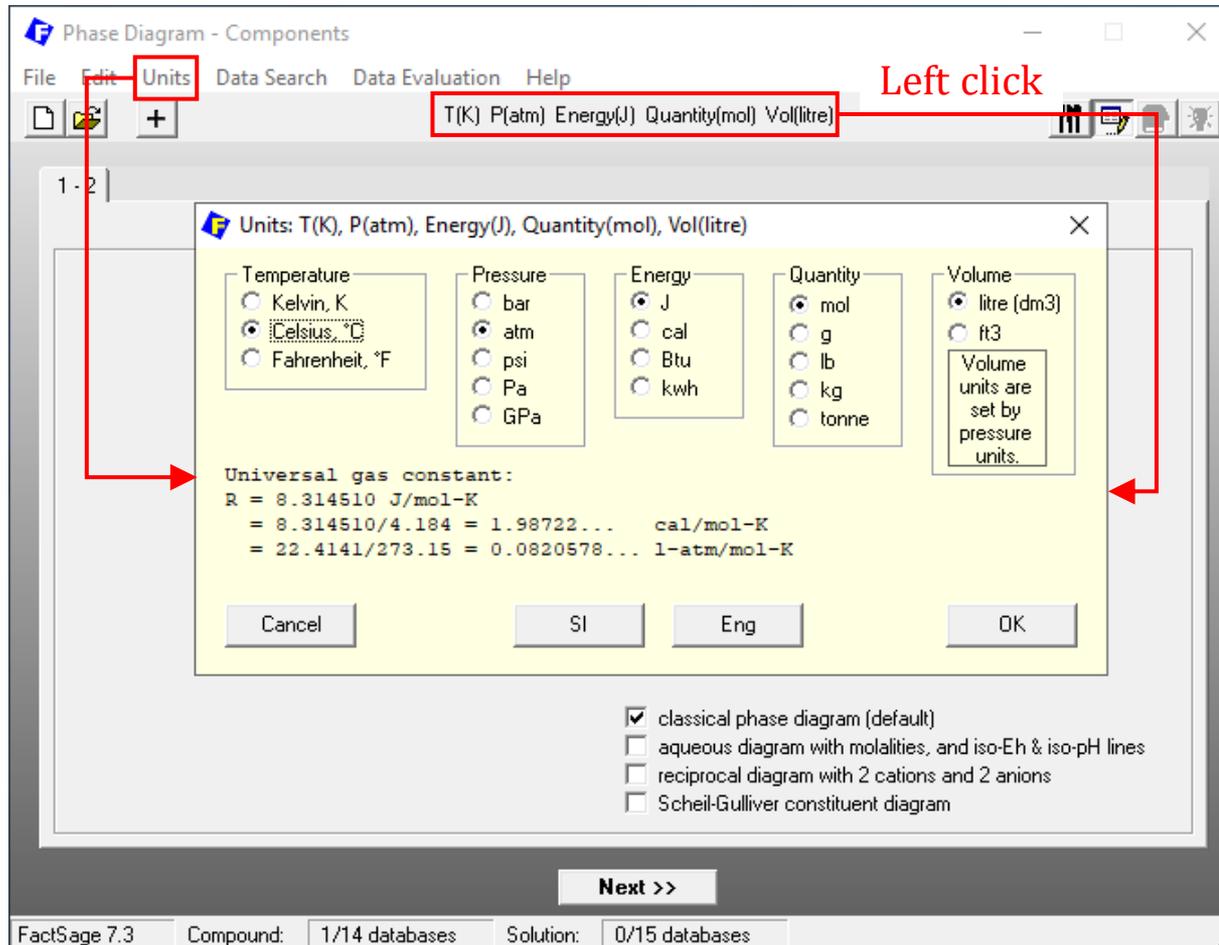
classical phase diagram (default)
 aqueous diagram with molalities, and iso-Eh & iso-pH lines
 reciprocal diagram with 2 cations and 2 anions
 Scheil-Gulliver constituent diagram

Next >>

FactSage 7.3 Compound: 1/14 databases Solution: 0/15 databases

Phase Diagram Module: Fe-Cr System

Components Window: Choose Units



Phase Diagram Module: Fe-Cr System

Menu Window: Choose Products/Phases (Compounds and Solution Phases)

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components [2]

Fe + Cr

Solution Phase FTlite-A2
BCC-A2 Prototype-W Strukturbericht = A2; Pearson = cI2; Space Group = Im-3m (229); []
C, H, N and B interstitial on tetrahedral sites

The components in FTlite-A2 for the current calculation are:
Cr, Fe-alpha

Products

Compound species

gas ideal real 0
aqueous 0
pure liquids 0
pure solids 0

Species: 0

Target
- none -
Estimate T(K): 1000

Legend

Show species:
solutions:

*	+	Base-Phase	Full Name
		FTlite-Liqu	Liquid
		FTlite-A1	FCC-A1
		FTlite-A2	BCC-A2
		FTlite-A3	HCP-A3
		FTlite-D8h	Sigma Prototype-FeCr

Custom Solutions
0 fixed activities Details...

assume molar volumes of solids and liquids = 0
include molar volume data and physical properties data

Variables

T(C)	Fe/(Fe+Cr)		
1000	0 (min)		

vs

FactSage 7.3

Left click on the column of "Base-Phase" or "Full Name" to display the solution description.

We need to tell FactSage which phases should be **considered** before performing equilibrium calculations. Then FactSage will only retrieve the models of the selected phases from the chosen database, and then perform the minimization of Gibbs energy under the conditions that will be specified later.

Phase Diagram Module: Fe-Cr System

Menu Window: Choose Products/Phases (Compounds and Solution Phases)

Note: the [I]-option only means we are considering the **possibility** of immiscibility, and it might not appear in the calculation results.

Solution FTlite-Liqu

- clear
- all end-members
- * - custom select end-members
- m - merge dilute solution from >
- + - single phase
- I - possible 2-phase immiscibility
- J - possible 3-phase immiscibility
- standard stable phase
- ! - dormant (metastable) phase
- F - formation target phase
- P - precipitate target phase
- O - Only plot this single phase
- S - Scheil cooling target phase
- Z - iso-activity lines ...
- Help ...

*		Base-Phase	Full Name
<input checked="" type="checkbox"/>		FTlite-Liqu	Liquid
<input type="checkbox"/>	I	FTlite-A1	FCC-A1
<input type="checkbox"/>	I	FTlite-A2	BCC-A2
<input type="checkbox"/>	I	FTlite-A3	HCP-A3
<input type="checkbox"/>	I	FTlite-D8b	Sigma Prototype-FeCr

Legend
I - immiscible 5

Show all selected

Custom Solutions:
0 fixed activities
0 ideal solutions

Pseudonyms:
apply Edit ...

Volume data:
 assume molar volumes of solids and liquids = 0
 include molar volume data and physical properties data

paraequilibrium & Gmin edit

Total Species (max 5000) 32

[+] - single phase: the solution phase is included as a possible product in the equilibrium calculation. Species of the phase will not appear the [Results Window] if their concentrations are below the Print Cut-off lower limit (click on Parameters in the Menu Window).

[I] - possible 2-phase immiscibility: the solution phase may be immiscible. For example select this option for FACT-SLAG when SiO₂ > 50%. If the phase is not immiscible the results of the calculation will be OK - the phase will appear twice with the same composition. Note this option tends to slow down the speed of the calculation.

Phase Diagram Module: Fe-Cr System

Menu Window: Choose Products/Phases (Compounds and Solution Phases)

A Note: for the calculation of phase diagrams of a **binary** system which has been optimized in the FactSage databases, we normally use the default settings when choose phases, that is, all pure solids and all solutions (some default setting is [I]-option). However, when calculating higher-order systems which requires the selection of multiple databases, caution must be exercised and screening of certain phases is necessary.

Phase Diagram Module: Fe-Cr System

Menu Window: Choose Variables

Phase Diagram - Menu: last system

File Units Parameters **Variables** Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (2)

Products

Compound species

gas ideal real

aqueous

pure liquids

pure solids

species: 12

Target: none

Estimate T(K): 1000

Variables: Fe-Cr T(C) vs composition #1.

Variables

Y-axis: T(C) 1/TK

log10(a): 0

X-axis: T(C) log10(composition)

Compositions Quantity(mol)

#1. 1 Fe + 0 Cr = 1 (max) 0 (min)

1 Fe + 1 Cr

T and P

Temperature

Y-axis: T(C)

Max: 2000

Min: 200

Pressure or Volume

P(atm) constant

log P

V(litre) 1

log V

OK

Left click

We are calculating $T \sim X_B$ phase diagram.

Temperature range.

Pressure, if not exceedingly high, has a negligible effect on phase equilibria of the Fe-Cr system. Put 1 atm.

$$\frac{n_{\text{Fe}}}{n_{\text{Fe}} + n_{\text{Cr}}} = X_{\text{Fe}}$$

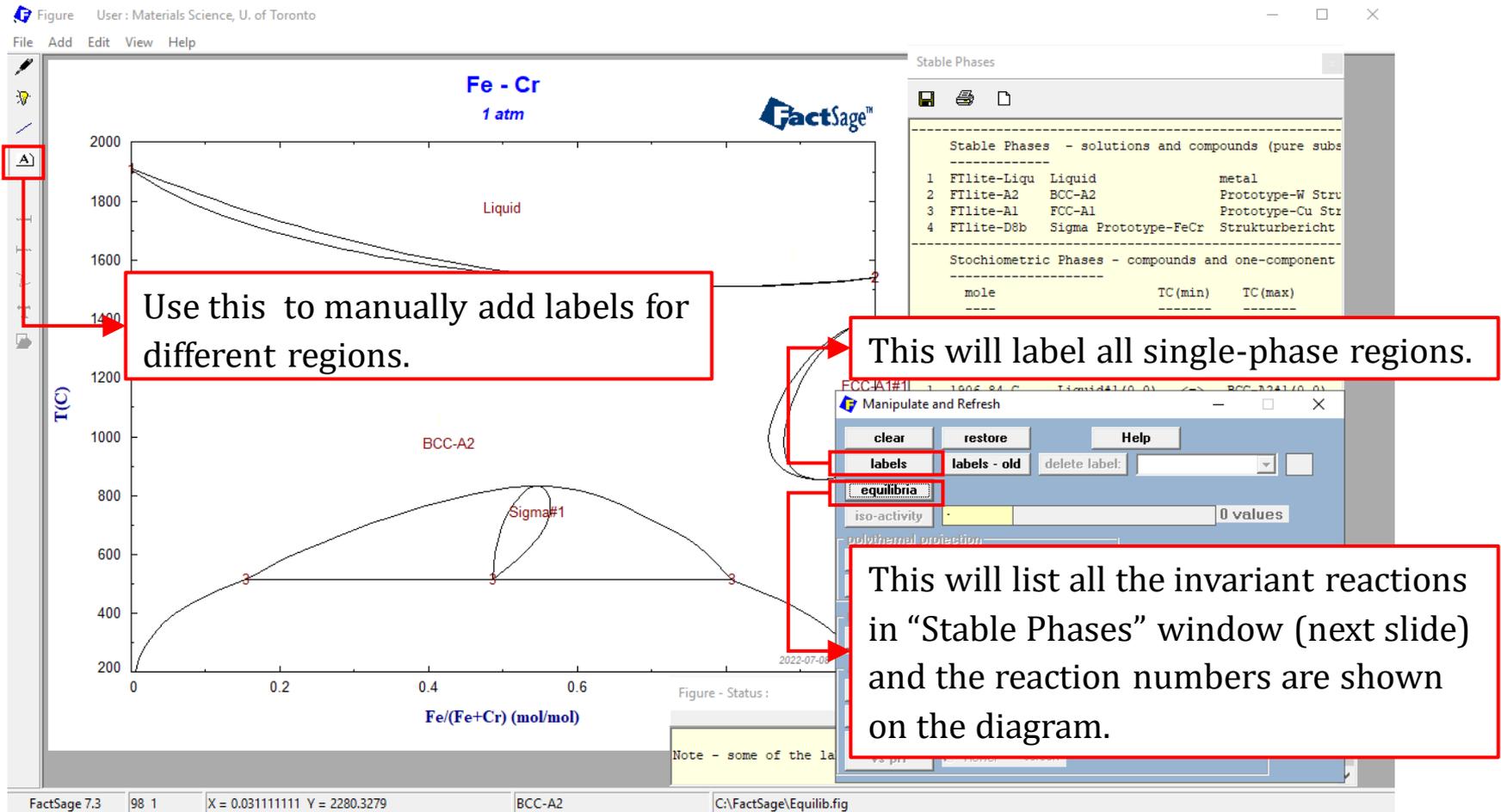
Variables	Fe/(Fe+Cr)
200 2000	0 1

T(C) vs Fe/(Fe+Cr)

FactSage 7.3

Phase Diagram Module: Fe-Cr System

Results: Click on “Calculate” to generate the phase diagram.



Phase Diagram Module: Fe-Cr System

Results: Click on “Calculate” to generate the phase diagram.

Stable Phases

All the stable phases (compounds and solutions) are listed. Also included are the structural information of these phases.

Phase	Structure	Prototype	Structural Information
1 FTlite-Liqu	Liquid	metal	
2 FTlite-A2	BCC-A2	Prototype-W	Strukturbericht = A2; Pearson = cI2
3 FTlite-A1	FCC-A1	Prototype-Cu	Strukturbericht = A1; Pearson = cF4
4 FTlite-D8b	Sigma	Prototype-FeCr	Strukturbericht = D8b; Pearson = tP30; Space gr

Stoichiometric

All the invariant reactions (the number of degree of freedom is zero) are listed.

Reaction	Temperature (C)	Phase 1	Phase 2
1	1906.84	Liquid#1(0.0)	BCC-A2#1(0.0)
2	1537.81	Liquid#1(1.0)	BCC-A2#1(1.0)
3	511.94	Sigma#1(0.486)	BCC-A2#1(0.1535) + BCC-A2#2(0.808)

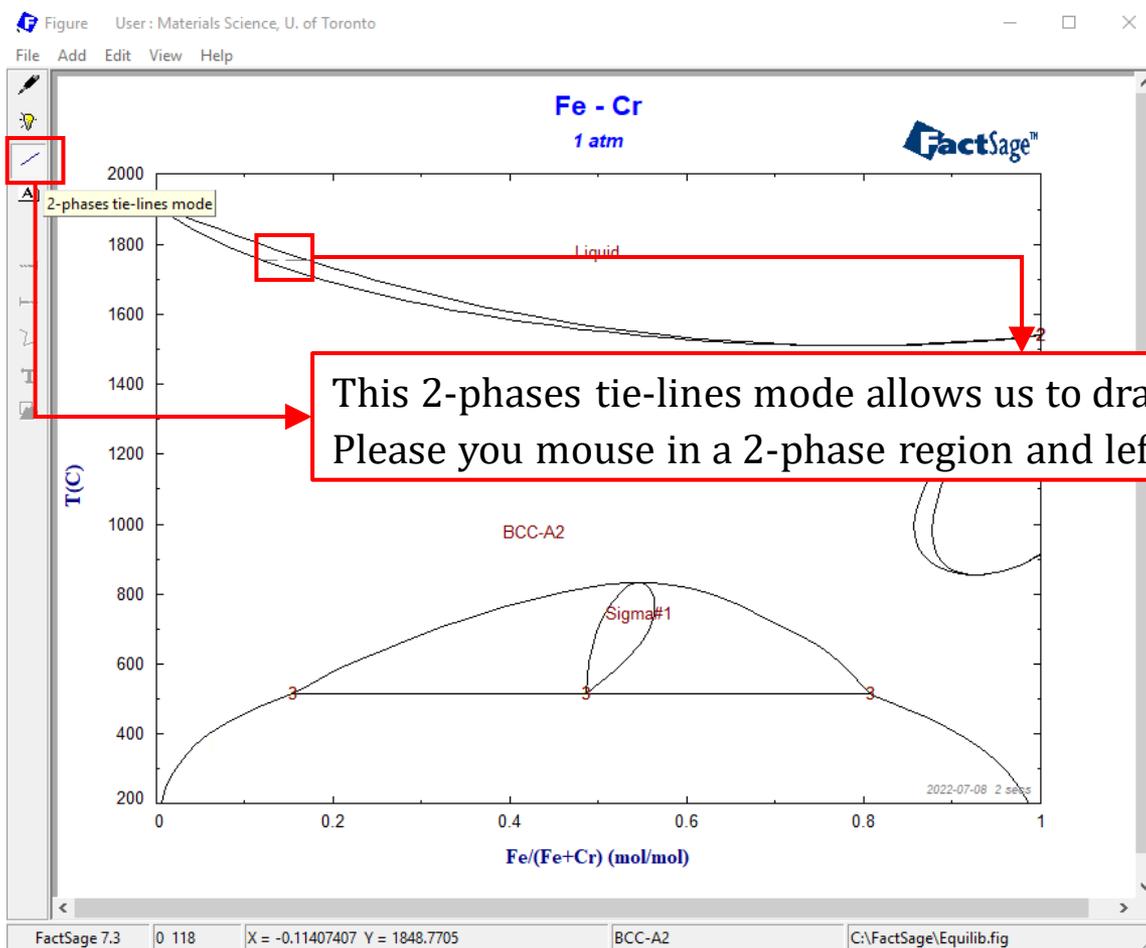
Phase Equilibria

Please note the number of components for these two equilibria is 1.

Equilibrium	Temperature (C)	Phase 1	Phase 2
1	1906.84	Liquid#1(0.0)	BCC-A2#1(0.0)
2	1537.81	Liquid#1(1.0)	BCC-A2#1(1.0)
3	511.94	Sigma#1(0.486)	BCC-A2#1(0.1535) + BCC-A2#2(0.808)

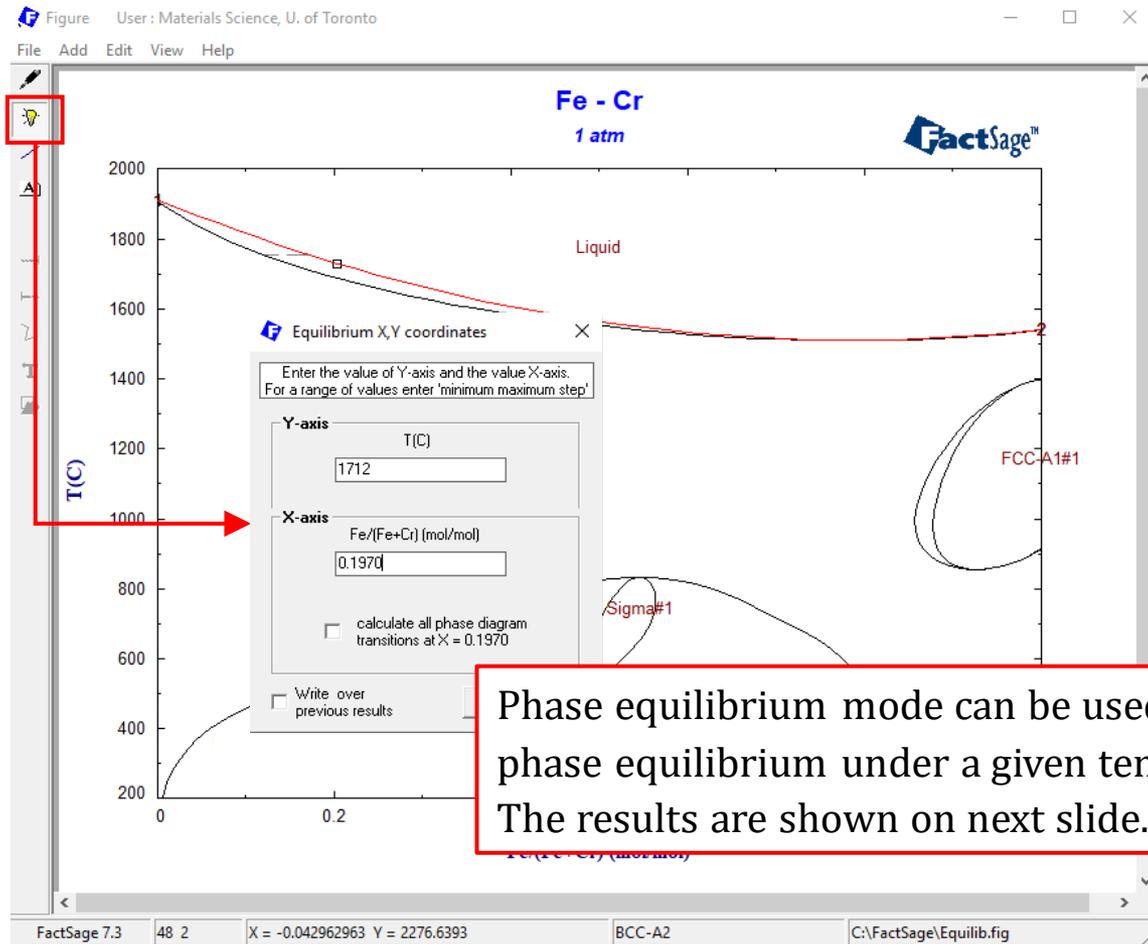
Phase Diagram Module: Fe-Cr System

Results: 2-phases tie-lines mode



Phase Diagram Module: Fe-Cr System

Results: phase equilibrium mode



Phase equilibrium mode can be used to quickly calculate the phase equilibrium under a given temperature and composition. The results are shown on next slide.

Phase Diagram Module: Fe-Cr System

Results: phase equilibrium mode

Phase Diagram Equilibrium

File Edit Format

1

Specified Temperature and Composition

$T(C) = 1712, Fe/(Fe+Cr) \text{ (mol/mol)} = 0.197$

FactSage 7.3

Fe + Cr =

0.52322 mol Liquid#1
(27.658 gram, 0.52322 mol)

+ 0 mol Liquid#2
(1712 C, 1 atm, a=1.0000)
(0.77559 Cr
+ 0.22441 Fe)

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	0.11742	6.5571	0.22441	0.23708
Cr	0.40581	21.100	0.77559	0.76292

+ 0.47678 mol BCC-A2#1
(25.097 gram, 0.47678 mol)

+ 0 mol BCC-A2#2
(1712 C, 1 atm, a=1.0000)
(0.83308 Cr
+ 0.16692 Fe-alpha)

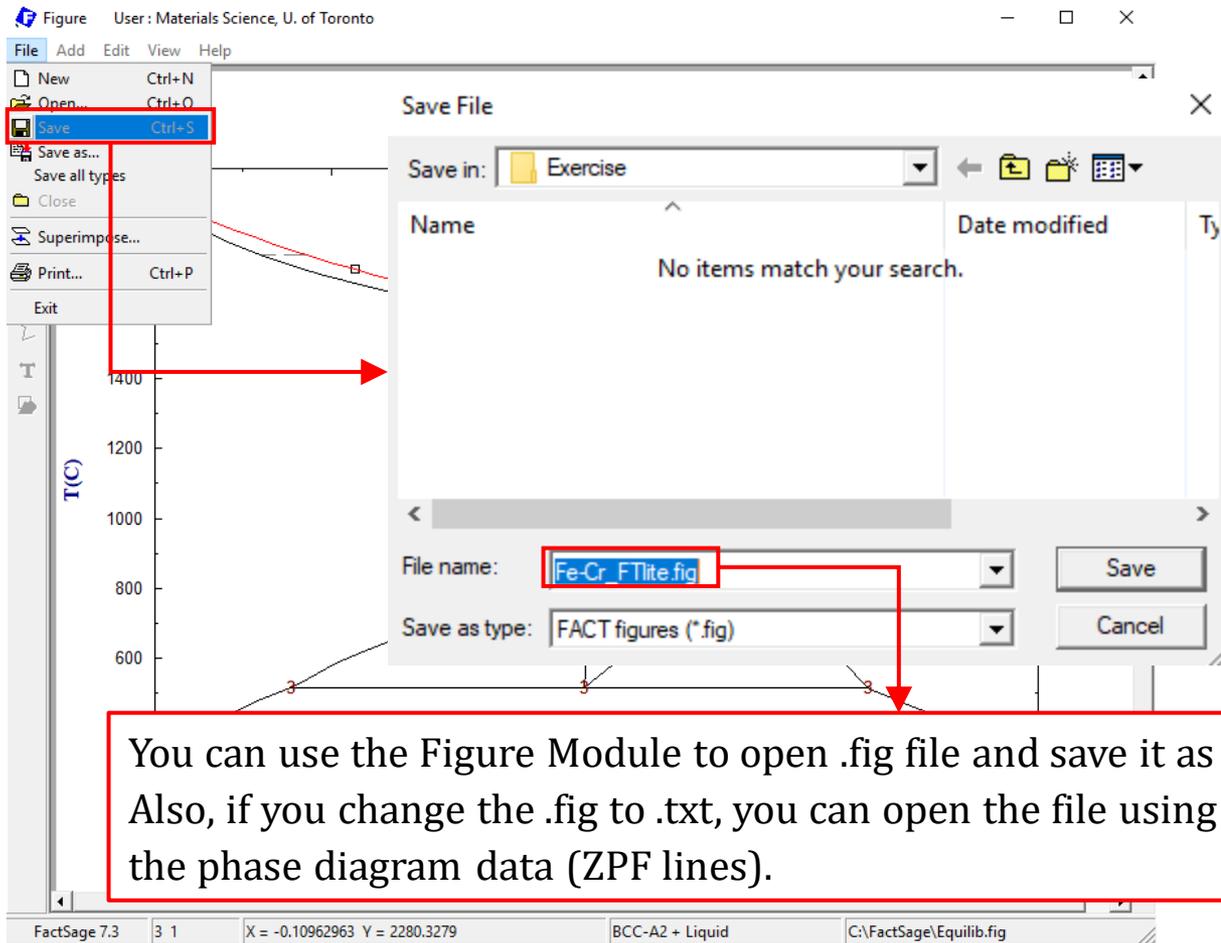
System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	7.9584E-02	4.4444	0.16692	0.17709
Cr	0.39719	20.652	0.83308	0.82291

The phases at equilibrium.

Phase compositions.

Phase Diagram Module: Fe-Cr System

Save Results



You can use the Figure Module to open .fig file and save it as other graph format. Also, if you change the .fig to .txt, you can open the file using NotePad and extract all the phase diagram data (ZPF lines).

Phase Diagram Module: Fe-O₂ System

The third example guides you through the calculation of the $T \sim X_B$ diagrams as well as two-potential phase diagrams. We will use the Fe-O₂ system as the example.

First, let us calculate the $T \sim X_B$ diagram for the Fe-O₂ system.

Phase Diagram Module: Fe-O₂ System

Search the Fe-O (not Fe-O₂) system in the Documentation Module.

The screenshot shows the FactSage Browser interface. The search bar contains "Fe O" and the results list includes "Fe - O : | FToxid | TDnucl |". A red box highlights this entry. Below the search results, a phase diagram is displayed with the title "Fe - O Gas phase suppressed" and "Data from FToxid - FACT oxide databases". The diagram plots Temperature (°C) on the y-axis (400 to 1800) against mole O/(Fe+O) on the x-axis (0 to 0.6). The diagram shows various phase regions such as ASiag+liq, AMonoxide, and Spinel. A red arrow points from the search results to the phase diagram.

FToxid should contain the optimized model parameters for all the possible **oxide** phases in the Fe-O system (FToxid database only contains the models for oxide phases).
Note we do not have the access to TDnucl database.

Phase Diagram Module: Fe-O₂ System

Components Window: Define Components

Phase Diagram - Components

File Edit Units Data Search Data Evaluation Help

T(K) P(atm) Energy(J) Quantity(mol) Vol(litre)

1 - 2

Choose units

Components

Fe

O₂

Don't forget to check your Directory.

classical phase diagram (default)

aqueous diagram with molalities, and iso-Eh & iso-pH lines

reciprocal diagram with 2 cations and 2 anions

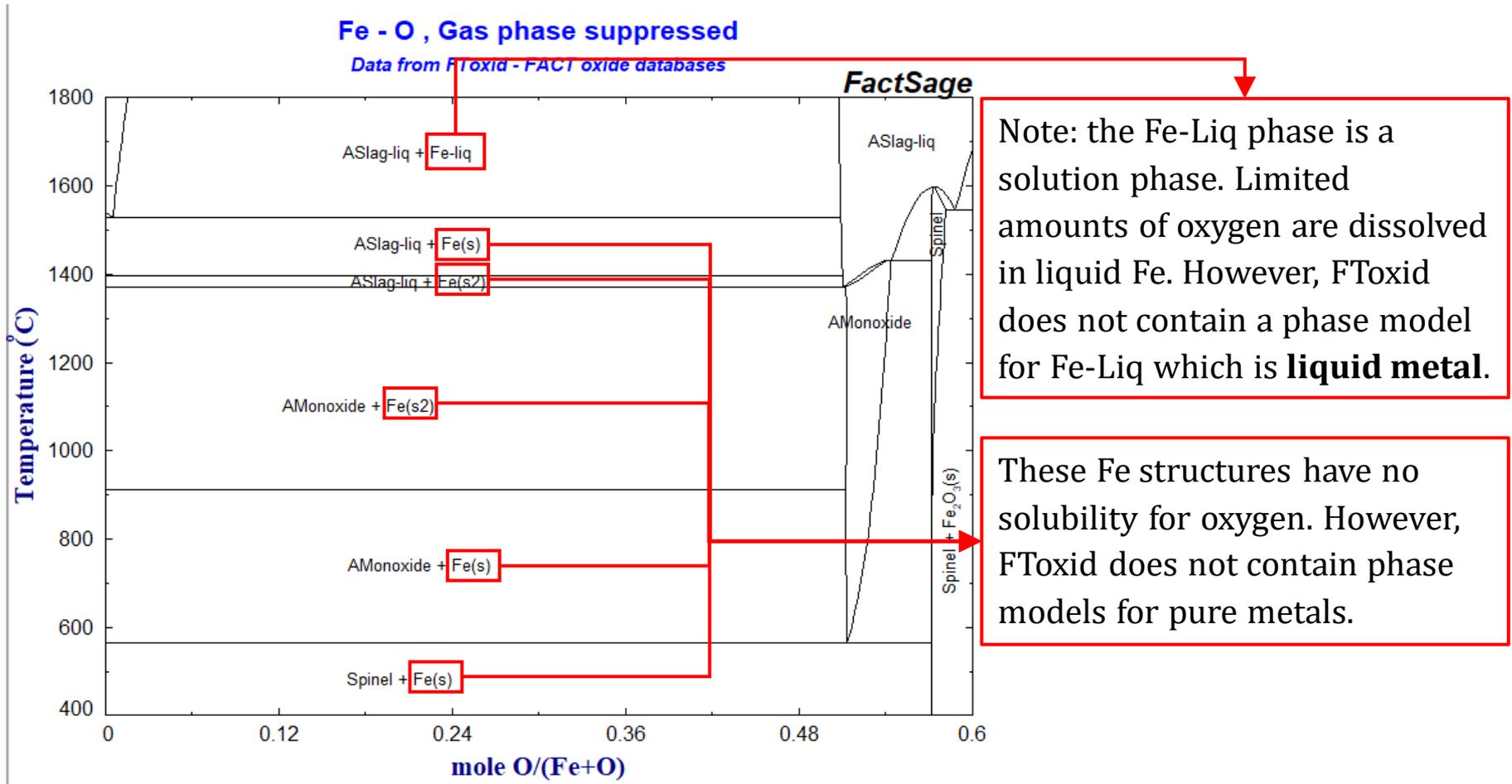
Scheil-Gulliver constituent diagram

Next >>

FactSage 7.3 Compound: 1/14 databases Solution: 0/15 databases

Phase Diagram Module: Fe-O₂ System

Before we choose the database(s), let us check the pre-made phase diagram.



Phase Diagram Module: Fe-O₂ System

We use the View Data Module to determine which other databases are needed.

First, check the Liquid Solution.

View Data

View solutions

Examples:
Ca Al O S - solutions with Ca, Al, O and/or S
H O Fe S - solutions (including aqueous) of H, O, Fe and/or S
ALL - ALL solutions

Pressure
 atm
 bar

Energy
 J
 cal

Data
 compound solution
minimum solution components
1 2 cpts

Solution Databases (16)
Summary ... Add ... Remove ... All Public Data ▾
All Public Databases
- 15 Solution Databases

Elements or ALL: Fe O

Exit Assessments ... Information ... OK

We want to find the Liquid Solution containing Fe and O.

View Data Fe-O

File Edit Sort Solution
16 Solutions

Phase	Name & End-members EMs	Information
5. FTdemo-CuLQ	Fe O	0.0 < X < 0.50 0.0 < X < 0.10
6. FSstel-Liqu	LIQUID 2 EMs 2 elements #99 Fe O	[I] Liquid steel phase
7. FSstel-FCC	FCC_A1 2 EMs 2 elements #12 Fe O	[J] Austenitic form of Fe with B, C, N and H in interstitial site. Use J op
8. FSstel-BCC	BCC_A2 2 EMs 2 elements #12 Fe O	Prototype_w-A2 c12 Im-3m (229) (use [I]-option) C, N and B interstitial
9. FTmisc-FeLQ	Fe-liq 2 EMs 2 elements #2 Fe !	steel([H Jung model]). Don't use with any other liq metal phase. Fo Iron/Steelmaking Processes, not solidification. Fe-rich(not for stain - this species must be present !

FactSage 7.3 | All public solution databa

This **might** be a suitable phase for the liquid metal. However, no solubility limit of oxygen is noted. This would make the liquid metal indistinguishable from the Slag phase.

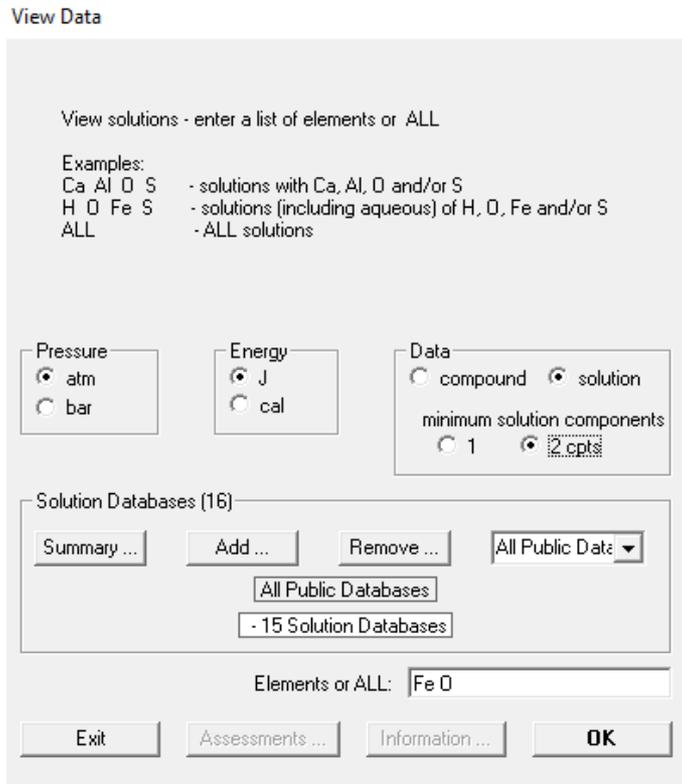
Number refers to the type of phase model. See the supplementary of Solution Module.

Note: there is no need to check the FTdemo database.

Phase Diagram Module: Fe-O₂ System

We use the View Data Module to determine which other databases are needed.

First, check the Liquid Metal.



This phase sets the solubility limit of oxygen in liquid Fe. This is exactly what we need for a liquid metal phase.

Phase	Name & End-members EMs	Information
8. FSstel-BCC	Fe O	
9. FTmisc-FeLQ	Fe-lq 2 EMs 2 elements #2	steel(l-H Jung model). Don't use with any other liq metal phase. For Iron/Steelmaking Processes, not solidification. Fe-rich(not for stainless steel). - this species must be present! 0.0 < X < 0.10
10. FT0xCN-Liqu	Liquid 2 EMs 2 elements #99	metal (Use l-option)
11. FToxid-SLAGA	ASlag-liq 2 EMs 2 elements #98	oxide Al,As,B,Ba,Ca,Co,Cr,Cu,Fe,Ge,K,Mg,Mn,Na,Ni,P,Pb,Si,Sn,S dilute S and F (Mis.gap at high SiO2, use [l] option).

Similar to FSstel-Liqu, no solubility limit of oxygen was set.

Note: there is no need to check the FTdemo database.

Phase Diagram Module: Fe-O₂ System

We use the View Data Module to determine which other databases are needed.

First, check the Liquid Metal.

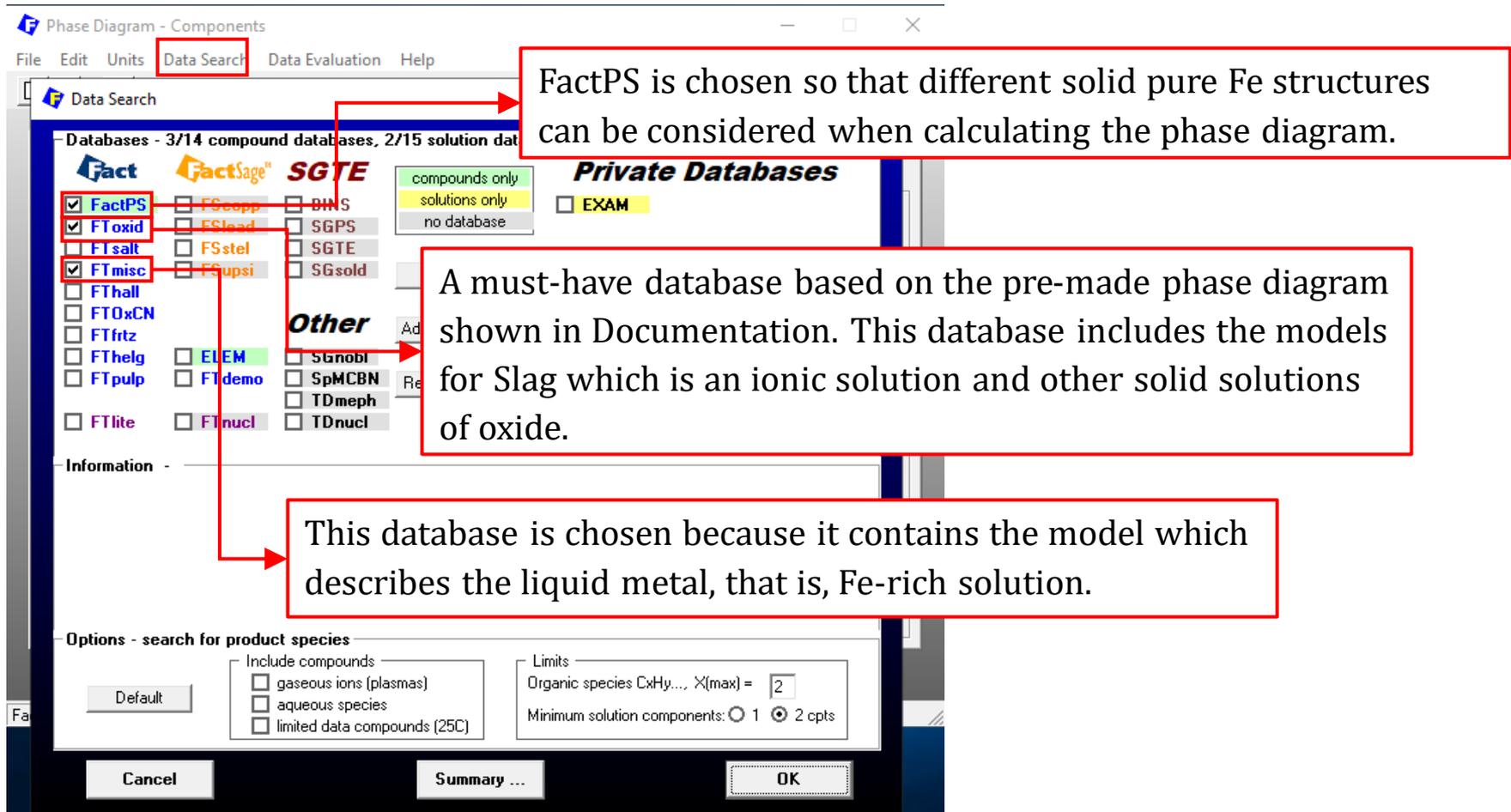
The above information shows that FTmisc-FeLQ is probably the best candidate for the liquid metal phase. Therefore, FTmisc database should be chosen.

For the solid **metallic Fe** phases, since the solubility is very low, you can choose either FactPS database which ignores the solubility of oxygen, or FSstel database which considers the dissolution of oxygen (FSstel-BCC and FSstel-FCC). Here, we choose FactPS .

Now let us reproduce the Fe-O phase diagram before we calculate the Fe-O₂ phase diagram.

Phase Diagram Module: Fe-O₂ System

Components Window: Choose Database(s)



Phase Diagram - Components

Data Search

Databases - 3/14 compound databases, 2/15 solution dat

Fact **FactSage[®]** **SGTE**

FactPS FScomp BINS EXAM

FToxid FSlead SGPS

FTsalt FSstel SGTE

FTmisc FSsupsi SGsold

Private Databases

compounds only
solutions only
no database

Other

Sgnobi Ad

SpMCBN Re

TDmeph

TDnucl

Information

Options - search for product species

Default

Include compounds

gaseous ions (plasmas)

aqueous species

limited data compounds [25C]

Limits

Organic species CxHy..., X(max) = 2

Minimum solution components: 1 2 cpts

Cancel Summary ... OK

FactPS is chosen so that different solid pure Fe structures can be considered when calculating the phase diagram.

A must-have database based on the pre-made phase diagram shown in Documentation. This database includes the models for Slag which is an ionic solution and other solid solutions of oxide.

This database is chosen because it contains the model which describes the liquid metal, that is, Fe-rich solution.

Phase Diagram Module: Fe-O₂ System

Menu Window: Choose Products/Phases (Compounds and Solution Phases)

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (2)

Fe + O

Select all the solutions and use the default settings of immiscibility gaps.

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

+ pure solids 5

* - custom selection species: 5

Target

- none -

Estimate T(K): 1000

Variables

T(C) O/(Fe+O)

400 1800 0 0.6

T(C) vs O/(Fe+O)

FactSage 7.3

Solution phases

*	+	Base-Phase	Full Name
	+	FTmisc-FeLQ	Fe-liq
	l	FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
	+	FToxid-MeO_A	A-Monoxide

Selection - Phase Diagram - no results -

File Edit Show Sort

Selected: 5/13 SOLID Duplicates selected. X denotes species excluded

no results -

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
+	9	Fe(s)	FactPS	bcc		V			
+	10	Fe(s2)	FactPS	fcc		V			
X	11	FeO(s)	FactPS	Wustite		V			
X	12	Fe2O3(s)	FactPS			V			
X	13	Fe2O3(s2)	FactPS			V			
X	14	Fe2O3(s3)	FactPS			V			
X	15	Fe3O4(s)	FactPS			V			
X	16	Fe3O4(s2)	FactPS			V			
X	17	Fe3O4(s3)	FactPS			V			
X	18	Fe3O4(s4)	FactPS			V			
+	19	Fe2O3(s)	FToxid	High-Pressure-H		V			
+	20	Fe2O3(s2)	FToxid	High-Pressure-H		V			
+	21	Fe2O3(s3)	FToxid	High-Pressure-H		V			

permit selection of X species Suppress Duplicates Edit priority list: Show Selected Select All Select/Clear... Clear OK

Choose all the pure solids. FactSage 7.3 version is quite "smart". When multiple databases contain the data for same species, FactSage will suppress the duplicates. You can edit the priority.

Phase Diagram Module: Fe-O₂ System

Menu Window: Choose Variables

Phase Diagram - Menu: last system

File Units Parameters **Variables** Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components [2]

Fe + O

Variables: Fe-O T(C) vs composition #1.

Variables

Y-axis: log10(a) 0

X-axis: compositions 1

T and P

Temperature: T(C) Max: 1800 Min: 400

Pressure or Volume: P(atm) constant

Compositions Quantity(mol)

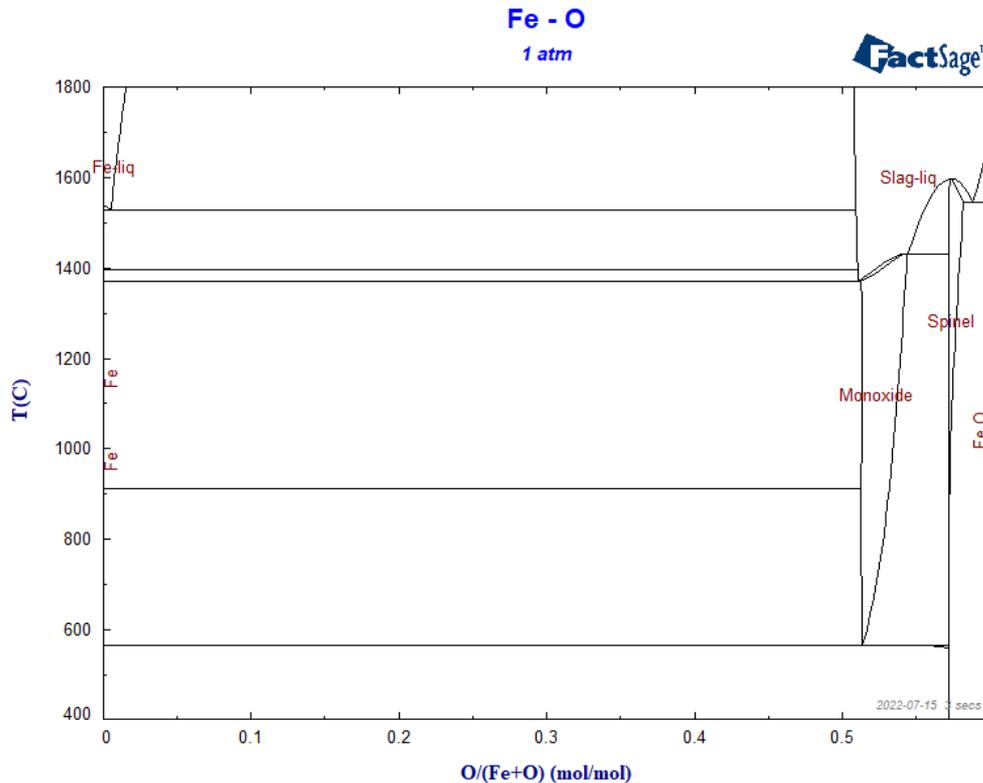
#	Quantity(mol)	Chemical Formula	X-axis
#1.	0	Fe + 1	0
	1	Fe + 1	0

$$\frac{n_O}{n_{Fe} + n_O} = X_O$$

Cancel OK

Phase Diagram Module: Fe-O₂ System

Results: Fe-O Phase Diagram ($T \sim X_O$ Phase Diagram)



Stable Phases

Stoichiometric Phases - compounds and one-component solutions

mole		TC(min)	TC(max)
1	0.0000 Fe(s)	400.00	1537.79
2	0.0000 Fe(s2)	911.66	1394.32
3	0.6000 Fe2O3(s)	400.00	1684.45

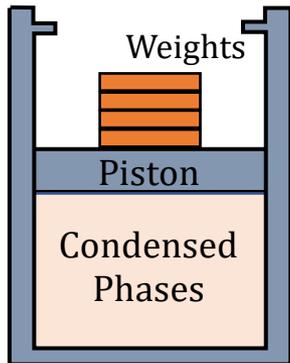
Phase Equilibria

1	1544.89 C	Slag-liq#1(0.5879)	<=>	Spinel(0.5815)	+	Fe2O3(s)(0.6)
2	1537.80 C	Fe-liq(0.0)	<=>	Fe(s)(0.0)		
3	1526.92 C	Fe-liq(0.005514)	<=>	Fe(s)(0.0)	+	Slag-liq#1(0.5088)
4	1430.24 C	Monoxide(0.5435)	<=>	Slag-liq#1(0.5434)	+	Spinel(0.5714)
5	1394.32 C	Fe(s2)(0.0)	<=>	Fe(s)(0.0)	+	Slag-liq#1(0.51)
6	1370.50 C	Slag-liq#1(0.5103)	<=>	Fe(s2)(0.0)	+	Monoxide(0.5124)
7	911.66 C	Fe(s)(0.0)	<=>	Fe(s2)(0.0)	+	Monoxide(0.5124)
8	563.55 C	Monoxide(0.5132)	<=>	Fe(s)(0.0)	+	Spinel(0.5714)

Phase Diagram Module: Fe-O₂ System

A Note on the Fe-O Phase Equilibrium: “Gas Suppression” Condition

It is worth noting that the Fe-O phase diagram shown on [Slide](#) does not include the gas phase. That is, the gas phase is suppressed.

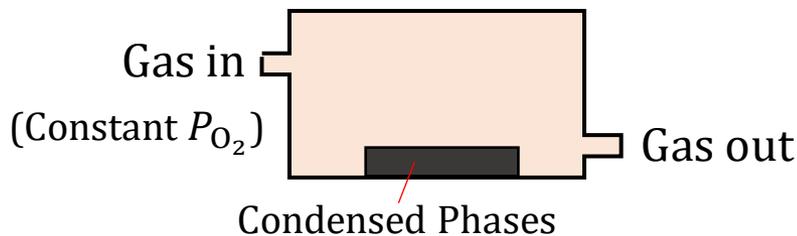


Say we fix a constant **hydrostatic** pressure of 1 atm by placing the condensed phases in a cylinder fitted with a piston (left graph). If the total gas pressure at equilibrium (i.e., sum of the partial pressures exerted by the gaseous species in the vapor phase generated by incomplete vaporization of the components) is less than 1 atm, there will be no gas phase present. This condition is referred to as “gas suppression” condition. Clearly, if we heat or cool the system, the **overall** composition of the condensed phases remain constant.

Phase Diagram Module: Fe-O₂ System

A Note on the Fe-O Phase Equilibrium: Fixed Oxygen Potential

Different from the previous condition under which the composition of the condensed phases remains unchanged, another condition is to control the oxygen content in the gas phase, i.e., constant partial pressure P_{O_2} .



Note: the mass ratio of gas to condensed phases is large enough so that the composition of gas-in and that gas-out is same.

When the above system reaches equilibrium, the condensed phases (solid and/or liquid) are equilibrated with a gas phase with fixed P_{O_2} . Say we wish to fix P_{O_2} in the range of 10^{-24} to 1 atm. Now let us plot the oxygen isobars on the Fe-O phase diagram.

Phase Diagram Module: Fe-O₂ System

Back to the Menu Window ([Slide](#))

Right click to open the Selection Window.

Right click

Click on OK and you will see "Z" appears.

Isobars (atm) of O₂(g)

Enter up to 10 isobars (atm) for O₂(g)

Enter 0 or Click on [Cancel] to delete the values.

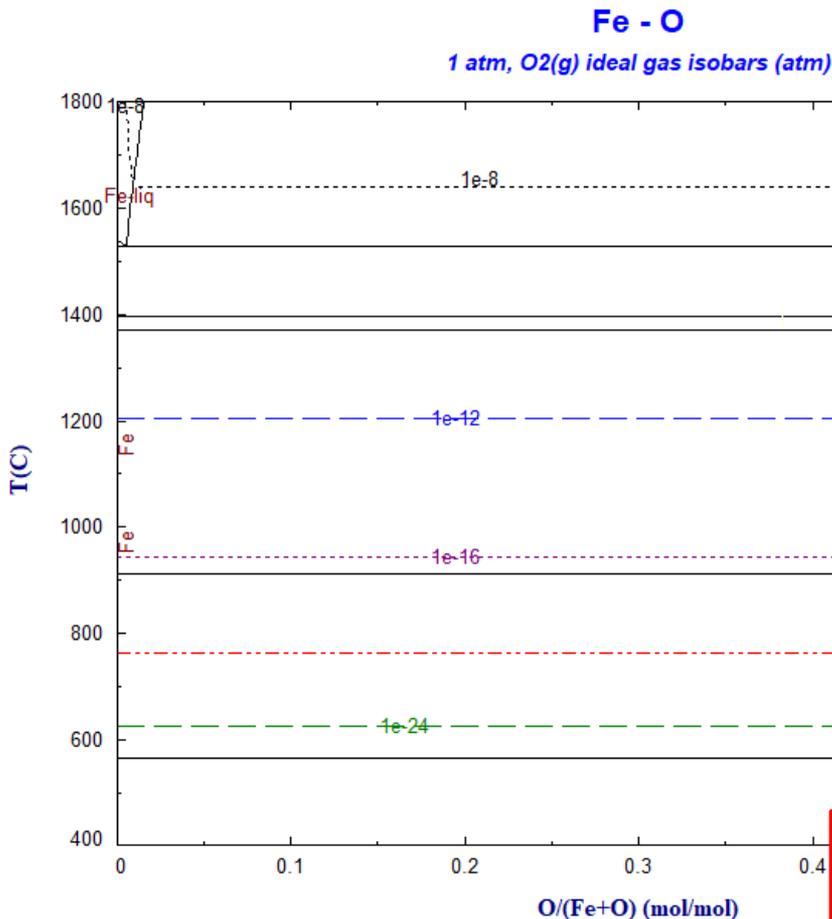
1e-24 1e-20 1e-16 1e-12 1e-8 1e-4 |

	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
1	O(g)	FactPS	gas						
2	O ₂ (g)	FactPS	gas						
3	O ₃ (g)	FactPS	gas						
4	Fe(g)	FactPS	gas						
5	FeO(g)	FactPS	gas						

permit selection of 'X' species Help Suppress Duplicates Edit priority list: Show Selected Select All Select/Clear... Clear OK

Phase Diagram Module: Fe-O₂ System

Back to the Menu Window ([Slide](#))



You may noticed this region is different from the case when gas is suppressed.

FactSage™

Stoichiometric Phases - compounds and one-com

mole		TC (min)	TC (max)
1	0.0000 Fe(s)	400.00	1537.71
2	0.0000 Fe(s2)	911.66	1394.31
3	0.6000 Fe2O3(s)	400.00	1456.41

Phase Equilibria

1	1580.04 C	Slag-liq#1(0.5814)	<=>	Spinel
2	1537.80 C	Fe-liq(0.0)	<=>	Fe(s) (0.0)

Manipulate and Refresh

clear restore Help

labels labels - old delete label: []

equilibria

iso-activity [] 1e-24 1e-20 1e-16 1e-12 1e-8 1e-4 1e-2 1e-1 7 value

polythermal projection

iso-therm T step: [100]

color T-bar clear

tie lines - isothermal diagram

all domains 1 domain hi med lo density clear

aqueous diagram

iso-Eh Eh step: [0] min: [] max: [] volts)

You are allowed to add other P_{O_2} values even after the calculation of phase diagram.

Phase Diagram Module: Fe-O₂ System

A Note on the Fe-O Phase Equilibrium: Fixed Oxygen Potential

The calculated Fe-O phase diagram with the P_{O_2} isobars can be used to study a heating or cooling process.

Say we are controlling the oxygen partial pressure $P_{O_2} = 10^{-8}$ atm. From the calculated Fe-O phase diagram, it is seen that along the line of $P_{O_2} = 10^{-8}$ atm, the highest temperature is > 1800 °C, and the condensed phase should be pure iron. Now, if we cool this system while keeping the oxygen partial pressure constant (10^{-8} atm), the composition of the condensed phase will be changed along the line of $P_{O_2} = 10^{-8}$ atm because of the oxidation.

The above simple analysis shows that the variables, i.e., temperature, composition of the condensed phases and P_{O_2} are correlated. As West and Saunders commented that the partial pressure of oxygen is a function of both temperature and composition.

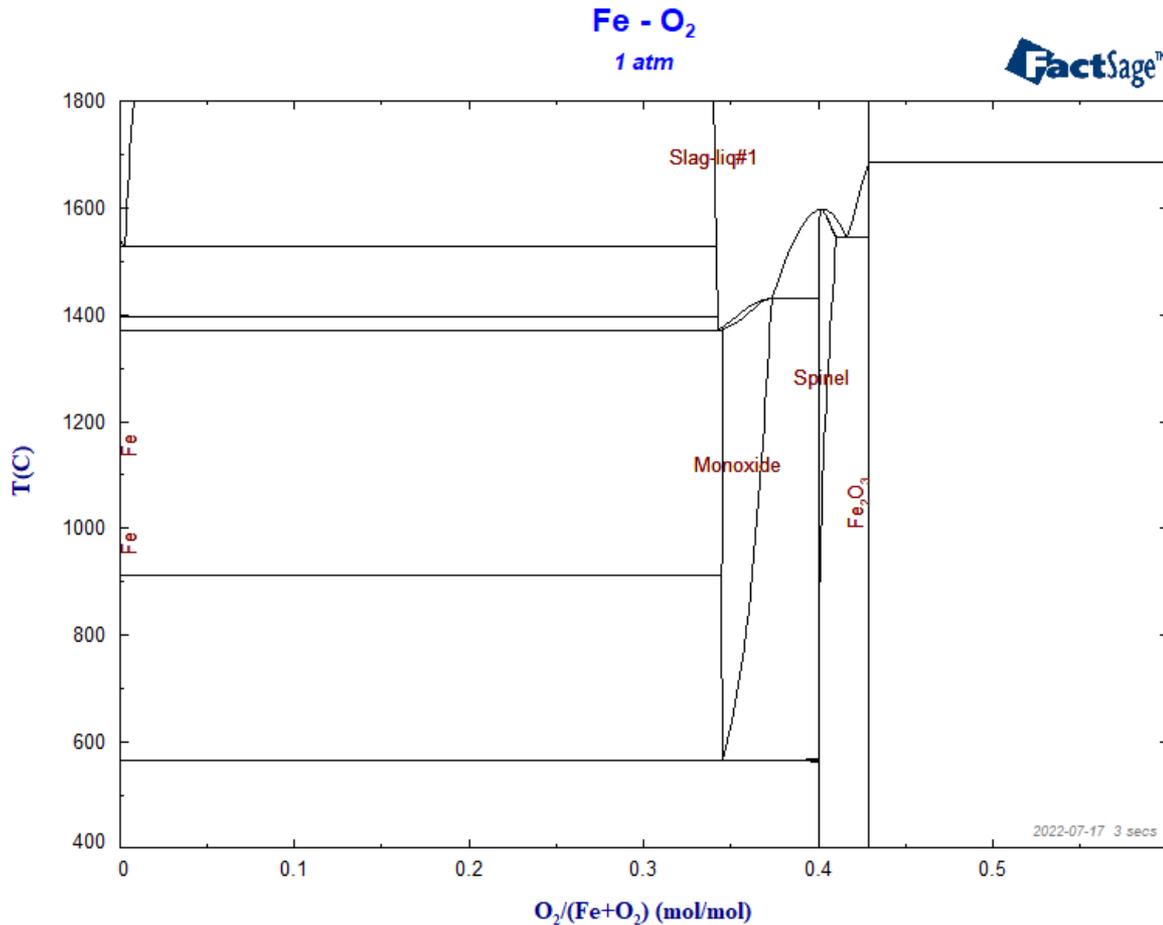
Phase Diagram Module: Fe-O₂ System

Now, we have successfully reproduce the Fe-O phase diagram shown in the Documentation. To calculate the Fe-O₂ phase diagram, we need to change the component “O” to “O₂”, but do not change the phase selection.

You can calculate either the condition under which the gas phase is suppressed, or the condition of fixed P_{O_2} . Here, we only show the calculation when the gas phase is suppressed.

Phase Diagram Module: Fe-O₂ System

Results: Fe-O₂ Phase Diagram ($T \sim X_{O_2}$ Phase Diagram)



Phase Diagram Module: Fe-O₂ System

Next, let us look at two-potential phase diagrams. We will again use the Fe-O₂ system as the example to calculate $T \sim \mu_{\text{O}_2}$ (thermal potential ~ chemical potential) for the Fe-O₂ system.

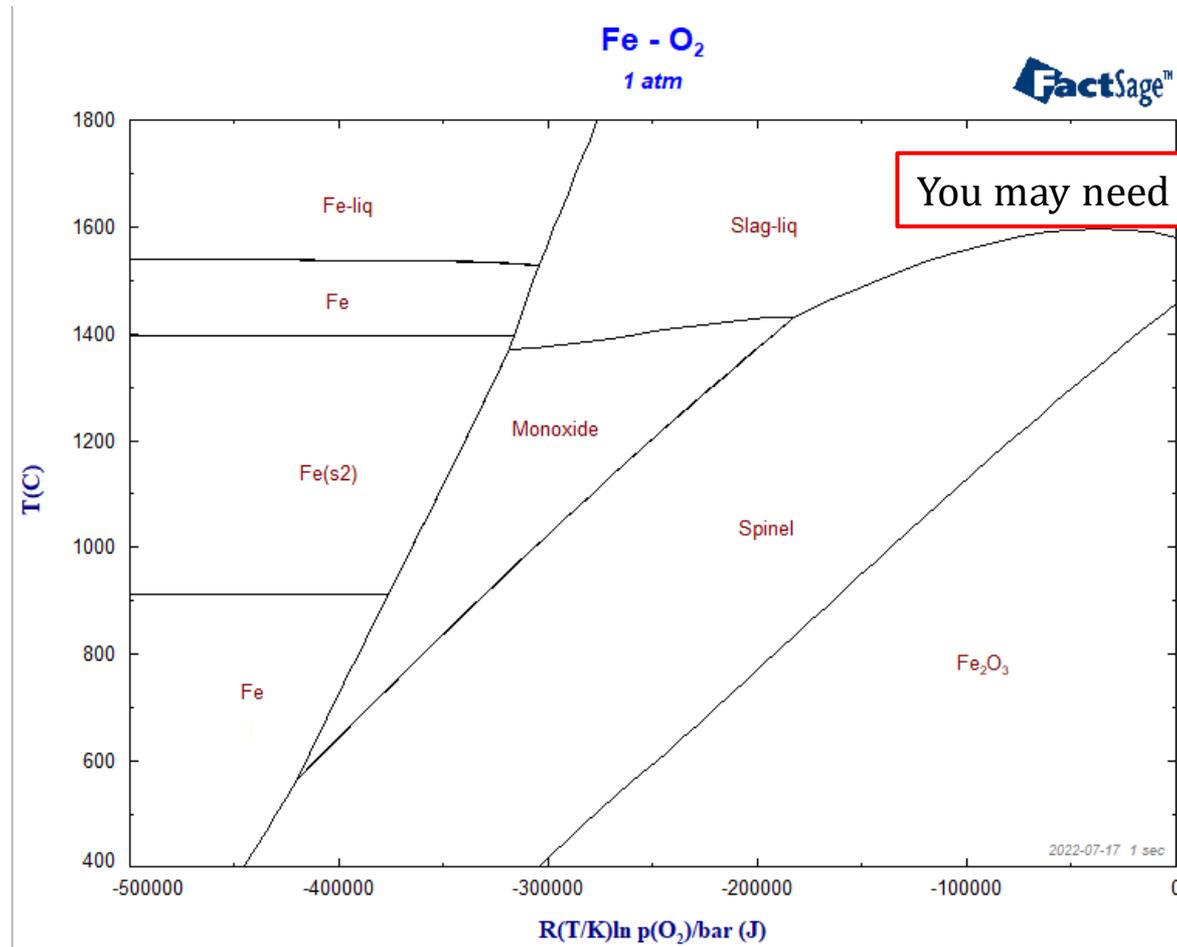
You might ask why we want to use μ_{O_2} as a variable? From the master equation, we know,

$$\mu_{\text{O}_2} = \mu^{\circ}_{\text{O}_2} + RT \ln(P_{\text{O}_2})$$

This means that, the topology of the $T \sim \mu_{\text{O}_2}$ diagram is same to that of the $T \sim RT \ln(P_{\text{O}_2})$ diagram. **Clearly**, we are very interested in the effect of P_{O_2} on the phase equilibria. However, you should note that the topology of the $T \sim \mu_{\text{O}_2}$ diagram is different from that of the $T \sim \ln(P_{\text{O}_2})$ diagram.

Phase Diagram Module: Fe-O₂ System

Results: Fe-O₂ Phase Diagram (Two-potential Phase Diagram)



You may need to add labels manually.

This is a very useful diagram. It shows the stability regions of various condensed phases.

FactSage Practical

MSE302

Practical 3. Phase Diagram Calculation

Phase Diagram Module: Ternary System

Phase Diagram Module

The phase diagram for a ternary system requires a space model. Because of this, we normally calculate **isothermal sections** and **liquidus projections** which are easier to view in a 2D space.

The Phase Diagram Module can be used to calculate above phase diagrams for ternary systems. Two examples will be presented, one is metallic system and the other is oxide system.

A Note: most binaries have been critically assessed using existing experimental data and therefore the binary phase diagrams reported by different accessors (or model developers) generally agree with each other. However, this is not true for ternary and higher-order systems. Since the amount of work in measuring even one isothermal section of a relatively simple **ternary** phase diagram is enormous, most of ternary phase diagrams and higher-order phase diagrams are estimates extrapolated from critically evaluated binaries, and validated using limited amounts of experimental data.

Phase Diagram Module: Al-Mg-Zn System

Let us review the FTlite database. Go to the Documentation Module, navigate to “[FTlite] – FACT Al-Alloy and Mg-alloy databases”, and open the PDF document of “general description and list of optimized systems”.

Al Alloys
Ag, Al , <u>As</u> , <u>Au</u> , B , Ba , Be , Bi , C , Ca , Ce , Co , Cr , Cu , Dy , Er , Eu , Fe , <u>Ga</u> , Gd , Ge , H , <u>Hf</u> , Ho , In , K , La , Li , Lu , Mg , Mn , <u>N</u> , Na , <u>Nb</u> , Nd , Ni , <u>P</u> , Pb , Pr , Sb , Sc , Si , Sm , Sn , Sr , <u>Ta</u> , Tb , Ti , Tm , V , <u>W</u> , Y , Yb , Zn , Zr
Mg Alloys
Ag, Al , B , Ba , Be , Bi , C , Ca , Ce , Co , Cr , Cu , Dy , Er , Eu , Fe , Ga , Gd , Ge , H , Ho , In , K , La , Li , Lu , Mg , Mn , Na , Nb , Nd , Ni , Pb , Pr , Sb , Sc , Si , Sm , Sn , Sr , Tb , Ti , Tm , V , Y , Yb , Zn , Zr
Color codes
Red : Al or Mg
Blue : Major alloying elements (full optimisations of binary systems with Al and Mg and with several minor alloying elements, Al-Mg-Xx ternary systems evaluated (good for Al+Mg-rich regions), several quaternary systems included);
Green : Minor alloying elements (full optimisations of binary systems with Al and Mg);
<u>Black</u> : Optimized for the Al-Zz system and few Al-Xx-Zz and Al-Yy-Zz systems;

Phase Diagram Module: Al-Mg-Zn System

The above description shows that the FTlite database could be used to calculate the Al-Mg-Zn system.

Note: for the FTlite database, no pre-made phase diagram for ternary systems by CRCT (only binary systems) is available. That is, you won't be able to find the Al-Mg-Zn phase diagrams calculated using the FTlite database from the Documentation Module. You might be able to find a few Al-Mg-Zn phase diagrams calculated using the SGTE (alloy) database. Unfortunately, we do not have the access to the SGTE database.

Phase Diagram Module: Al-Mg-Zn System

Components Window: Define Components

Phase Diagram - Components

File Edit Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Choose Units.

Don't forget to check your Directory.

Components

Al

Mg

Zn

classical phase diagram (default)

aqueous diagram with molalities, and iso-Eh & iso-pH lines

reciprocal diagram with 2 cations and 2 anions

Scheil-Gulliver constituent diagram

Next >>

FactSage 7.3 Compound: 1/14 databases Solution: 1/15 databases

Phase Diagram Module: Al-Mg-Zn System

Menu Window: Choose Products/Phases (Compounds and Solution Phases)

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (3)

Al + Mg + Zn

Select all the solutions and use the default settings of immiscibility gaps.

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

pure solids 35

species: 35

Target

- none -

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
	I	FTlite-Liqu	Liquid
	I	FTlite-A1	FCC-A1
	I	FTlite-A2	BCC-A2
	I	FTlite-A3	HCP-A3
	I	FTlite-A3''	HCP-Zn Prototype-Mg
	I	FTlite-A12	CBCC-A12 Prototype-Mn
	I	FTlite-C14	C14 Prototype-MgZn2
	I	FTlite-C36	C36 Prototype-MgNi2

Legend

I - immiscible 9

+ - selected 6

species: 118

solutions: 24

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

paraequilibrium & Gmin edit

Total Species (max 5000) 153

Total Solutions (max 200) 24

Total Phases (max 1500) 59

Select

Add all solutions containing >

Add all solutions from database >

Select all solutions

Make all unselected solutions dormant

Change all [I] to [+] (2-phase to 1-phase)

Change all [I] to [I] (3-phase to 2-phase)

Clear all solutions containing >

Clear all solutions from database >

Clear all solutions

Clear all dormant solutions

Choose all the pure solids. You should know that selection of some of the pure solids is not necessary, e.g., Mg(hcp_A3), Mg₂Zn(C36) etc., because there are corresponding solution phases which include these pure solids as endmembers. For example, FTlite-A3 (HCP-A3) in the Solution phases, if $X_{Mg} = 1$, FTlite-A3 becomes Mg(hcp_A3). However, in most cases, it does no harm if these phases are selected.

Phase Diagram Module: Al-Mg-Zn System

A Note on the Selection of Products/Phases

To make FactSage more user-friendly, the developers of **commercial** databases have added some key features to the databases, for example:

- ✓ [+] , [I] , and [J] indicate the possibility of miscibility, two-phase immiscibility, and three-phase immiscibility.
- ✓ All the endmembers of solution phases are included in the pure solids.

These features permit the FactSage users who do not have a good knowledge of thermodynamics to perform relatively reliable calculations for simple systems. **However**, for complex real-world problems, an advanced FactSage user always performs screening of products to avoid the appearance of unreasonable phases in the equilibrium calculations.

Phase Diagram Module: Al-Mg-Zn System

Menu Window: Set up the Variables (**Liquidus Projections**)

For ternary systems, we use Gibbs triangle to describe the composition (only 2 are needed).

This will permit the calculation of projection diagrams. Also, the isotherms are specified by max, min and increments.

A-Corner would be Zn.

$$\frac{n_{Zn}}{n_{Al} + n_{Mg} + n_{Zn}} = X_{Zn}$$

Phase Diagram Module: Al-Mg-Zn System

Menu Window: Choose Products/Phases (Compounds and Solution Phases)

Right click to change FTlite-Liqu to the option of “P – precipitate target phase”.

We are calculating the liquidus projection, which means other solids phases (primary crystallization solids) are precipitating from the liquid.

The options of “univariants” and “isotherms” must be selected. They are important elements of liquidus projection diagrams.

*	+	Base-Phase	Full Name
*		IP	FTlite-Liqu
	I		FTlite-A1
	I		FTlite-A2
	I		FTlite-A3
	I		FTlite-A3''
	I		FTlite-A12

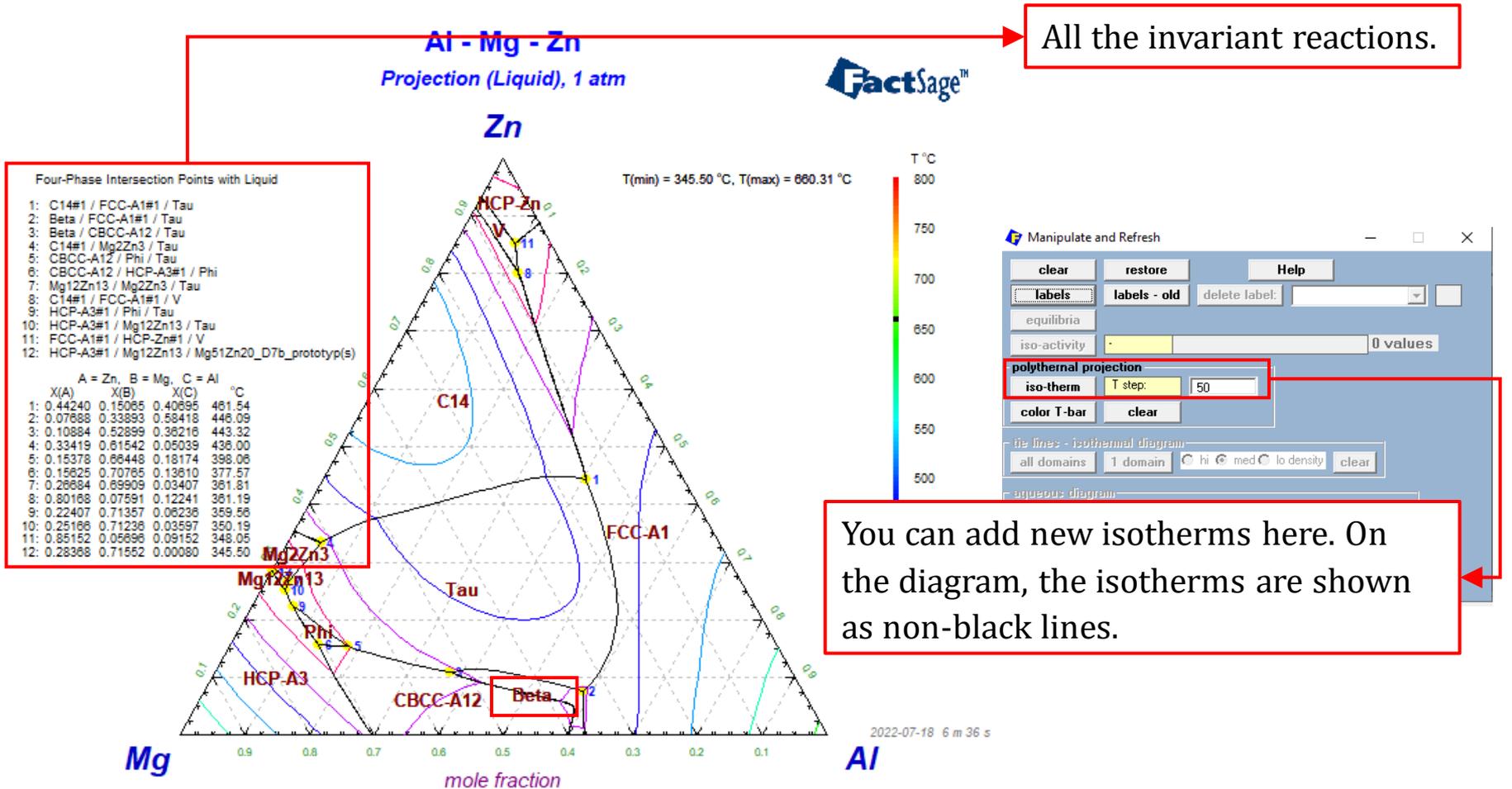
Phase Diagram Projection

univariants
 isotherms (9)

Calculate >>

Phase Diagram Module: Al-Mg-Zn System

Results: Liquidus Projection of the Al-Mg-Zn System (FTlite Database)



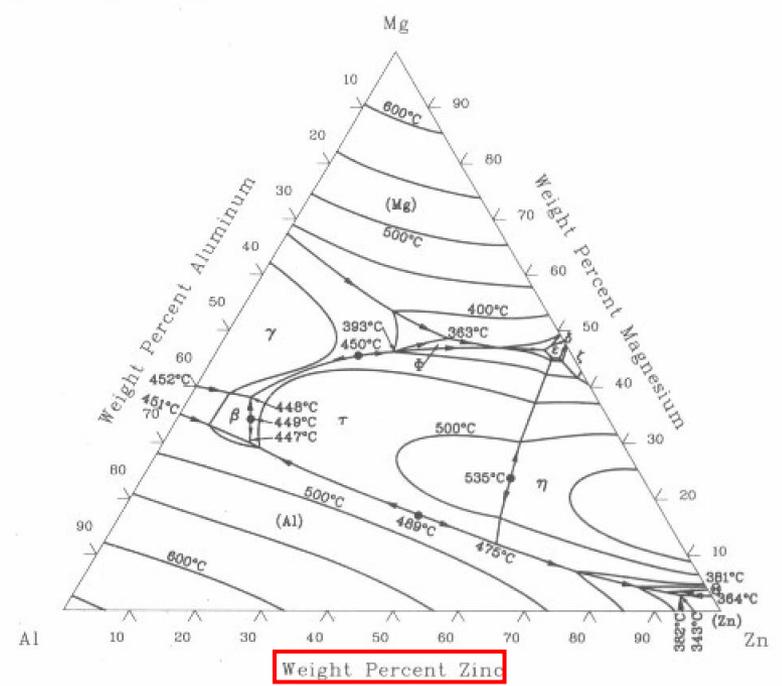
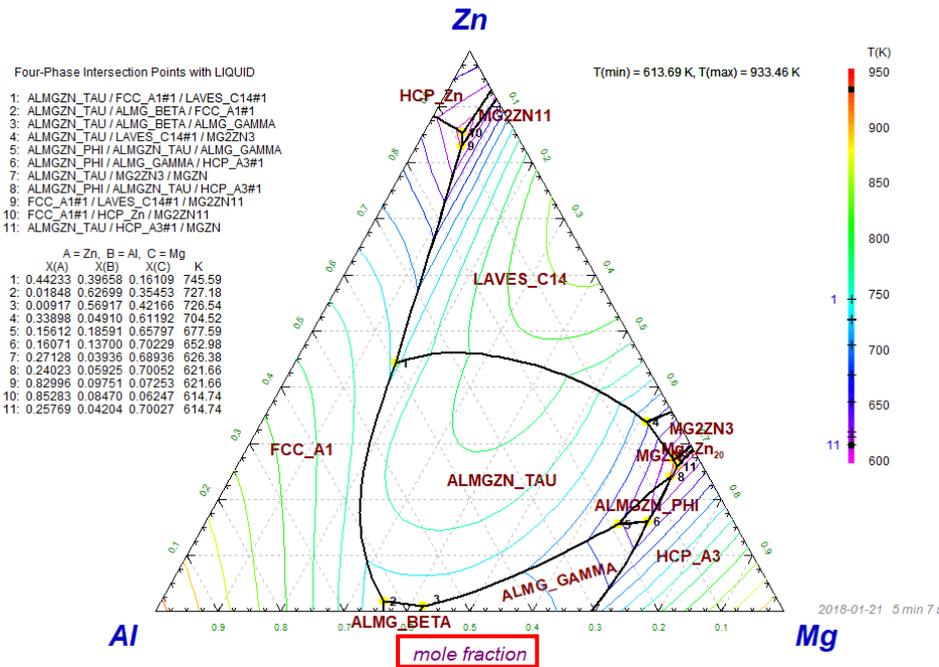
Phase Diagram Module: Al-Mg-Zn System

Comparison with the diagrams from [SGTE2017](#) and [ASM Handbook](#).

Al - Mg - Zn
Projection (LIQUID), 1 bar



Al-Mg-Zn liquidus projection [73Wil]



Don't be surprised if you find that the discrepancy exists for the liquidus Al-Mg-Zn projections from different sources. After all, they are all just estimates!!!

Phase Diagram Module: Al-Mg-Zn System

Back to Variable Window ([Slide](#)): Isothermal Sections

Phase Diagram - Menu: last system

File Units Parameters **Variables** Help

Variables: Al-Mg-Zn composition #1. vs composition #1.

Variables

compositions 2

log10(a) 0

Next >>

T and P

Temperature

T(C)

constant

20

Pressure or Volume

P(atm) constant

log P

V(litre) 1

log V

Compositions Quantity(mol)

#1. 0 Al + 0 Mg + 1 Zn = 1 (max)
1 Al + 1 Mg + 1 Zn = 0 (min)

A-Corner

#2. 1 Al + 0 Mg + 0 Zn = 1 (max)
1 Al + 1 Mg + 1 Zn = 0 (min)

C-Corner

#3. 0 Al + 1 Mg + 0 Zn = 1 (max)
1 Al + 1 Mg + 1 Zn = 0 (min)

B-Corner

Cancel OK

Now we want to calculate the isothermal section of the Al-Mg-Zn system at 20 °C.

Phase Diagram Module: Al-Mg-Zn System

Menu Window: Choose Products/Phases (Compounds and Solution Phases)

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components [3]

Change FTlite-Liqu to the option of "standard stable phase".

Solution FTlite-Liqu

- clear
- all end-members
- * - custom select end-members ...
- m - merge dilute solution from >
- + - single phase
- I - possible 2-phase immiscibility
- J - possible 3-phase immiscibility
- standard stable phase
- ! - dormant (metastable) phase
- F - formation target phase
- P - precipitate target phase
- O - Only plot this single phase
- S - Scheil cooling target phase
- Z - iso-activity lines ...
- Help ...

Products

Compound species

gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	0
aqueous			0
pure liquids			0
pure solids			35
species:			35

Solution phases

*	+	Base-Phase	Full Name
<input checked="" type="checkbox"/>	<input type="checkbox"/>	FTlite-Liqu	Liquid
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-A1	FCC-A1
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-A2	BCC-A2
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-A3	HCP-A3
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-A3"	HCP-Zn Prototype-Mg
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-A12	CBCC-A12 Prototype-Mn
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-C14	C14 Prototype-MgZn2
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-C36	C36 Prototype-MgNi2

Legend
I - immiscible 9
+ - selected 6

Show all selected

species: 118
solutions: 24

Variables

T(C)	Zn/(Al+Mg+Zn)	Al/(Al+Mg+Zn)		
20	01	01		

A = Zn, B = Mg, C = Al

Target
- none -
Estimate T(K):

Custom Solutions
0 fixed activities
0 ideal solutions

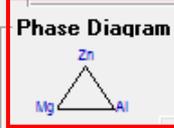
Pseudonyms
apply

Volume data
 assume molar volumes of solids and liquids = 0
 include molar volume data and physical properties data

paraequilibrium & Gmin

Total Species (max 5000) 153
Total Solutions (max 200) 24
Total Phases (max 1500) 59

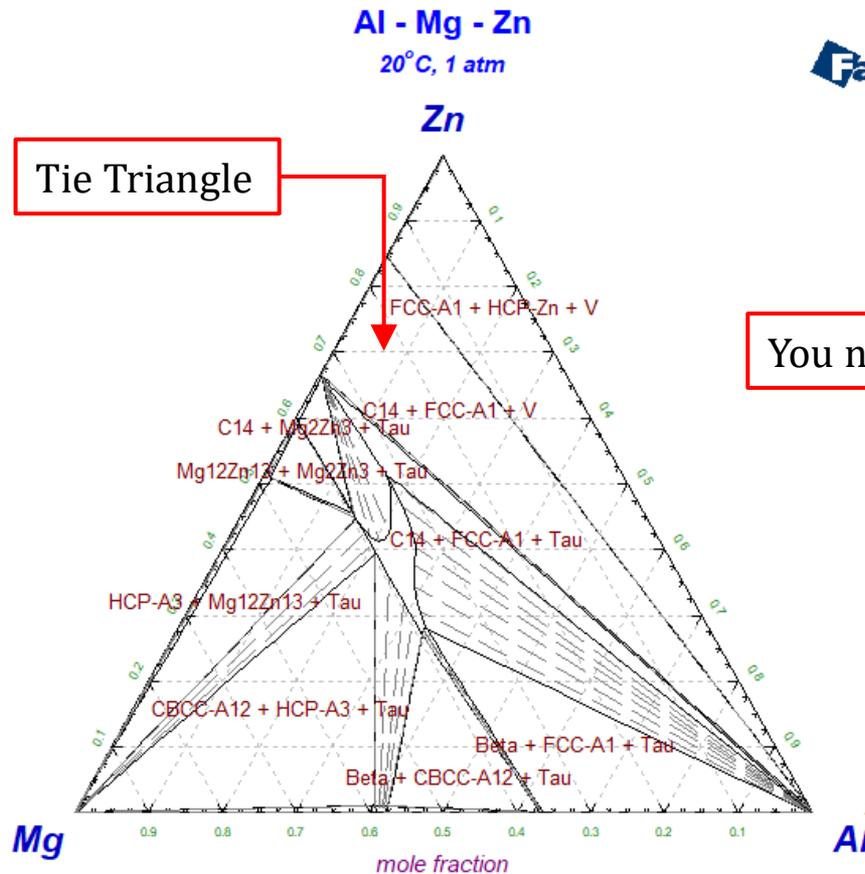
Phase Diagram



FactSage 7.3

Phase Diagram Module: Al-Mg-Zn System

Results: Isothermal Section of the Al-Mg-Zn System (FTlite Database)



Stable Phases - solutions and compounds (pure)

- 1 FTlite-Beta Beta Prototype-Mg₂₈Al₄₅ Pears
- 2 FTlite-C14 C14 Prototype-MgZn₂ (Lave
- 3 FTlite-Al₂ CBCC-Al₂ Prototype-Mn Struk
- 4 FTlite-Al₁ FCC-Al Protc
- 5 FTlite-A₃ HCP-A₃ Protc
- 6 FTlite-A₃" HCP-Zn Prototype-Mg Struk
- 7 FTlite-MgZn Mg₁₂Zn₁₃ Mg-Zn

Manipulate and Refresh

clear restore Help

labels labels - old delete label: C14 + Mg₂Zn₁₃ + Tau 9

equilibria

iso-activity 0 values

polythermal projection

iso-therm T step: 100

color T-bar clear

tie lines - isothermal diagram

all domains 1 domain hi med lo density clear

aqueous diagram

iso-Eh Eh step: 0 min: max: (volts)

iso-pH pH step: 0 min: max:

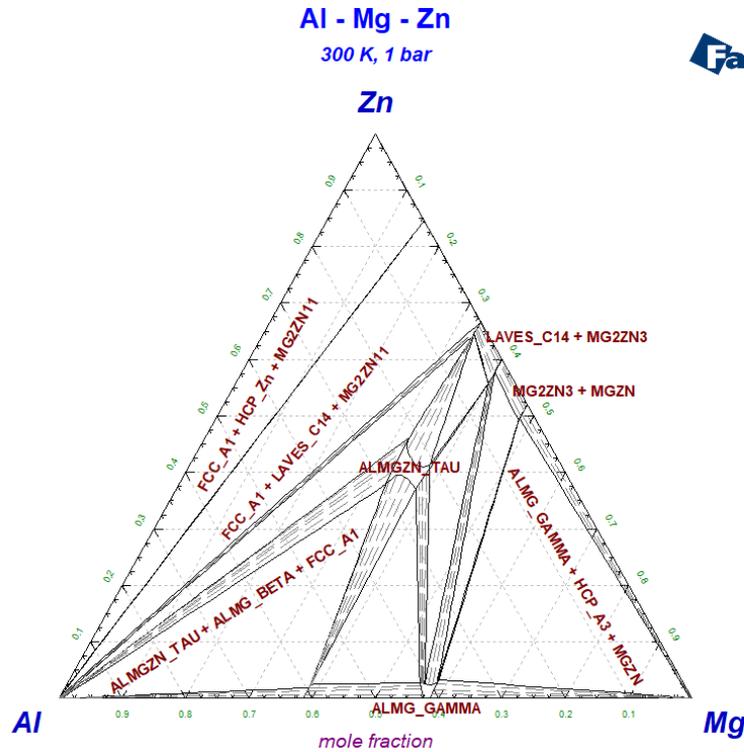
Figure viewer full screen

You need to manually label the regions.

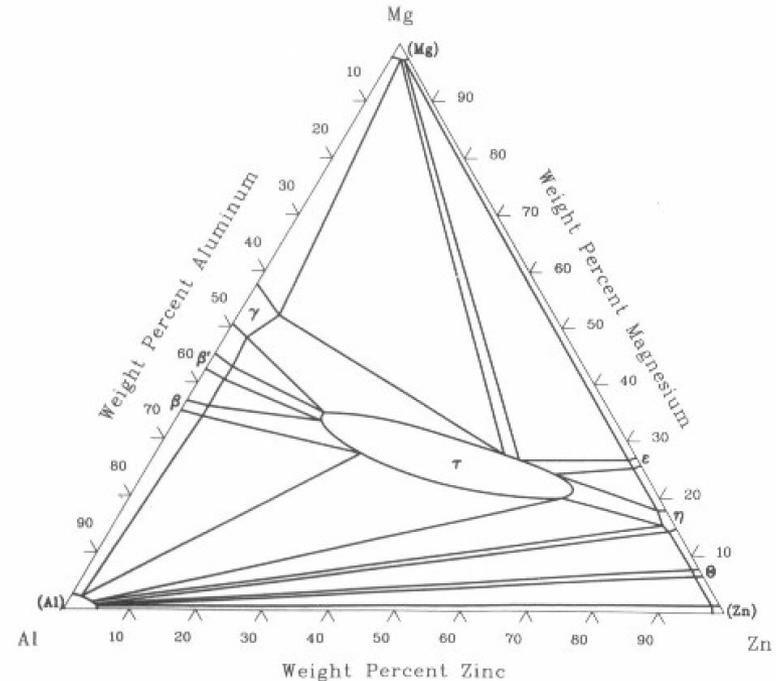
This allows us to plot the tie lines for two-phase regions.

Phase Diagram Module: Al-Mg-Zn System

Comparison with the diagrams from [SGTE2017](#) and [ASM Handbook](#).



Al-Mg-Zn isothermal section at 20 °C [36Kos]



Again, there is a discrepancy between different phases diagrams reported from different sources.

Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

Now let us calculate an oxide system which consists of SiO_2 , CaO , and Al_2O_3 . It is worth mentioning that the ternary SiO_2 - CaO - Al_2O_3 phase diagram is actually an isopleth of the quaternary Si-Ca-Al-O system along the line:

$$n_{\text{O}} = 2n_{\text{Si}} + n_{\text{Ca}} + 1.5n_{\text{Al}}$$

This relationship is met in every condensed phases. Therefore, strictly speaking, the ternary SiO_2 - CaO - Al_2O_3 phase diagram is a “**quasi-**” ternary phase diagram.

You also should note that the pressure, more specifically, P_{O_2} , has a negligible effect on the phase equilibria of the SiO_2 - CaO - Al_2O_3 system because all the metals have only one oxidation state.

Phase Diagram Module: $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ System

First, let us search this system in the Documentation Module.

The screenshot shows the FactSage Browser interface with search results for the $\text{CaO-Al}_2\text{O}_3\text{-SiO}_2$ system. The search criteria are $\text{CaO Al}_2\text{O}_3 \text{ SiO}_2$ and the search scope is set to 'Search phase diagrams'. The results page displays a list of phase diagrams, with three entries from the FToxid database highlighted in red:

- CaO - Al₂O₃ - SiO₂ : | FToxid |
- CaO - Al₂O₃ - SiO₂ : | FToxid |
- CaO - Al₂O₃ - SiO₂ : | FToxid |

Other results include diagrams from the TDnucl database for CaO-SiO₂ and ZrO₂-SiO₂-CaO, and FToxid diagrams for CaO-SiO₂-TiO₂-O₂ and P₂O₅-CaO-SiO₂.

A red box highlights the three FToxid results, and a red arrow points from this box to a text box containing the following text:

Three isothermal sections calculated using the FToxid database are found. Let us first reproduce these diagrams. (In doing so, we will find out if some phases should not be selected.)

The interface also shows a list of database files on the left and a 'Revised: 3/3/2019' timestamp at the bottom right.

Phase Diagram Module: $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ System

Components Window: Define Components

Phase Diagram - Components

File Edit Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

1 - 3

Components

SiO₂

CaO

Al₂O₃

classical phase diagram (default)

aqueous diagram with molalities, and iso-Eh & iso-pH lines

reciprocal diagram with 2 cations and 2 anions

Scheil-Gulliver constituent diagram

Next >>

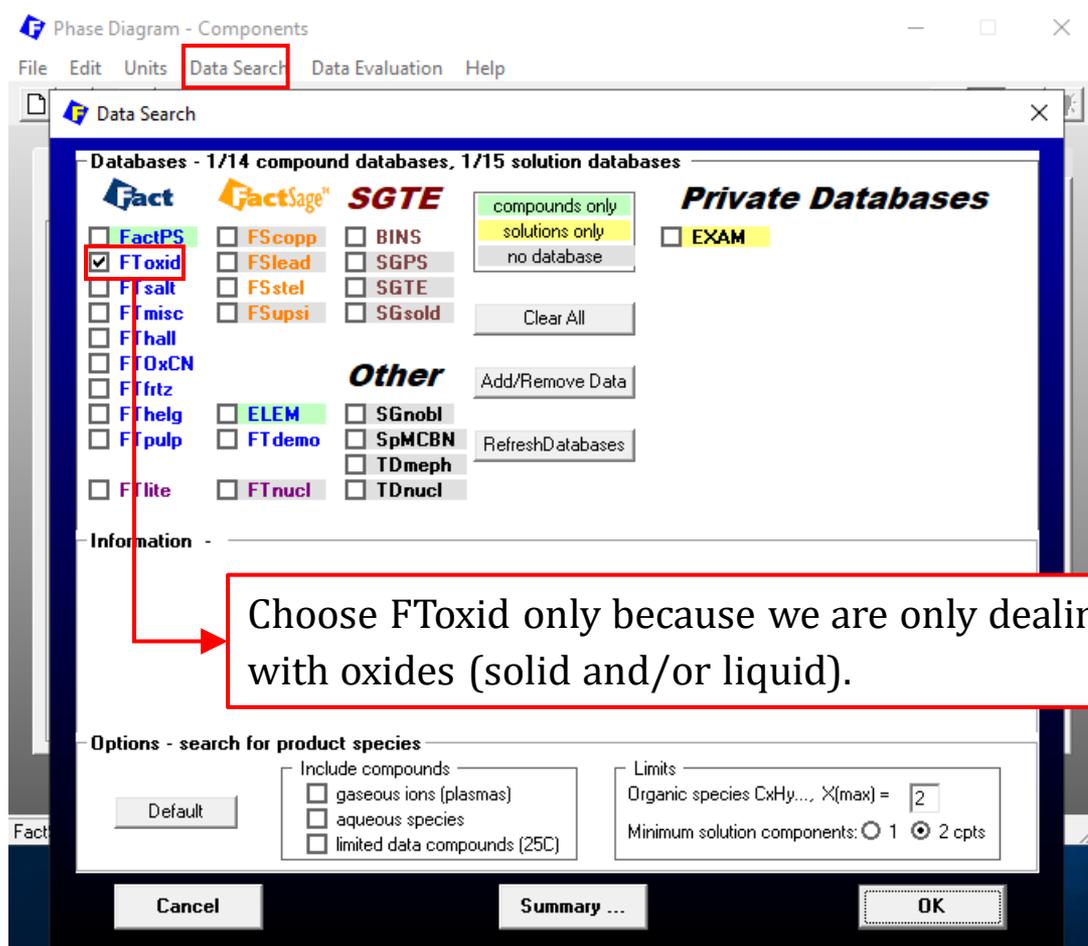
FactSage 7.3 Compound: 1/14 databases Solution: 1/15 databases

Don't forget to check your Directory.

Choose Units.

Phase Diagram Module: SiO₂-CaO-Al₂O₃ System

Components Window: Choose Database(s)



Phase Diagram Module: SiO₂-CaO-Al₂O₃ System

Menu Window: Choose Products/Phases (Compounds and Solution Phases)

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (3)

SiO₂ + CaO + Al₂O₃

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

+ pure solids 30

species: 30

Target

- none -

Estimate T(K): 1000

Variables

T(C)

1200

A = SiO₂, B = CaO, C = Al₂O₃

Solution phases

*	+	Base-Phase	Full Name
		FToxid-SLAGA	A-Slag-liq all oxides + S
		FToxid-MeO_A	A-Monoxide
	+	FToxid-Mel_A	A-Melilite
		FToxid-Mull	Mullite

Custom Solutions

0 fixed activities Details ...

0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

paraequilibrium & Gmin edit

Virtual species: 6

Total Species (max 5000) 50

Total Solutions (max 200) 7

Total Phases (max 1500) 37

Legend

| - immiscible 3

+ - selected 1

Show all selected

species: 20

solutions: 7 Select

FactSage 7.3

Let us choose all pure solids and all solution phases. For solution phases, choose the default setting of immiscibility. If the three isothermal sections found from the Documentation Module can be reproduced, then probably no phase is required to be removed.

Phase Diagram Module: $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ System

Menu Window: Set the Variables (**Isothermal Sections**)

Phase Diagram - Menu: last system

File Units Parameters **Variables** Help

Variables: $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ composition #1. vs composition #1.

Variables

compositions 2

T and P

Temperature

T(C) constant 1200

Pressure or Volume

P(atm) constant

log P

V(litre) 1

log V

Gibbs triangle.

Compositions Quantity(mol)

Corner	SiO ₂	CaO	Al ₂ O ₃
A-Corner	1 (max)	0 (min)	0 (min)
C-Corner	0 (min)	0 (min)	1 (max)
B-Corner	0 (min)	1 (max)	0 (min)

A corner: pure SiO_2 .

C corner: pure Al_2O_3 .

B corner: pure CaO.

Cancel OK

Phase Diagram Module: SiO₂-CaO-Al₂O₃ System

Menu Window: Set up the Variables

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (3)

SiO₂ + CaO + Al₂O₃

Products

Compound species

gas ideal real 0
aqueous 0
pure liquids 0
pure solids 30

species: 30

Target
- none -
Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
		FToxid-SLAGA	A-Slag-liq all oxides + S
		FToxid-MeO_A	A-Monoxide
	+	FToxid-Mel_A	A-Mellite
		FToxid-Mull	Mullite

Legend
| - immiscible 3
+ - selected 1

Show all selected
species: 20
solutions: 7

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
apply

Volume data
 assume molar volumes of solids and liquids = 0
 include molar volume data and physical properties data

paraequilibrium & Gmin

Virtual species: 6
Total Species (max 5000) 50
Total Solutions (max 200) 7
Total Phases (max 1500) 37

Variables

T(C)	SiO ₂ /	Al ₂ O ₃ /		
1200	0.1	0.1		

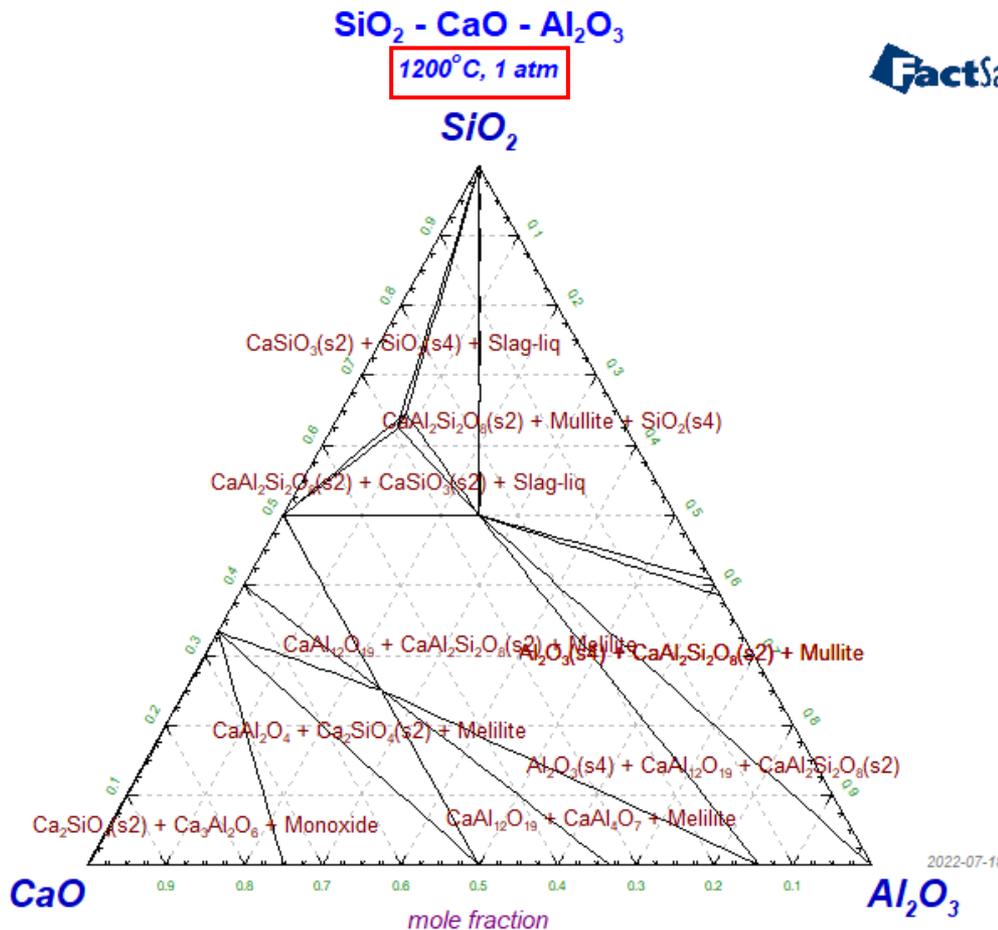
A = SiO₂, B = CaO, C = Al₂O₃

Phase Diagram

FactSage 7.3

Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

Results: Isothermal Section of the SiO_2 - CaO - Al_2O_3 System (FToxid Database)



Stable Phases

Stable Phases - solutions and compounds (pure)			
1	FToxid-SLAG	Slag-liq	oxide Al,As,B,Ba,C
2	FToxid-Mel_	Melilite	(Ca,Sr,Ba,Pb,Na)2[
3	FToxid-MeO_	Monoxide	Rocksalt-str. Fe(2
4	FToxid-Mull	Mullite	[Al,Fe]2[Al,Si,B,E
5	FToxid (PS)	Al2O3 (s4)	corundum(alpha)
6	FToxid (PS)	Ca2SiO4 (s2)	Alpha-prime
7	FToxid (PS)	Ca3Al2O6 (s)	solid
8	FToxid (PS)	Ca3Si2O7 (s)	Rankinite
9	FToxid (PS)	CaAl12O19 (s)	solid
10	FToxid (PS)	CaAl2O4 (s)	solid
11	FToxid (PS)	CaAl2Si2O8 (s2)	Anorthite

Manipulate and Refresh

clear restore Help

labels labels - old delete label: $\text{Al}_2\text{O}_3(\text{s4}) + \text{CaAl}_2$

equilibria

iso-activity 0 values

polythermal projection

iso-therm T step: 100

color T-bar clear

tie lines - isothermal diagram

all domains 1 domain hi med lo density clear

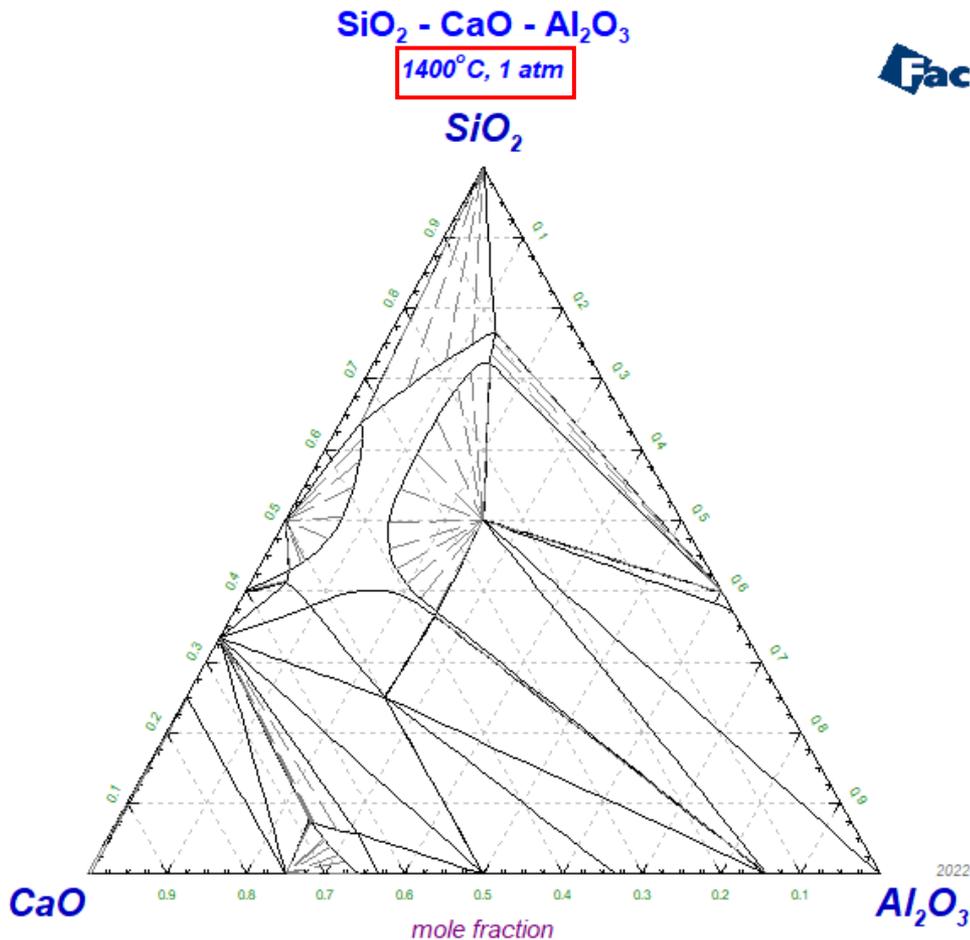
aqueous diagram

iso-Eh Eh step: 0 min: max: (volts)

pH step: 0 min: max:

Phase Diagram Module: $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ System

Results: Isothermal Section of the $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ System (FToxid Database)



Stable Phases

Stable Phases - solutions and compounds (pure)			
1	FToxid-SLAG	Slag-liq	oxide Al,As,B,Ba,C
2	FToxid-Mel_	Melilite	(Ca,Sr,Ba,Pb,Na) ₂ [
3	FToxid-MeO_	Monoxide	Rocksalt-str. Fe(2
4	FToxid-Mull	Mullite	[Al,Fe] ₂ [Al,Si,B,F
5	FToxid (PS)	Al ₂ O ₃ (s4)	corundum(alpha)
6	FToxid (PS)	Ca ₂ SiO ₄ (s2)	Alpha-prime
7	FToxid (PS)	Ca ₃ Al ₂ O ₆ (s)	solid
8	FToxid (PS)	Ca ₃ Si ₂ O ₇ (s)	Rankinite
9	FToxid (PS)	Ca ₃ SiO ₅ (s)	Hatrumite
10	FToxid (PS)	CaAl ₁₂ O ₁₉ (s)	solid

Manipulate and Refresh

clear restore Help

labels labels - old delete label: [dropdown]

equilibria

iso-activity [input] 0 values

polythermal projection

iso-therm T step: [input] 100

color T-bar clear

tie lines - isothermal diagram

all domains 1 domain hi med lo density clear

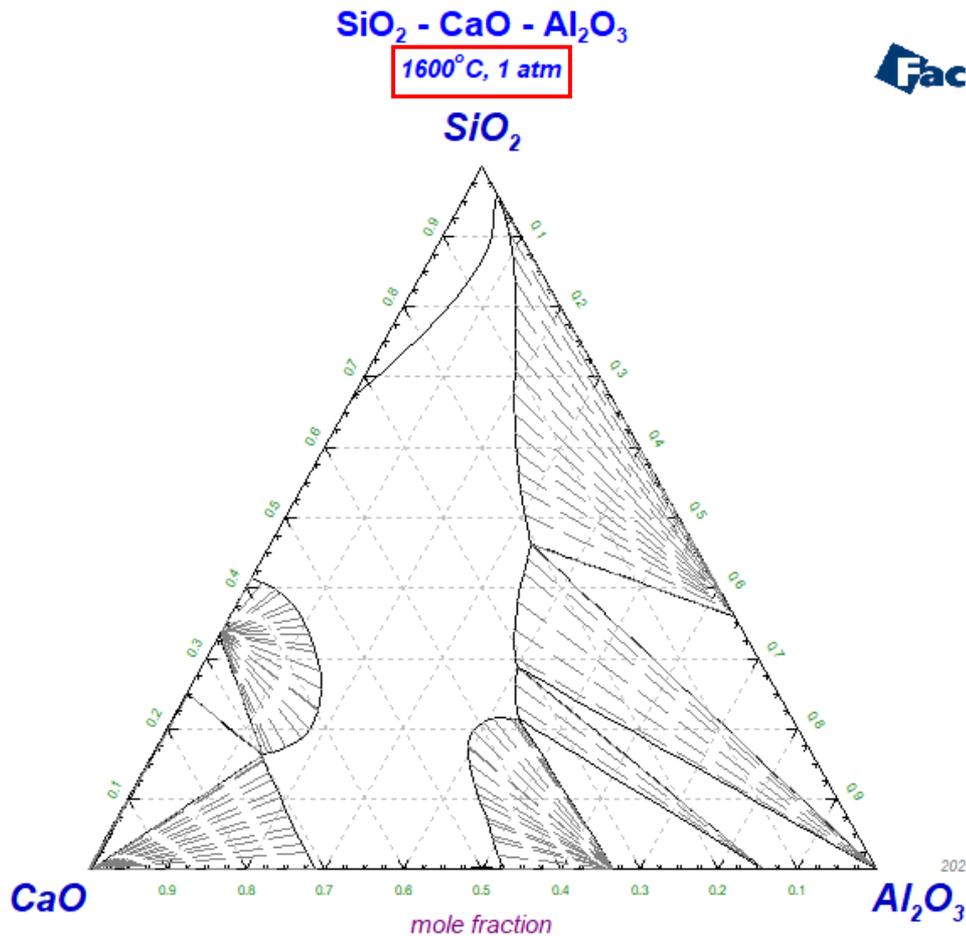
aqueous diagram

iso-Eh Eh step: [input] 0 min: [input] max: [input] (volts)

iso-pH pH step: [input] 0 min: [input] max: [input]

Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

Results: Isothermal Section of the SiO_2 - CaO - Al_2O_3 System (FToxid Database)



Stable Phases

Stable Phases - solutions and compounds (pure)			
1	FToxid-SLAG	Slag-liq	oxide Al,As,B,Ba,Ca,
2	FToxid-MeO_	Monoxide	Rocksalt-str. Fe(2),
3	FToxid-Mull	Mullite	[Al,Fe]2[Al,Si,B,Fe]
4	FToxid (PS)	Al2O3(s4)	corundum(alpha)
5	FToxid (PS)	Ca2SiO4(s3)	Alpha
6	FToxid (PS)	Ca3SiO5(s)	Hatrurite
7	FToxid (PS)	CaAl12O19(s)	solid
8	FToxid (PS)	CaAl2O4(s)	solid
9	FToxid (PS)	CaAl4O7(s)	solid
10	FToxid (PS)	SiO2(s6)	Cristobalite(h)

Manipulate and Refresh

clear restore Help

labels labels - old delete label: [dropdown]

equilibria

iso-activity [input] 0 values

polythermal projection

iso-therm T step: [input] 100

color T-bar clear

tie lines - isothermal diagram

all domains 1 domain hi med lo density [clear]

aqueous diagram

iso-Eh Eh step: [input] 0 min: [input] max: [input] (volts)

Phase Diagram Module: $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ System

Comparison with the three pre-made isothermal sections indicates that choosing all the pure solids and solution phases from the FToxid database permits one to generate reliable phase diagrams for the $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ system.

Now, we can calculate the isothermal sections at other temperatures using the same selection of the phases. Please try to calculate the isothermal sections at 1800 °C, 1500 °C, and 1100 °C.

Phase Diagram Module: $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ System

Before we calculate the liquidus projection of the $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ system, let us think about the following question:

Who critically assessed the $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ system?

The development of CALPHAD databases (e.g., FactSage databases) is based on numerous thermodynamic assessment work for binaries, ternaries, etc. These work was either published in journals or communicated internally.

For FactSage, the references of thermodynamic assessments are compiled as “List of references” in the Documentation Module. Then the next question is how can we find the references which were used to build the FactSage databases?

Phase Diagram Module: $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ System

What are the references used for the $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ system?

Phase Diagram - Menu: last system

File Units Parameters Variables Help

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

Components (3)

Products

Compound species

gas ideal real
aqueous

Right click

Information...

Solution Phase FToxid-Mull
Mullite $[\text{Al,Fe}]_2[\text{Al,Si,B,Fe}][\text{O,Va}]_5$, accounts for non-stoichiometry.
Replaces MULL and MulF. Use [I] option.

The components in FToxid-Mull for the current calculation are:
 $\text{Al}_2\text{Al}_1\text{O}_5[-1]$, $\text{Al}_2\text{Al}_1\text{Va}_5[+9]$, $\text{Al}_2\text{Si}_1\text{O}_5[0]$, $\text{Al}_2\text{Si}_1\text{Va}_5[+10]$

IP	FToxid-SLAGA	A-Slag-liq all oxides + S
I	FToxid-MeO_A	A-Monoxide
+	FToxid-Mel_A	A-Melilite
I	FToxid-Mull	Mullite

Custom Solutions
0 fixed activities
0 ideal solutions
Details ...

FToxid-Mull

File Edit

[FToxid-Mull] Mullite
OXIDE solution - mullite with borate in solution

Solid solution of non-stoichiometric mullite with B_2O_3 and Fe_2O_3 in solution.

Replaces former FToxid-MulF and FToxid-MULL.

$[\text{Al,Fe}]_2[\text{Al,Si,B,Fe}][\text{O,Va}]_5$

Possible miscibility gap. (Use I option.)

End-members in pure compound database FToxidBase.cdb: $\text{Al}_6\text{Si}_2\text{O}_{13}$ solid.

References: 2004, 2025, 2044, 2047, 2055, 6009, 6020

One way to find the **references of assessments** for a given system is to look at the “Information” of solution phases. It is recommended to choose the solid solutions which are unique to the system of interest. Here, we use Mullite. The reference numbers are shown at the bottom.

Phase Diagram Module: $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ System

What are the references used for the $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ system?

FACT reference list - FactSage Browser - [FACT_reference_List.htm]

File View About...

Search phase diagrams: <chemical formula> + must contain: <ex: CaO>

[FToxid] - FACT oxide database:
[FTsalt] - FACT salt database:
[FTmisc] - FACT sulfide, alloy, miscellaneous databases:
[FTOxCN] - FACT high-T oxycarbonitride database:
[FTfrtz] - FACT fertilizer database:
[FThall] - FACT database for Hall aluminum process:
[FThelg] - FACT aqueous (Helgeson) database:
[FTpulp] - FACT pulp and paper database:
[FTlite] - FACT Al-alloy and Mg-alloy databases:
[FTnuc] - FACT nuclear database for the nuclear industry:

[FS Copp] - FactSage copper alloy database:
[FSlead] - FactSage lead alloy database:
[FSstl] - FactSage steel alloy database:
[FSups] - FactSage ultrapure silicon database:

[SGsold] - SGTE solder alloy database:
[SGTE] - SGTE 2011 alloy database:
[SGTE] - SGTE 2014 alloy database:
[SGTE] - SGTE 2017 alloy database:
[BINS] - SGTE free binary alloy database:
[SGUN] - SGTE unary database:

[SGnobl] - SGnobl noble metal alloy database:
[SpMCBN] - Spencer Group carbide-nitride-boride-silicide systems
[TDmeph] - MEPHISTA database for new generation nuclear fuels:
[TDnuc] - NUCLEA nuclear database:

List of database files stored in \FACTDATA
List of references

[2002] P. Wu, G. Eriksson and A.D. Pelton, "Critical Evaluation and Optimization of the Thermodynamic Properties and Phase Diagrams of the CaO-Al₂O₃, Al₂O₃-SiO₂ and CaO-Al₂O₃-SiO₂ Systems", *J. Alloys and Compounds*, **179**, 259-287 (1992).

[2003] P. Wu, G. Eriksson and A.D. Pelton, "Critical Evaluation and Optimization of the Thermodynamic Properties and Phase Diagrams of the CaO-Al₂O₃, Al₂O₃-SiO₂ and CaO-Al₂O₃-SiO₂ Systems", *Ceram. Soc.*, **76**, 2059-64 (1993).

[2004] G. Eriksson and A.D. Pelton, "Critical Evaluation and Optimization of the Thermodynamic Properties and Phase Diagrams of the CaO-Al₂O₃, Al₂O₃-SiO₂ and CaO-Al₂O₃-SiO₂ Systems", *Metall. Trans.*, **24B**, 807-816 (1993).

[2005] G. Eriksson and A.D. Pelton, "Critical Evaluation and Optimization of the Thermodynamic Properties and Phase Diagrams of the MnO-TiO₂, MgO-TiO₂, FeO-TiO₂, Ti₂O₃-TiO₂, Na₂O-TiO₂ and K₂O-TiO₂ Systems", *Metall. Trans.*, **24B**, 795-805 (1993).

Done Revised: 3/3/2019

A complete thermodynamic assessment for the $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ system was detailed in this paper. Also included are the calculated phase diagrams.

[Link](#)

Phase Diagram Module: $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ System

Back to the Menu Window ([Slide](#)): Change the mass unit to gram.

The screenshot shows the 'Phase Diagram - Menu: last system' window. The 'Components (3)' section displays '(gram) SiO2 + CaO + Al2O3'. A red box highlights the '(gram)' unit, with an arrow pointing to a text box that says 'Mass unit: gram'. Below this, the 'Units: T(C), P(atm), Energy(J), Quantity(g), Vol(litre)' dialog box is open. In this dialog, the 'Quantity' section has 'g' selected, and it is highlighted with a red box. Other sections include 'Temperature' (Celsius, °C selected), 'Pressure' (atm selected), 'Energy' (J selected), and 'Volume' (litre (dm3) selected). Buttons for 'Cancel', 'SI', 'Eng', and 'OK' are visible at the bottom of the dialog.

Phase Diagram Module: SiO₂-CaO-Al₂O₃ System

Back to the Variables Window ([Slide](#))

Choose the projection option and set the isotherms.

A corner: pure SiO₂.

$$\frac{m_{\text{SiO}_2}}{m_{\text{SiO}_2} + m_{\text{Al}_2\text{O}_3} + m_{\text{CaO}}} = \text{mass fraction}_{\text{SiO}_2}$$

Note: mass fraction is not wt.%.

Phase Diagram Module: SiO₂-CaO-Al₂O₃ System

Menu Window ([Slide](#)): Choose Liquid (Slag) as the precipitate target phase.

Phase Diagram - Menu: comments

File Units Parameters Variables Help

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

Components [3]

[gram] SiO2 + CaO + Al2O3

Solution FToxid-SLAGA

- clear
- all end-members
- * - custom select end-members
- m - merge dilute solution from >
- + - single phase
- I - possible 2-phase immiscibility
- J - possible 3-phase immiscibility
- standard stable phase
- ! - dormant (metastable) phase
- F - formation target phase
- P - precipitate target phase
- O - Only plot this single phase
- S - Scheil cooling target phase
- Z - iso-activity lines ...
- Help ...

*	+	Base-Phase	Full Name
	<input checked="" type="checkbox"/>	FToxid-SLAGA	A-Slag-liq all oxides + S
	<input type="checkbox"/>	FToxid-MeO_A	A-Monoxide
	<input type="checkbox"/>	FToxid-Mel_A	A-Melilite
	<input type="checkbox"/>	FToxid-Mull	Mullite

Legend

- immiscible
- P - precipitate
- selected

Custom Solutions

0 fixed activities Details ...

0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data

Phase Diagram

SiO2

CaO Al2O3

Projection

univariants

isotherms (13)

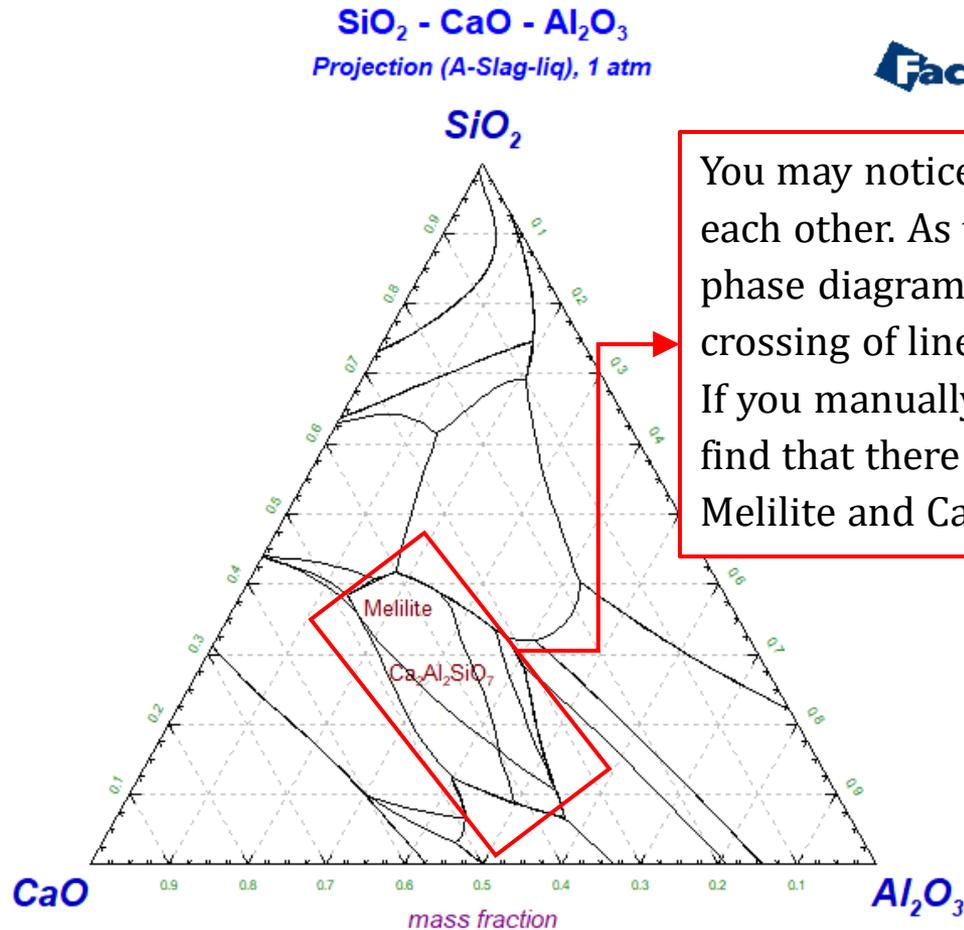
Calculate >>

3age\PhasSCA.DAT

We are calculating the liquidus projection, which means other solids phases (primary crystallization solids) are precipitating from the liquid.

Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

Results: the Liquidus Projection of the SiO_2 - CaO - Al_2O_3 System



You may notice there are lines which cross with each other. As the equilibrium state shown on a phase diagram must be uniquely defined, the crossing of lines is not permitted. If you manually label the phase regions, you will find that there is a region which is labeled both as Melilite and $\text{Ca}_2\text{Al}_2\text{SiO}_7$.

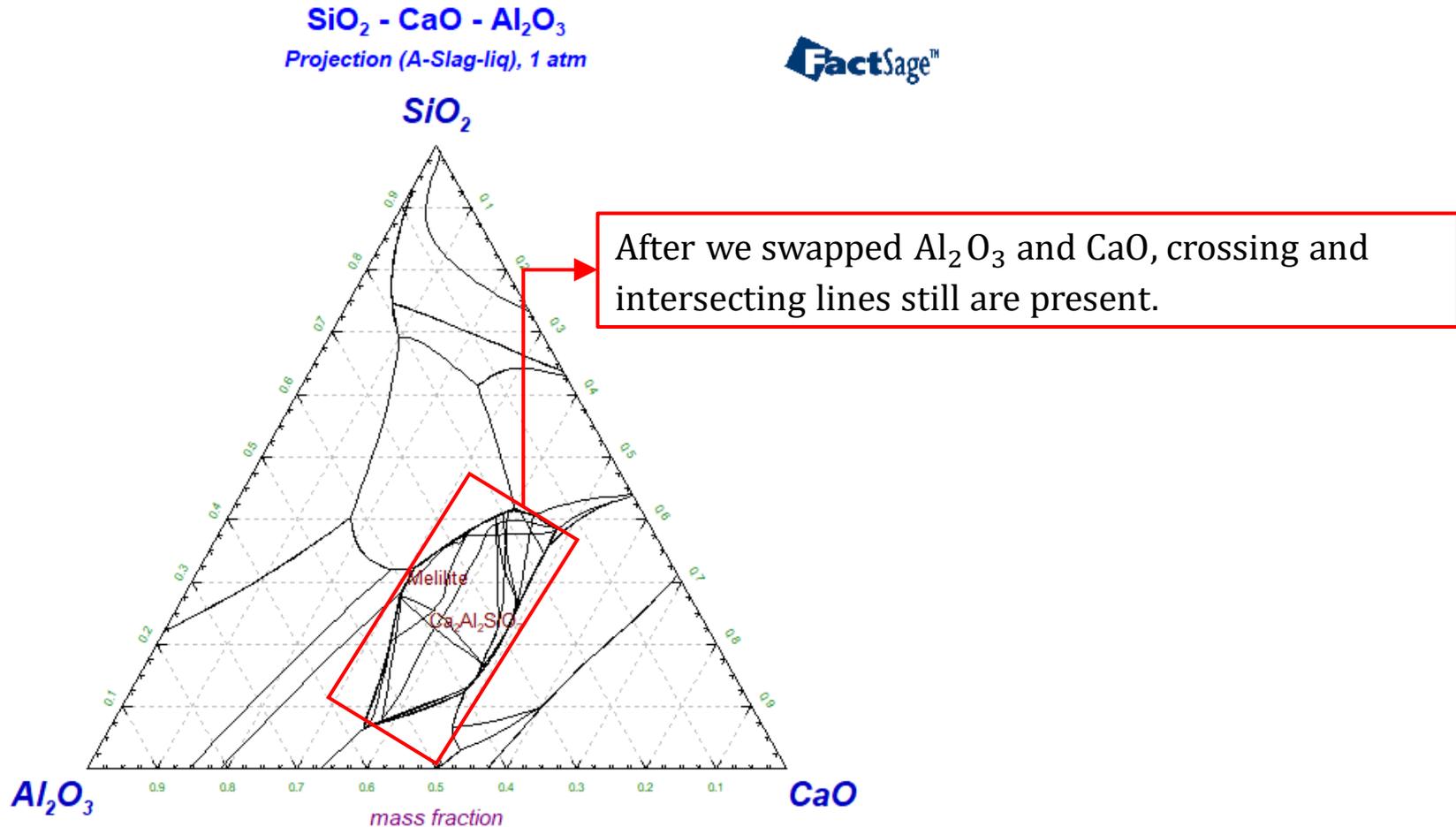
Phase Diagram Module: $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ System

The issue of having crossing or redundant lines when calculating the liquidus projection is usually because we choose both the solution phase and its **endmembers** from pure solids.

It is worth mentioning that the topology of the space model for a ternary system like the $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ system is quite complex. When FactSage is performing the “Gibbs energy minimization” calculation, if there are two Gibbs energy functions of which the values are close (e.g., the Gibbs energy of a solution phase and its endmembers), the calculation which gives single-value solutions might be challenging. Furthermore, the algorithm of the “Gibbs energy minimization” is based on numerical methods (not analytical!!!). Because of this, if we rearrange the A, B, and C corner, the complexity of the “Gibbs energy minimization” might be different, and the diagrams might look slightly different. Actually, one strategy of resolving the issue when the calculated phase diagram contains crossing and redundant lines is to switch the components at the A, B, and C corner.

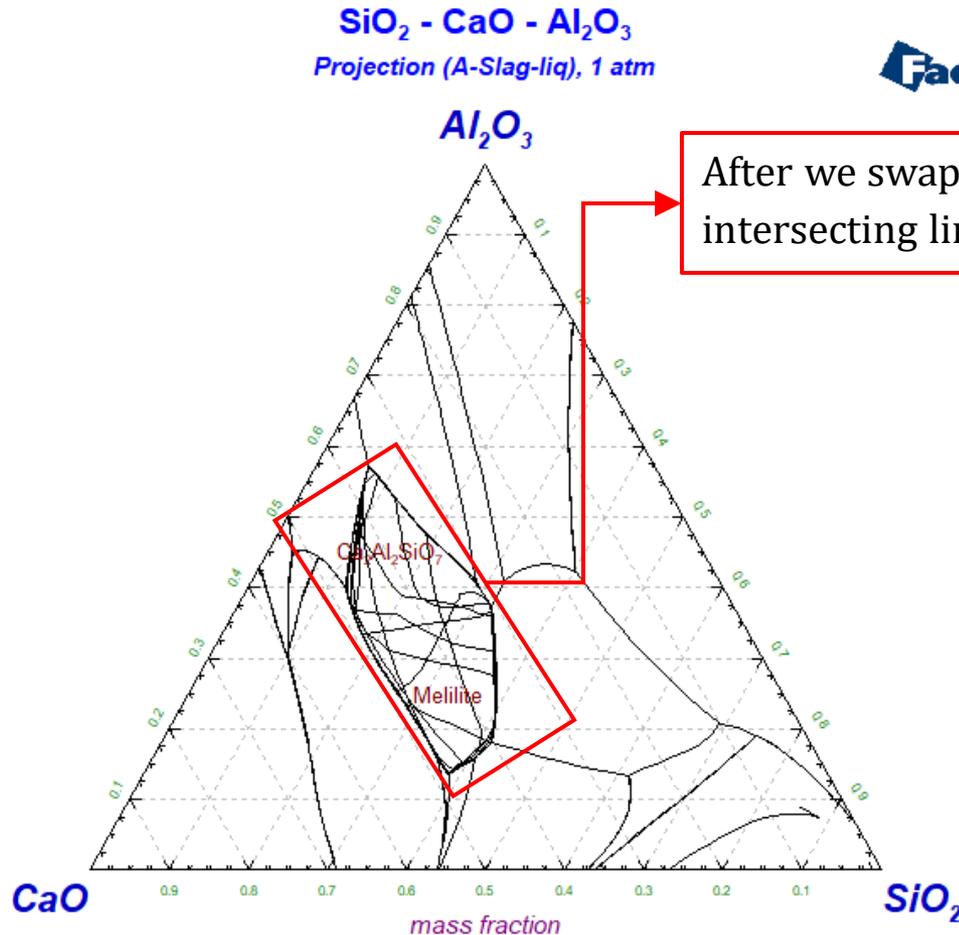
Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

Results: the Liquidus Projection of the SiO_2 - CaO - Al_2O_3 System



Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

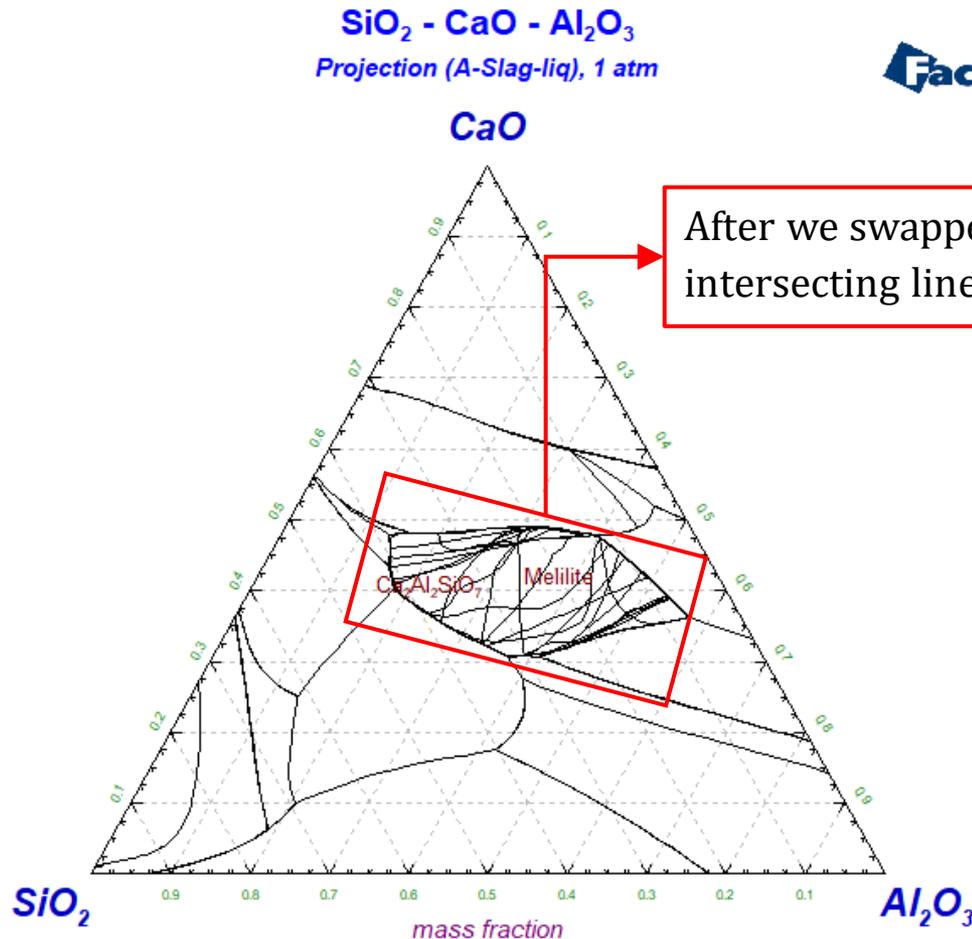
Results: the Liquidus Projection of the SiO_2 - CaO - Al_2O_3 System



After we swapped SiO_2 and Al_2O_3 , crossing and intersecting lines still are present.

Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

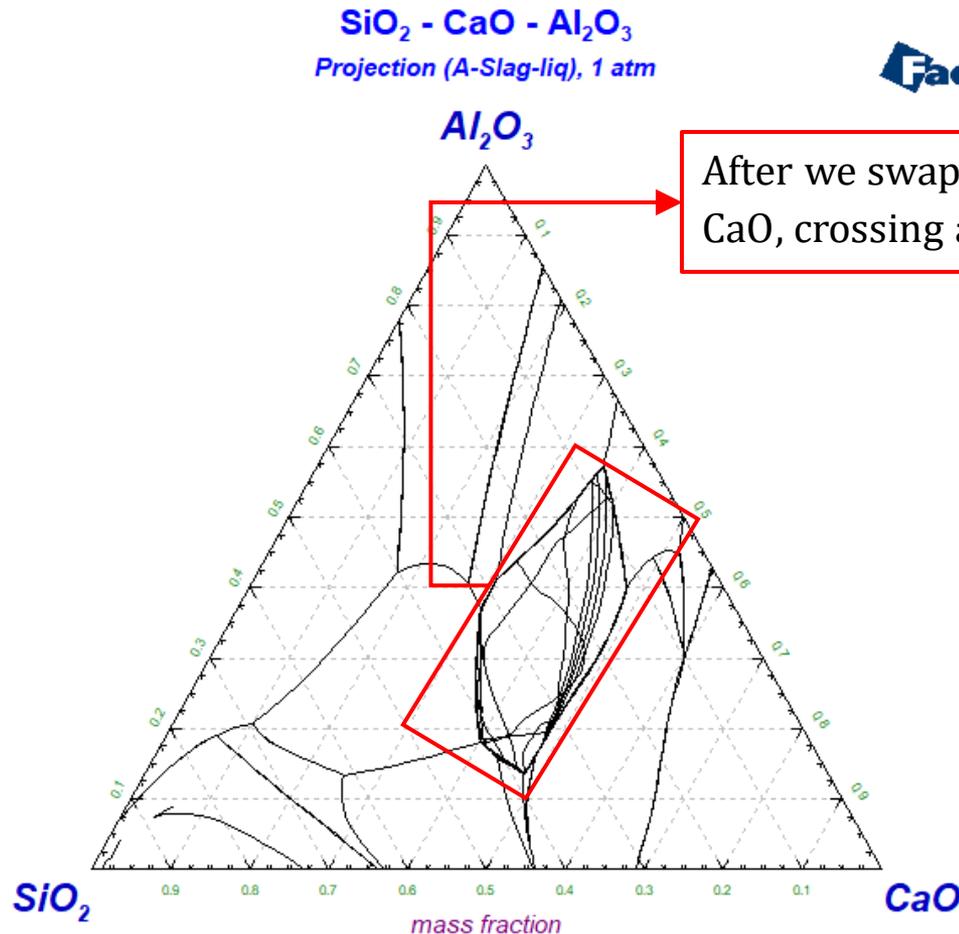
Results: the Liquidus Projection of the SiO_2 - CaO - Al_2O_3 System



After we swapped SiO_2 and CaO , crossing and intersecting lines still are present.

Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

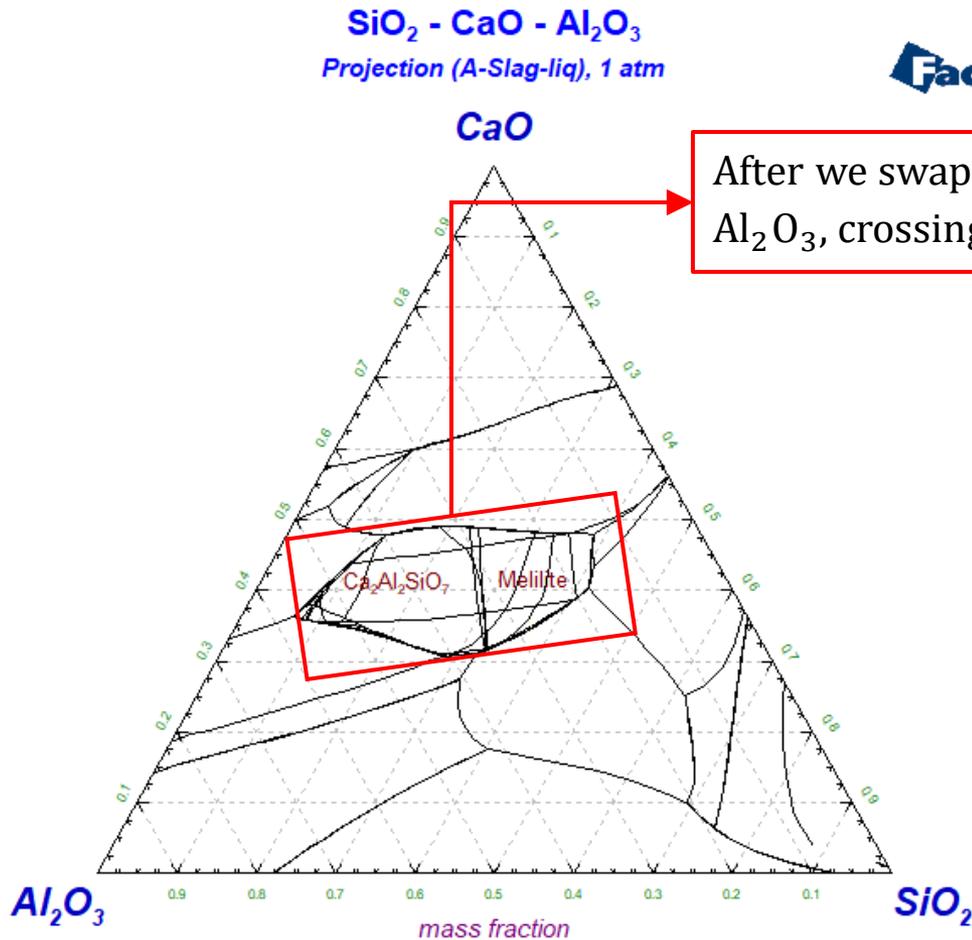
Results: the Liquidus Projection of the SiO_2 - CaO - Al_2O_3 System



After we swapped SiO_2 and Al_2O_3 , then SiO_2 and CaO , crossing and intersecting lines still are present.

Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

Results: the Liquidus Projection of the SiO_2 - CaO - Al_2O_3 System



After we swapped SiO_2 and CaO , and then SiO_2 and Al_2O_3 , crossing and intersecting lines still are present.

Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

The above phase diagram calculations show that the process of “Gibbs energy minimization” might be impeded when both the solution phases and some pure solids which are the endmembers of these solution phases are selected.

How to resolve the issue of having crossing and intersecting lines? The solution is very simple: remove all the pure solids which are the endmembers of the solution phases.

Phase Diagram Module: $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3$ System

Find the endmembers of solid phases

1. Show the Information of a solid phase.
2. Click on “Information”, and find the section which describes the Endmembers in pure compound database.
The endmember of FToxid-MeO_A for the current SCA system is CaO.

[FToxid-MeO_A] A-Monoxide
OXIDE monoxide (rocksalt structure) solution
Approved sub-system of FToxid-MeO_
Note that the former phase FToxid-MONO has now been combined with FToxid-MeO and merged into it.
Fe(II)O,CaO,MgO,SrO,BaO,Mn(II)O,NiO,CoO at all compositions + (Al,Fe(III),Cr(III),Na,Ti(IV),Zn,Zr :
Mineralogical names: Wustite (Fe_xO), Lime (CaO), Periclase (MgO), Magnesiowustite (MgO- Fe_xO), Mang:
End-members in pure compound database FToxidBase.cdb: CaO, MgO, SrO, BaO, MnO, NiO, and CoO :
Evaluated and optimized at all compositions.
Can be used for wustite (Fe_xO) solutions at all oxygen contents. However, Mn(III) is not included in FToxid-

Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

Find the endmembers of solid phases

The endmember of FToxid-Mel_A for the current SCA system is $\text{Ca}_2\text{Al}_2\text{SiO}_7$.

Information...

Quantity	Phase	Endmember
0		FToxid-MeO_A A-Monoxide
0	+	FToxid-Mel_A A-Melilite
28		FToxid-Mull Mullite

FToxid-Mel_A
OXIDE solution melilite

Distribution of cations over the three cation sites are taken into account as follows:
 $(\text{Ca,Pb})_2[\text{Mg,Fe(II),Fe(III),Al,Zn}]\{\text{Al,Fe(III),Si}\}_2\text{O}_7$

Mineralogical names: Akermanite ($\text{Ca}_2\text{MgSi}_2\text{O}_7$), Iron-akermanite ($\text{Ca}_2\text{FeSi}_2\text{O}_7$), **Gehlenite ($\text{Ca}_2\text{Al}_2\text{SiO}_7$)**, Iron-gehle

End-members in pure compound database FToxidBase.cdb: $\text{Ca}_2\text{MgSi}_2\text{O}_7$, $\text{Ca}_2\text{FeSi}_2\text{O}_7$, **$\text{Ca}_2\text{Al}_2\text{SiO}_7$** , $\text{Ca}_2\text{ZnSi}_2\text{O}_7$, 1

Evaluated and optimized at all compositions where data are available.

Phase Diagram Module: SiO₂-CaO-Al₂O₃ System

Find the endmembers of solid phases

Phase Diagram - Menu: comments

File Units Parameters Variables Help

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

Components (3)

Solution Phase FToxid-Mull
Mullite [Al,Fe]₂[Al,Si,B,Fe][O,Va]₅, accounts for non-stoichiometry.
Replaces MULL and MulF. Use [I] option.

The components in FToxid-Mull for the current calculation are:
Al₂Al₁O₅[-1], Al₂Al₁Va₅[+9], Al₂Si₁O₅[0], Al₂Si₁Va₅[+10]

Products

Compound species

gas ideal real 0
aqueous 0
pure liquids 0
* + pure solids 28
* - custom selection

IP	FToxid-SLAGA	A-Slag-liq all oxides + S
I	FToxid-MeO_A	A-Monoxide
+	FToxid-Mel_A	A-Mellite
I	FToxid-Mull	Mullite

Information...

FToxid-Mull

File Edit

End-members in pure compound database FToxidBase.cdb: Al₄Fe₂Si₅O₁₈ and Al₄Mg₂Si₅O₁₈ solids.

[FToxid-Mull] Mullite
OXIDE solution - mullite with borate in solution

Solid solution of non-stoichiometric mullite with B₂O₃ and Fe₂O₃ in solution.

Replaces former FToxid-MulF and FToxid-MULL.

[Al,Fe]₂[Al,Si,B,Fe][O,Va]₅

Possible miscibility gap. (Use I option.)

End-members in pure compound database FToxidBase.cdb: Al₆Si₂O₁₃ solid.

The endmember of FToxid-Mel_A for the current SCA system is Al₆Si₂O₁₃.

Phase Diagram Module: SiO₂-CaO-Al₂O₃ System

Remove the endmembers of solid phases from pure solids

Phase Diagram - Menu: comments

Selection - Phase Diagram - no results -

Selected: 28/30 **SOLID**

- no results -

	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
+	13	SiO2(s6)	FToxid	Cristobalite(h)		V			
+	14	SiO2(s7)	FToxid	coesite		V			
+	15	SiO2(s8)	FToxid	stishovite		V			
+	16	Al2Si2O7(s)	FToxid	solid		V			
	17	CaO(s)	FToxid	Lime		V			
+	18	CaAl2O4(s)	FToxid	solid		V			
+	19	CaAl4O7(s)	FToxid	solid		V			
+	20	CaAl12O19(s)	FToxid	solid		V			
+	21	Ca3Al2O6(s)	FToxid	solid		V			
+	22	CaSiO3(s)	FToxid	Wollastonite		V			
+	23	CaSiO3(s2)	FToxid	Ps-wollastonite		V			
+	24	Ca2SiO4(s)	FToxid	Gamma(olivine)		V			
+	25	Ca2SiO4(s2)	FToxid	Alpha-prime		V			
+	26	Ca2SiO4(s3)	FToxid	Alpha		V			
+	27	Ca3SiO5(s)	FToxid	Hatrunite		V			
+	28	Ca3SiO7(s)	FToxid	Rankinite		V			
+	29	CaAl2SiO6(s)	FToxid	Ca-Tschermak		V			
+	30	CaAl2Si2O8(s)	FToxid	Hexagonal		o			
+	31	CaAl2Si2O8(s2)	FToxid	Anorthite		V			
	32	Ca2Al2SiO7(s)	FToxid	Gehlenite		V			
+	33	Ca3Al2Si3O12(s)	FToxid	Grossularite		V			

Remove these two pure solids.
(Ignore Al₆Si₂O₁₃ because it is not found.)

Components (3)

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

* + pure solids 28

* - custom selection species: 28

Target - none -

Estimate T(K): 1000

Variables

T(C) SiO2/

800 2000 0 1

A = SiO2, B = Al2O3, C = CaO

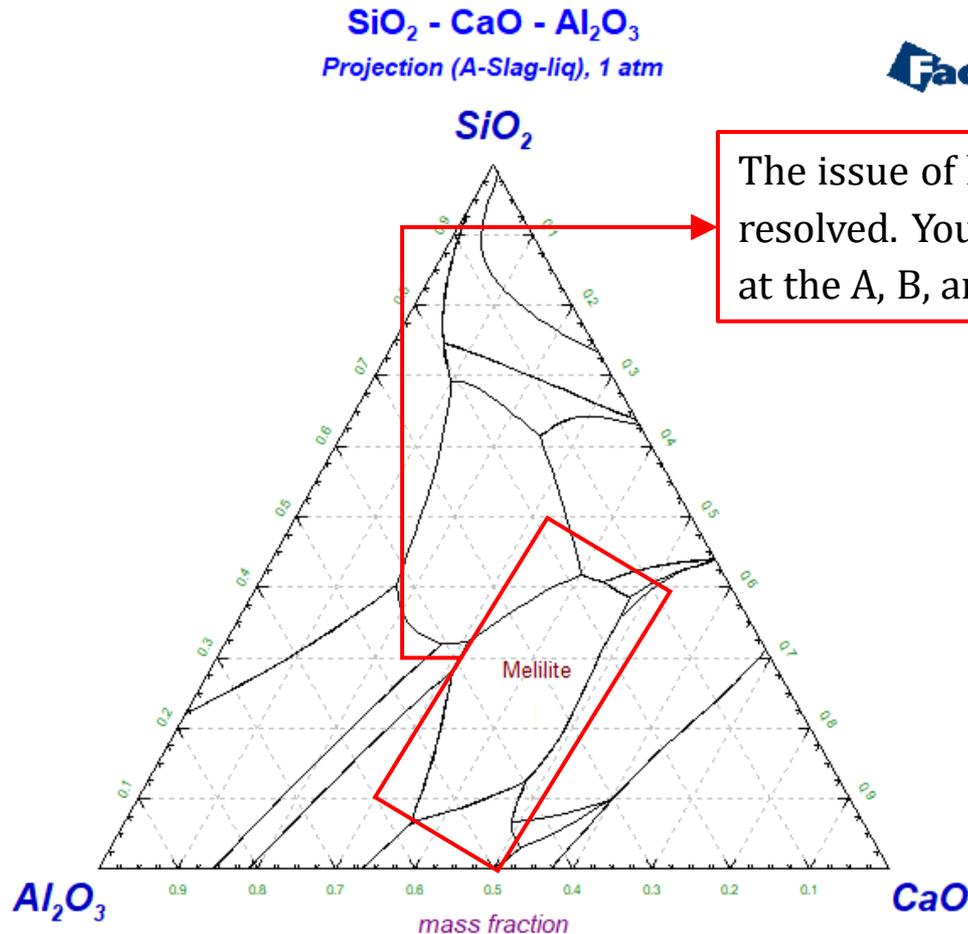
FactSage 7.3 C:\FactSa

permit selection of 'X' species Help Suppress Duplicates Edit priority list:

Show Selected Select All Select/Clear... Clear OK

Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

Then, perform the phase diagram calculation again.



The issue of having crossing and intersecting lines is resolved. You can try other component arrangements at the A, B, and C corner.

Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

Results: the Liquidus Projection of the SiO_2 - CaO - Al_2O_3 System.

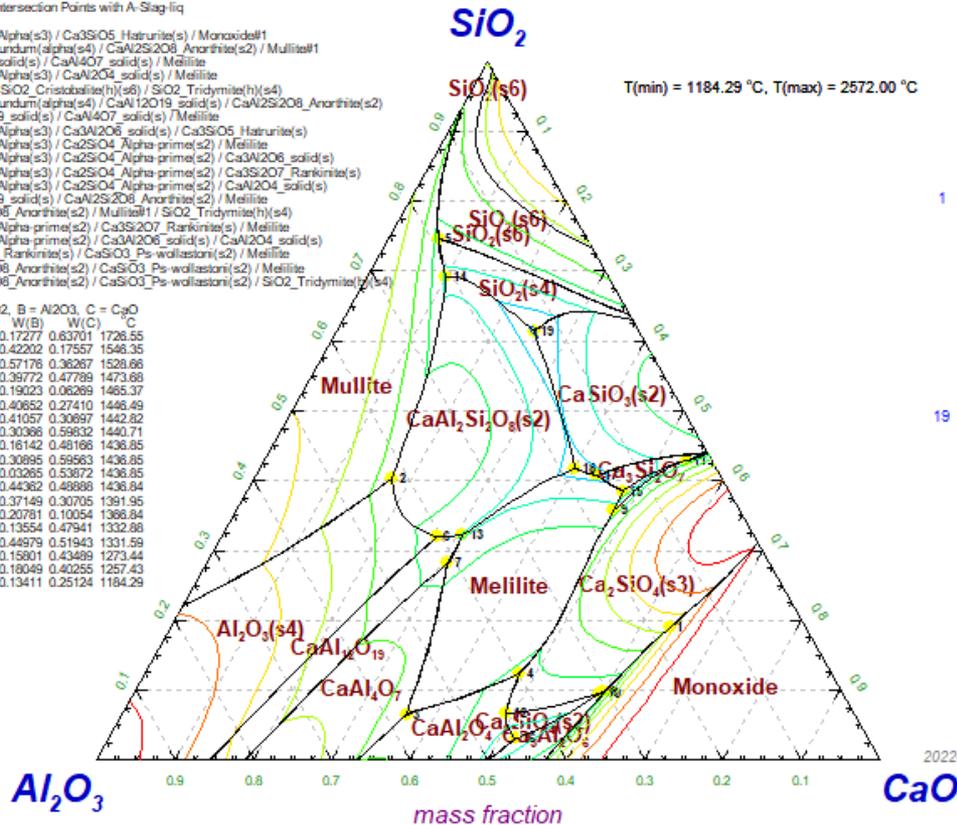
SiO_2 - CaO - Al_2O_3
Projection (A-Slag-liq), 1 atm

Four-Phase Intersection Points with A-Slag-liq

- 1: Ca_2SiO_4 _Alpha(s3) / Ca_3SiO_5 _Hatrurite(s) / Monoxide(l)
- 2: Al_2O_3 _corundum(alpha(s4)) / $\text{CaAl}_2\text{Si}_2\text{O}_8$ _Anorthite(s2) / Mullite(l)
- 3: $\text{CaAl}_2\text{Si}_2\text{O}_8$ _solid(s) / CaAl_2O_7 _solid(s) / Melilite
- 4: Ca_2SiO_4 _Alpha(s3) / $\text{CaAl}_2\text{Si}_2\text{O}_8$ _solid(s) / Melilite
- 5: Mullite(l) / SiO_2 _Cristobalite(h)(s6) / SiO_2 _Tridymite(h)(s4)
- 6: Al_2O_3 _corundum(alpha(s4)) / $\text{CaAl}_2\text{Si}_2\text{O}_8$ _solid(s) / $\text{CaAl}_2\text{Si}_2\text{O}_8$ _Anorthite(s2)
- 7: $\text{CaAl}_2\text{Si}_2\text{O}_8$ _solid(s) / CaAl_2O_7 _solid(s) / Melilite
- 8: Ca_2SiO_4 _Alpha(s3) / $\text{Ca}_3\text{Al}_2\text{Si}_2\text{O}_8$ _solid(s) / Ca_3SiO_5 _Hatrurite(s)
- 9: Ca_2SiO_4 _Alpha(s3) / Ca_2SiO_4 _Alpha-prime(s2) / Melilite
- 10: Ca_2SiO_4 _Alpha(s3) / Ca_2SiO_4 _Alpha-prime(s2) / $\text{Ca}_3\text{Al}_2\text{Si}_2\text{O}_8$ _solid(s)
- 11: Ca_2SiO_4 _Alpha(s3) / Ca_2SiO_4 _Alpha-prime(s2) / $\text{Ca}_3\text{Si}_2\text{O}_7$ _Rankinite(s)
- 12: Ca_2SiO_4 _Alpha(s3) / Ca_2SiO_4 _Alpha-prime(s2) / $\text{CaAl}_2\text{Si}_2\text{O}_8$ _solid(s)
- 13: $\text{CaAl}_2\text{Si}_2\text{O}_8$ _solid(s) / $\text{CaAl}_2\text{Si}_2\text{O}_8$ _Anorthite(s2) / Melilite
- 14: $\text{CaAl}_2\text{Si}_2\text{O}_8$ _Anorthite(s2) / Mullite(l) / SiO_2 _Tridymite(h)(s4)
- 15: Ca_2SiO_4 _Alpha-prime(s2) / $\text{Ca}_3\text{Si}_2\text{O}_7$ _Rankinite(s) / Melilite
- 16: Ca_2SiO_4 _Alpha-prime(s2) / $\text{Ca}_3\text{Al}_2\text{Si}_2\text{O}_8$ _solid(s) / $\text{CaAl}_2\text{Si}_2\text{O}_8$ _solid(s)
- 17: $\text{Ca}_3\text{Si}_2\text{O}_7$ _Rankinite(s) / Ca_3SiO_3 _Ps-wollastonite(s2) / Melilite
- 18: $\text{CaAl}_2\text{Si}_2\text{O}_8$ _Anorthite(s2) / Ca_3SiO_3 _Ps-wollastonite(s2) / Melilite
- 19: $\text{CaAl}_2\text{Si}_2\text{O}_8$ _Anorthite(s2) / Ca_3SiO_3 _Ps-wollastonite(s2) / SiO_2 _Tridymite(h)(s4)

A = SiO_2 , B = Al_2O_3 , C = CaO

	W(A)	W(B)	W(C)	C
1:	0.19022	0.17277	0.63701	1726.55
2:	0.40241	0.42202	0.17557	1546.35
3:	0.06557	0.57176	0.36267	1526.66
4:	0.12439	0.39772	0.47799	1473.66
5:	0.74708	0.19023	0.06269	1465.37
6:	0.31938	0.40652	0.27410	1446.49
7:	0.28246	0.41057	0.30697	1442.82
8:	0.09801	0.30366	0.59832	1440.71
9:	0.35692	0.16142	0.48166	1436.85
10:	0.09542	0.30695	0.59663	1436.85
11:	0.42963	0.02065	0.53972	1436.85
12:	0.06751	0.44382	0.48868	1436.84
13:	0.32148	0.37149	0.30705	1391.95
14:	0.69165	0.20781	0.10054	1386.84
15:	0.38505	0.13554	0.47941	1332.88
16:	0.03079	0.44979	0.51943	1331.59
17:	0.40710	0.15601	0.43489	1273.44
18:	0.41696	0.18049	0.40255	1257.43
19:	0.61465	0.13411	0.25124	1184.29



FactSage

Stable Phases

This allows you to remove all the labels and isotherms.

2	FToxid-MeO	Mullite	(Ca, Si, Al, Fe, Na)
3	FToxid-MeO	Monoxide	Rocksalt-str. Fe
4	FToxid-Mull	Mullite	[Al, Fe]2[Al, Si, I
5	FToxid (PS)	Al_2O_3 (s4)	corundum (alpha)
6	FToxid (PS)	Ca_2SiO_4 (s2)	Alpha-prime
7	FToxid (PS)	Ca_2SiO_4 (s3)	Alpha
8	FToxid (PS)	$\text{Ca}_3\text{Al}_2\text{O}_6$ (s)	solid
9	FToxid (PS)	$\text{Ca}_3\text{Si}_2\text{O}_7$ (s)	Rankinite

Manipulate and Refresh

clear restore Help

labels labels - old delete label: []

equilibria

iso-activity [] 0 val

polythermal projection

iso-therm T step: [100]

color T-bar clear

tie lines - isothermal diagram

all domains 1 domain hi med lo density clear

aqueous diagram

iso-Eh Eh step: [0] min: [] max: [] (volts)

iso-pH pH step: [0] min: [] max: []

replot as Eh vs pH Figure full Viewer screen

2022-07-20 12 m

Phase Diagram Module: SiO_2 - CaO - Al_2O_3 System

A Note on the Phase Selection:

Although the selection of CaO and $\text{Ca}_2\text{Al}_2\text{SiO}_7$ from the list of pure solids did not produce any redundant lines when the isothermal sections were calculated, it is still recommended that all the endmembers of the solutions phases be removed.

Comparison with the phase diagram reported by Eriksson and Pelton:

You might notice that the liquidus projection of the SCA system calculated by the current FToxid database is not exactly same to the one reported by Eriksson and Pelton (CRCT Team). This is because FToxid is being constantly updated by CRCT to improve the accuracy of models and to include other oxides.

Phase Diagram Module: MgF_2 - CaF_2 System

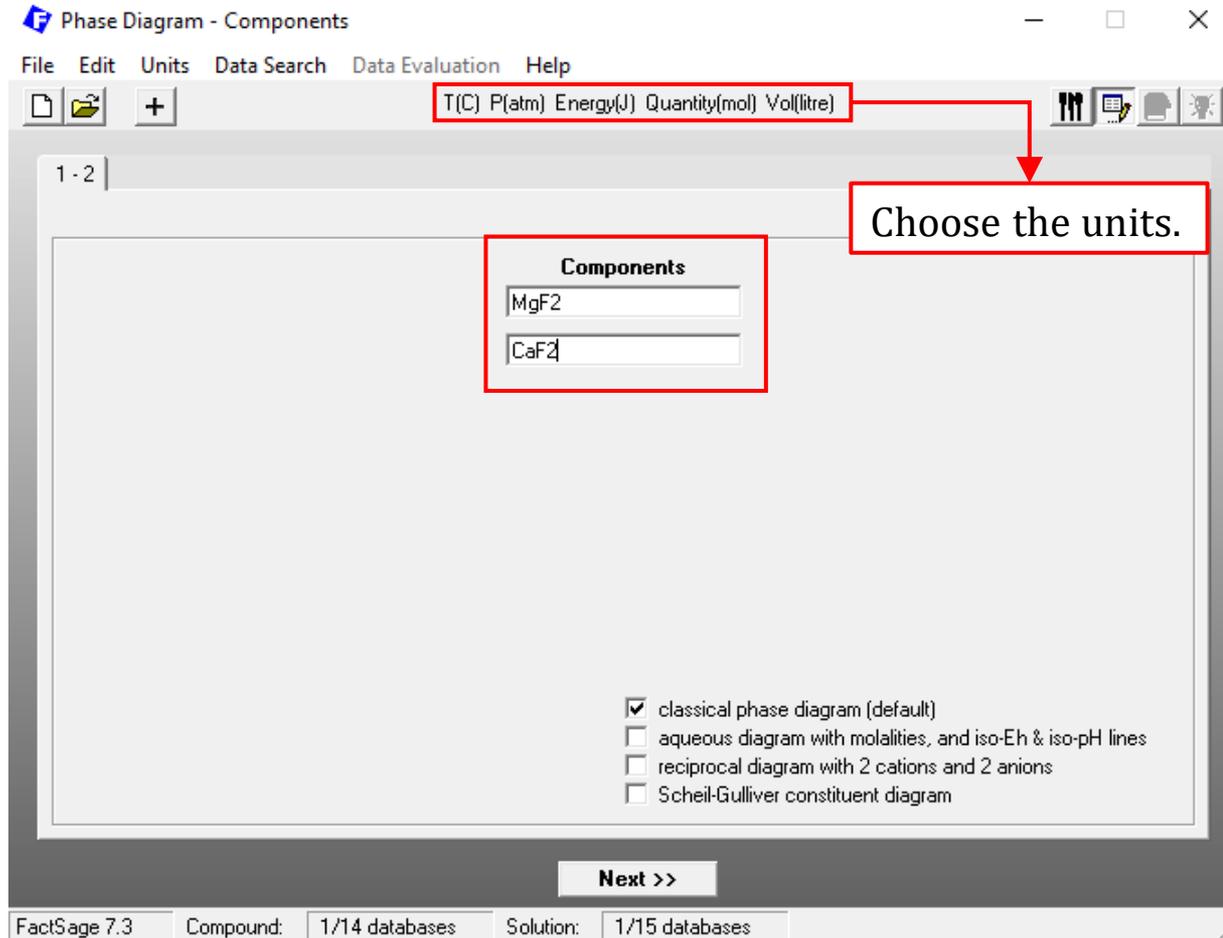
From previous examples, it is seen that the FactSage databases (e.g., FTlite, FToxid) always contain a model for **liquid solution**. The model usually gives a quite accurate description of the interactions between solution constituents. In most cases, the model is non-ideal solution model. However, the Phase Diagram Module permits one to choose instead of non-ideal liquid solution from the FactSage databases, an ideal liquid solution.

Say we are looking at a simple eutectic system, MgF_2 - CaF_2 . Let us calculate the phase diagram of the MgF_2 - CaF_2 system using both the ideal solution model and the non-ideal solution model for the liquid MgF_2 - CaF_2 solution.

Note: for these two scenarios, only the liquid phase is different.

Phase Diagram Module: MgF₂-CaF₂ System

Components Window: Define Components



Phase Diagram Module: MgF₂-CaF₂ System

Components Window: Choose Database(s)

Phase Diagram - Components

Data Search

Databases - 1/14 compound databases, 1/15 solution databases

Fact **FactSage™** **SGTE**

FactPS FScomp BINS EXAM

FToxid FSlead SGPS

FTsalt FSstel SGTE

FTmisc FSupsi SGsold

FTall

FToxCN

FTfritz

FThelp ELEM SGnobl

FTpulp FTdemo SpMCBN

FTlite FTnucl TDmeph

TDnucl

Private Databases

compounds only
solutions only
no database

Clear All

Add/Remove Data

RefreshDatabases

Information

Click on a box to select a database (when a database is selected, it is highlighted in yellow). To 'uncouple' a database click-mouse-right-button (note, this is NOT recommended).

Normally databases are 'coupled' - that is both the compound and solution databases (when available) will be selected. To 'uncouple' a database click-mouse-right-button (note, this is NOT recommended).

If database is stored on your PC but not listed here then you must 'add the database to the list' - click on 'Add/Remove ...'.

Options - search for product species

Default

Include compounds

gaseous ions (plasmas)

aqueous species

limited data compounds (25C)

Limits

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

Cancel Summary ... OK

Phase Diagram Module: MgF₂-CaF₂ System

Menu Window: Choose Products/Phases (Compounds and Solution Phases)

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (2)

MgF₂ + CaF₂

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

+ pure solids 3

species: 3

Target

- none -

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
	I	FTsalt-SALTA	A-Salt-liquid
	I	FTsalt-C1	Fluorite
	J	FTsalt-C4	Rutile
	I	FTsalt-C23	Cotunnite

Legend

I - immiscible 3

J - 3-immiscible 1

Show all selected

species: 18

solutions: 9

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

paraequilibrium & Gmin

Total Species (max 5000) 21

Total Solutions (max 200) 9

Total Phases (max 1500) 12

Phase Diagram

univariants

isotherms (13)

Projection

Variables

T(C)	MgF ₂ /			
800 2000	0 1			

MgF₂/(MgF₂+CaF₂) vs -

FactSage 7.3

Choose all pure solids and all solution phases (use default immiscibility settings).
Note: FTsalt-SALTA is the non-ideal solution model for the MgF₂-CaF₂ liquid.

Phase Diagram Module: MgF₂-CaF₂ System

Menu Window: Set up the Variables

Phase Diagram - Menu: last system

File Units Parameters **Variables** Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (2)
Variables: MgF2-CaF2 T(C) vs composition #1.

Variables

compositions 1

log10(a) 0

Next >>

T and P

Temperature

T(C) Y-axis

Max: 1500

Min: 0

1/TK

Pressure or Volume

P(atm) constant

log P

V(litre) 1

log V

Compositions Quantity(mol)

#1.	MgF2	+	CaF2	Quantity(mol)
1	1		0	X-axis
1	1		1	1 (max)
				0 (min)

#1 log10(composition)

Cancel

$$\frac{n_{\text{MgF}_2}}{n_{\text{MgF}_2} + n_{\text{CaF}_2}} = X_{\text{MgF}_2}$$

MgF2/(MgF2+CaF2) vs -

Projection Calculate >>

FactSage 7.3

We wish to calculate $T \sim X_B$ type of phase diagram.

Phase Diagram Module: MgF₂-CaF₂ System

Menu Window: Calculate

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (2)

MgF2 + CaF2

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 3

species: 3

Target

- none -

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
	I	FTsalt-SALTA	A-Salt-liquid
	I	FTsalt-C1	Fluorite
	J	FTsalt-C4	Rutile
	I	FTsalt-C23	Cotunnite

Legend

I - immiscible 3
J - 3-immiscible 1

Show all selected

species: 18
solutions: 9

Custom Solutions

0 fixed activities
0 ideal solutions

Pseudonyms

apply

Volume data

assume molar volumes of solids and liquids = 0
 include molar volume data and physical properties data

paraequilibrium & Gmin

Total Species (max 5000) 21
Total Solutions (max 200) 9
Total Phases (max 1500) 12

Variables

T(C)	MgF2/			
0 1500	0 1			

T(C) vs MgF2/(MgF2+CaF2)

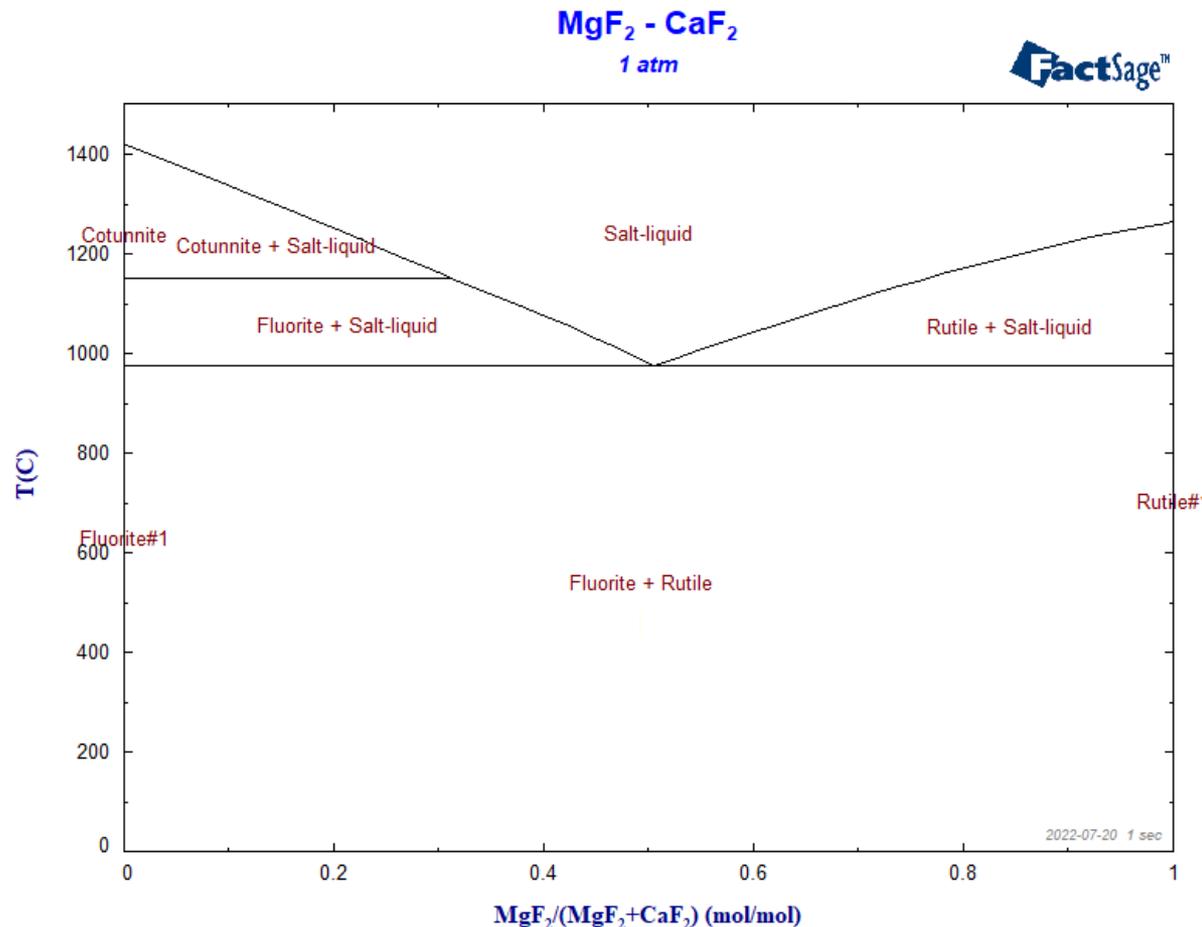
Phase Diagram

Y
X

FactSage 7.3

Phase Diagram Module: MgF_2 - CaF_2 System

Results: the MgF_2 - CaF_2 Phase Diagram



Stable Phases

Stable Phases - solutions and compounds (pu: ^

1	FTsalt-SALT	Salt-liquid	(main ions : Li,Na
2	FTsalt-C23	Cotunnite	Strukturbericht : C
3	FTsalt-C1	Fluorite	Strukturbericht : F
4	FTsalt-C4	Rutile	Strukturbericht : R

Stoichiometric Phases - compounds and one-comp

mole	TC (min)	TC (max)
----	----	----

Manipulate and Refresh

clear restore Help

labels labels - old delete label: Fluorite + Rutile

equilibria

iso-activity . 0 ve

polythermal projection

iso-therm T step: 100

color T-bar clear

tie lines - isothermal diagram

all domains 1 domain hi med lo density clear

aqueous diagram

iso-Eh Eh step: 0 min: max: (volts)

iso-pH pH step: 0 min: max:

replot as Eh vs pH

Figure Viewer full screen

Phase Diagram Module: MgF₂-CaF₂ System

Results: Invariant Reactions

Stable Phases

Stable Phases - solutions and compounds (pure substances PS)

1	FTsalt-SALT	Salt-liquid	(main ions : Li,Na,K,Rb,Cs,Mg,Ca,Sr,Ba,Al,Fe[2+,3+],Mn,Co,Ni,Zn,Pb,I
2	FTsalt-C23	Cotunnite	Strukturbericht : C23; Pearson : oP12; Space group : Pnma (62); Prot
3	FTsalt-C1	Fluorite	Strukturbericht : FCC_C1; Pearson : cF12; Space group : Fm-3m (225);
4	FTsalt-C4	Rutile	Strukturbericht : C4; Pearson : tP6; Space group : P42/mnm (136); Pr

Stoichiometric Phases - compounds and one-component solutions

mole	TC(min)	TC(max)
- none -		

Phase Equilibria

1	1418.05 C	Salt-liquid#1(0.0)	<=>	Cotunnite#1(0.0)
2	1262.85 C	Salt-liquid#1(1.0)	<=>	Rutile#1(1.0)
3	1150.85 C	Fluorite#1(0.0002255)	<=>	Cotunnite#1(0.0002255) + Salt-liquid#1(0.3109)
4	974.01 C	Salt-liquid#1(0.5047)	<=>	Fluorite#1(0.0003127) + Rutile#1(0.9997)

The invariant reaction labeled as "4" is the eutectic reaction.

Manipulate and Refresh

clear restore Help

labels labels - old delete label: Fluorite + Rutile

equilibria

iso-activity 0 value

polythermal projection

iso-therm T step: 100

color T-bar clear

tie lines - Isothermal diagram

all domains 1 domain hi med lo density clear

aqueous diagram

iso-Eh Eh step: 0 min: max: (volts)

iso-pH pH step: 0 min: max:

replot as Eh vs pH Figure Viewer full screen

Phase Diagram Module: MgF₂-CaF₂ System

Now, let us choose the MgF₂-CaF₂ liquid which is modeled as an ideal solution.

Back to the Menu Window.

The screenshot shows the 'Phase Diagram - Menu: last system' window. The 'Components (2)' section contains 'MgF2 + CaF2'. The 'Products' section has 'pure liquids' selected. The 'Solution phases' table is as follows:

*	+	Base-Phase	Full Name
		FTsalt-SALTA	A-Salt-liquid
I		FTsalt-C1	Fluorite
J		FTsalt-C4	Rutile
I		FTsalt-C23	Cotunnite

A red box highlights the 'pure liquids' option in the 'Products' section. Another red box highlights the 'FTsalt-SALTA' row in the 'Solution phases' table, with an arrow pointing to the text 'Remove FTsalt-SALTA.'.

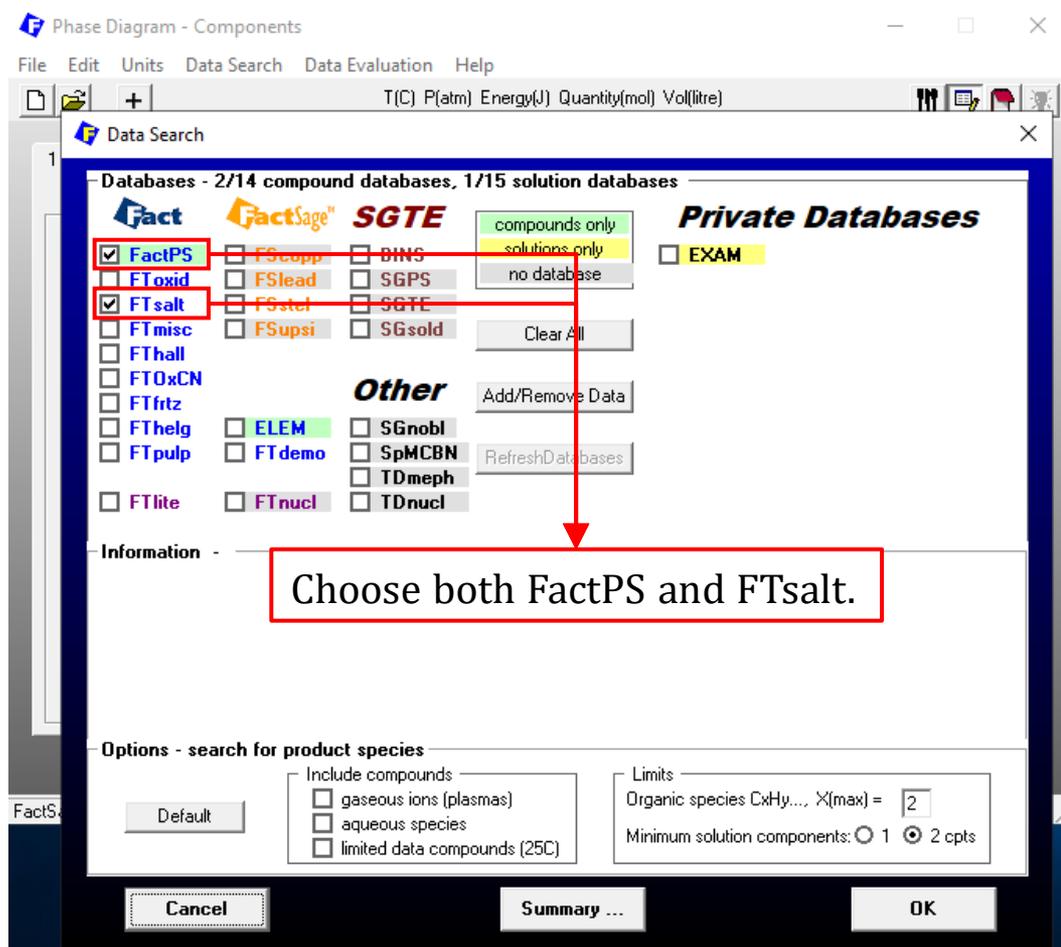
The 'Selection - Phase Diagram - no results -' window is open, showing 'Selected: 1/1 LIQUID' and a table with the following data:

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
+	1	MgF2(liq)	FTsalt	liquid		V			

To define an ideal liquid MgF₂-CaF₂ solution, we need both pure liquid MgF₂ and pure liquid CaF₂. However, the FTsalt database does not include the model for pure liquid CaF₂. Therefore, another database (normally FactPS) must be used.

Phase Diagram Module: MgF₂-CaF₂ System

Bac to Components Window: Add FactPS



Phase Diagram Module: MgF₂-CaF₂ System

Pure Solids: Remove all the pure solids from the FactPS database

Phase Diagram - Menu: last system

File Units Parameters Variables Help

Components [2]

Products

- Compound species
- gas ideal real 0
- aqueous 0
- * pure liquids 3
- * pure solids 7
- * custom selection species: 10

Target

Estimate T(K): 1000

Variables

T(C)	MgF ₂ /
0 1500	0 1

T(C) vs MgF₂/(MgF₂+CaF₂)

FactSage 7.3

Selection - Phase Diagram - no results -

File Edit Show Sort

Selected: 7/10 SOLID Duplicates selected. X denotes sp

- no results -

	+	Code	Species	Data	Phase	T	V
	+	17	Mg(s)	FactPS	solid		V
	X	18	MgF ₂ (s)	FactPS	Sellaite_(TiO2_r)		V
	+	19	Ca(s)	FactPS	Solid_Alpha		V
	+	20	Ca(s2)	FactPS	Solid_Beta		V
	X	21	CaF ₂ (s)	FactPS	Solid-alpha		V
	X	22	CaF ₂ (s2)	FactPS	Solid-beta		V
	+	23	Mg ₂ Ca(s)	FactPS	Laves_C-14		V
	+	24	MgF ₂ (s)	FTsalt	Sellaite_(TiO2_r)		V
	+	25	CaF ₂ (s)	FTsalt	alpha_Fluorite_C		V
	+	26	CaF ₂ (s2)	FTsalt	beta_C23_oP12		V

Because we included the FactPS database, more pure solids were added to the selection list. We can manually remove all the pure solids from the FactPS database. However, you don't have to do so.

Remove all species from database

- FactPS
- FTsalt

Show Selected Select All Select/Clear... Clear OK

Phase Diagram Module: MgF₂-CaF₂ System

Pure Liquids: Define Ideal Liquid MgF₂-CaF₂ Solution

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (2)

Products

Compound species

gas ideal real
aqueous
*** + pure liquids**
* + pure solids

* - custom selection species:

Target
- none -
Estimate T(K): 1000

Variables

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
	12	Mg(liq)	FactPS	liquid		V			
+ X	13	MgF2(liq)	FactPS	liquid		V			
	14	Ca(liq)	FactPS	liquid		V			
+ X	15	CaF2(liq)	FactPS	liquid		V			
	16	MgF2(liq)	FT salt	liquid		V			

Selected: 2/5 LIQUID Duplicates selected X denotes species excluded by default

- no results -

permit selection of 'X' species Help Suppress Duplicates Edit priority list: FactPS FT salt

Show Selected Select All Select/Clear... Clear OK

Choose pure liquids of MgF₂ and CaF₂.

Permit selection of "X" species.
Note: "X" species are those with a lower priority.

Phase Diagram Module: MgF₂-CaF₂ System

Pure Liquids: Define Ideal Liquid MgF₂-CaF₂ Solution

The screenshot displays the 'Selection - Phase Diagram' window. The main table lists species and their phases. A context menu for '13 MgF2(liq)' is open, with 'Ideal Solution' selected. A dialog box for '13 MgF2(liq) dissolved in Ideal Solution #1' is also open, showing parameters for an ideal solution: A=0, B=0, and P=1.

+ Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
12	Mg(liq)	FactPS	liquid		V			
+X 13 #1	MgF2(liq)	FactPS	liquid		V			
14	Ca(liq)	FactPS	liquid		V			
+X 15	CaF2(liq)	FactPS	liquid		V			
16	MgF2(liq)	FTsalt	liquid		V			

Context Menu for 13 MgF2(liq):

- clear
- + - select
- standard stable phase
- ! - dormant (metastable) phase
- F - formation target phase
- P - precipitate target phase
- 16
- L - cooling calculation ...
- Ideal Solution**
- Z - isobars ...
- Help ...

Dialog Box: 13 MgF2(liq) dissolved in Ideal Solution #1

13 MgF2(liq) - Henrian activity coefficient, gamma
 $\log_{10}(\text{gamma}) = A/TK + B$

A = 0
B = 0

New mixing particles: P = 1 (P > 0)

#1 Ideal Solution name: Ideal-1 (max 10 chars)

For ideal behaviour A = 0, B = 0, P = 1.

Buttons: Cancel, Help, OK

Phase Diagram Module: MgF₂-CaF₂ System

Pure Liquids: Define Ideal Liquid MgF₂-CaF₂ Solution

Repeat for CaF₂

The screenshot shows the 'Selection - Phase Diagram' window. The table below lists the selected species:

+ Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
12	Mg(liq)	FactPS	liquid		V			
+X 13 #1	MgF2(liq)	FactPS	liquid		V			
14	Ca(liq)	FactPS	liquid		V			
+X 15	CaF2(liq)	FactPS	liquid		V			
16	MgF2(liq)	FTsalt	liquid		V			

The '15 CaF2(liq) dissolved in Ideal Solution #1' dialog box is open, showing the following configuration:

- Equation: $\log_{10}(\gamma) = A/TK + B$
- A = 0
- B = 0
- New mixing particles P = 1 (P > 0)
- #1 Ideal Solution name: Ideal-1 (max 10 chars)

- 15 CaF2(liq)
- clear
- ✓ + - select
- ✓ - standard stable phase
- ! - dormant (metastable) phase
- F - formation target phase
- P - precipitate target phase
- 16
- L - cooling calculation ...
- Ideal Solution >
- Z - isobars ...
- Help ...

- Ideal Solution #1 ...
- Ideal Solution #2 ...
- Ideal Solution #3 ...
- Ideal Solution #4 ...
- Ideal Solution #5 ...
- Ideal Solution #6 ...
- Ideal Solution #7 ...
- Ideal Solution #8 ...
- Ideal Solution #9 ...
- Ideal Solution #10 ...
- Clear

Phase Diagram Module: MgF₂-CaF₂ System

Menu Window: Calculate when the liquid solution is ideal

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (2)
MgF2 + CaF2

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 2
- pure solids 3
- * - custom selection species: 5

Target
- none -
Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
		FTsalt-SALTA	A-Salt-liquid
I		FTsalt-C1	Fluorite
J		FTsalt-C4	Rutile
I		FTsalt-C23	Cotunnite

Legend
I - immiscible 2
J - 3-immiscible 1

Show all selected
species: 14
solutions: 7

Custom Solutions
0 fixed activities
1 ideal solutions

Pseudonyms
apply

Volume data
 assume molar volumes of solids and liquids = 0
 include molar volume data and physical properties data

paraequilibrium & Gmin

Total Species (max 5000) 19
Total Solutions (max 200) 8
Total Phases (max 1500) 12

Variables

T(C)	MgF2/			
0 1500	0 1			

T(C) vs MgF2/(MgF2+CaF2)

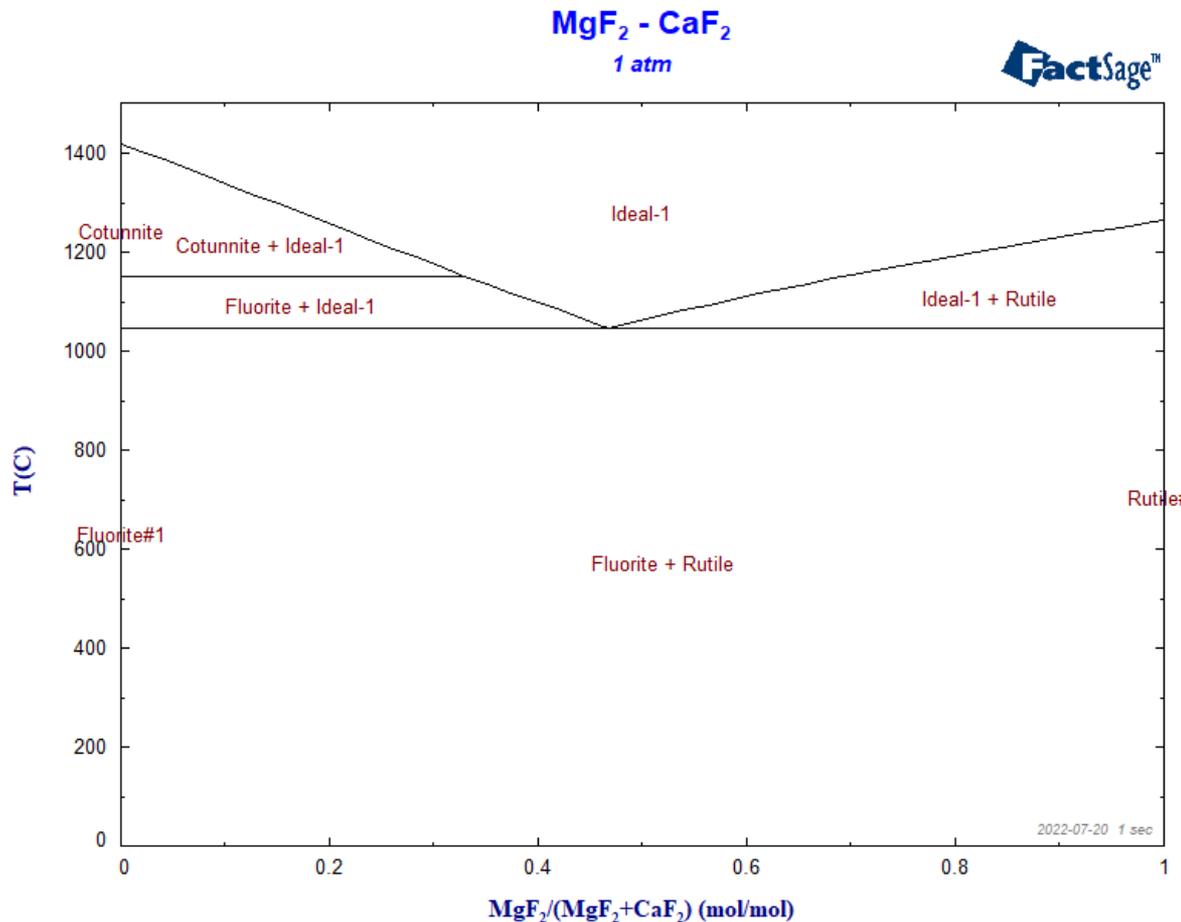
Phase Diagram

Y
X

FactSage 7.3

Phase Diagram Module: MgF_2 - CaF_2 System

Results: the MgF_2 - CaF_2 Phase Diagram (when the liquid solution is ideal)



Stable Phases

2	FTsalt-C1	Fluorite	Strukturbericht : FC
3	Ideal-1	Cotunnite	????
4	FTsalt-C4	Rutile	Strukturbericht : C4

- missing stored phase names and descriptions. Stable Phases you must first calculate the phases

Stoichiometric Phases - compounds and one-comp

mole	TC (min)	TC (max)
- none -	-	-

Manipulate and Refresh

clear restore Help

labels labels - old delete label: Fluorite + Rutile

equilibria

iso-activity

polythermal projection

iso-therm T step: 100

color T-bar clear

tie lines - isothermal diagram

all domains 1 domain hi med lo density clear

aqueous diagram

iso-Eh Eh step: 0 min: max: (volts)

iso-pH pH step: 0 min: max:

replot as Eh vs pH

Figure Viewer full screen

Phase Diagram Module: MgF₂-CaF₂ System

Results: Invariant Reactions (when the liquid solution is ideal)

```
Stable Phases
-----
1 FTsalt-C23 Cotunnite Strukturbericht : C23; Pearson : oP12; Space group : Pnma (62); Pr
2 FTsalt-C1 Fluorite Strukturbericht : FCC_C1; Pearson : cF12; Space group : Fm-3m (225
3 Ideal-1 Cotunnite ?????
4 FTsalt-C4 Rutile Strukturbericht : C4; Pearson : tP6; Space group : P42/mnm (136);

- missing stored phase names and descriptions. To list all the
Stable Phases you must first calculate the phase diagram.

-----
Stoichiometric Phases - compounds and one-component solutions
-----
mole          TC(min)    TC(max)
-----
- none -

-----
Phase Equilibria
-----
1 1417.86 C Ideal-1(0.0) + (1.0) <=> Cotunnite#1(0.0)
2 1262.85 C Ideal-1(0.0) + (1.0) <=> Rutile#1(0.0)
3 1150.85 C Fluorite#1(0.0004005) <=> Cotunnite#1(0.0004005) + Ideal-1(0.3274)
4 1045.02 C Ideal-1(0.4676) <=> Fluorite#1(0.000483) + Rutile#1(0.9995)
-----
```

Manipulate and Refresh

clear restore Help

labels labels - old delete label: Fluorite + Rutile

equilibria

iso-activity 0 value

polythermal projection

iso-therm T step: 100

color T-bar clear

tie lines - isothermal diagram

all domains 1 domain hi med lo density clear

aqueous diagram

iso-Eh Eh step: 0 min: max: (volts)

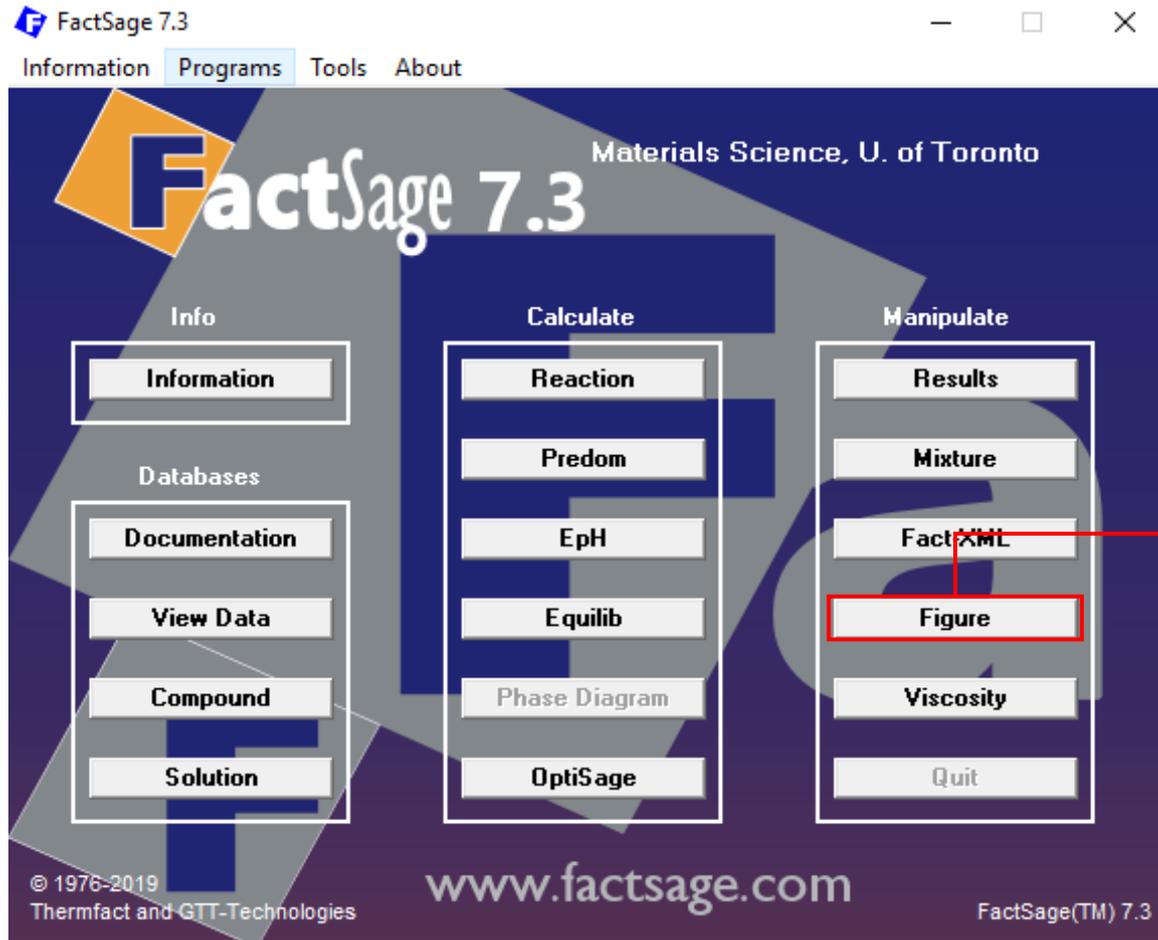
iso-pH pH step: 0 min: max:

replot as Eh vs pH

Figure Viewer full screen

Phase Diagram Module: $\text{MgF}_2\text{-CaF}_2$ System

Comparison: Open the Figure Module

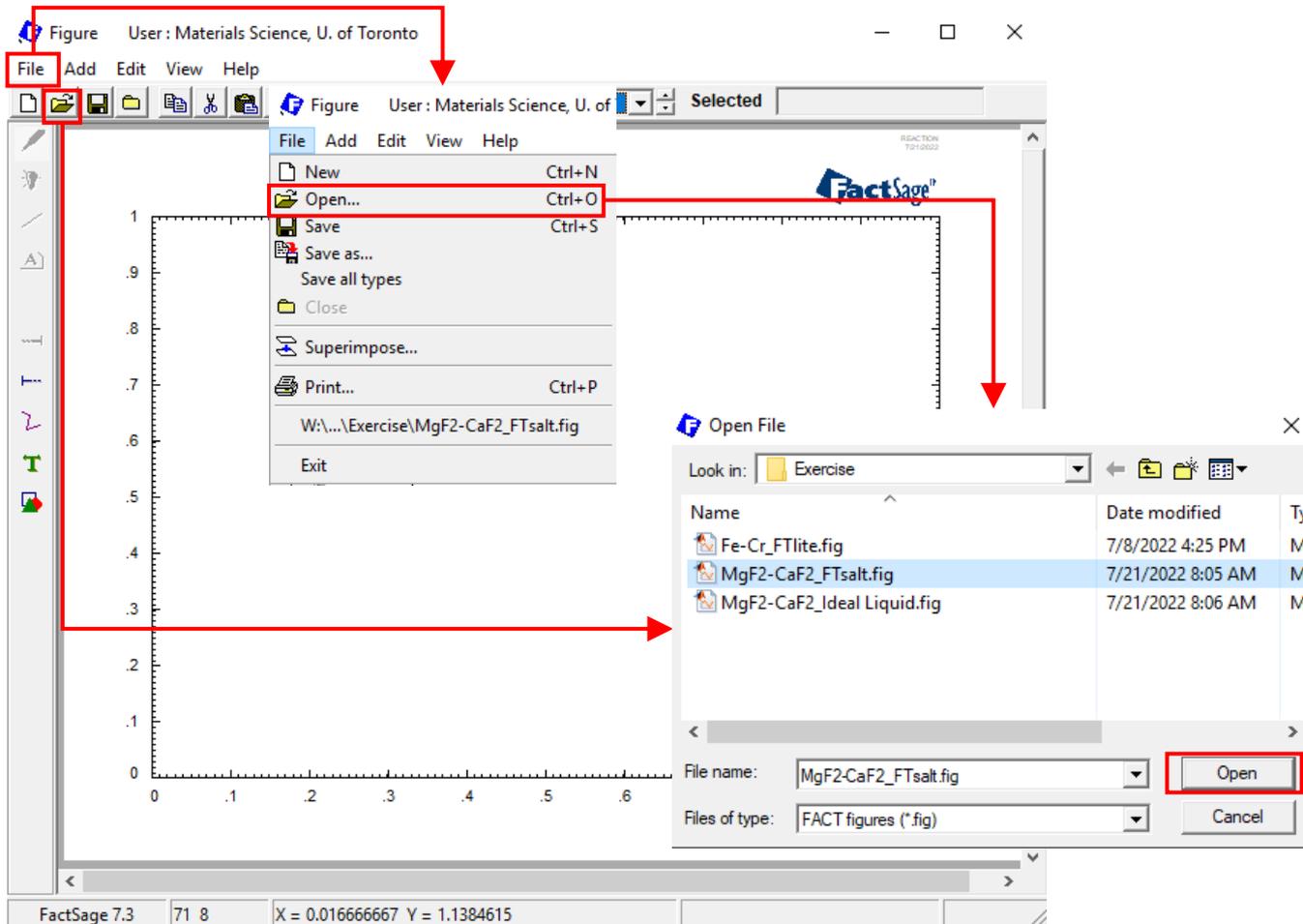


We will use the Figure Module to superimpose the two phases diagrams of the $\text{MgF}_2\text{-CaF}_2$ system.

Run Figure

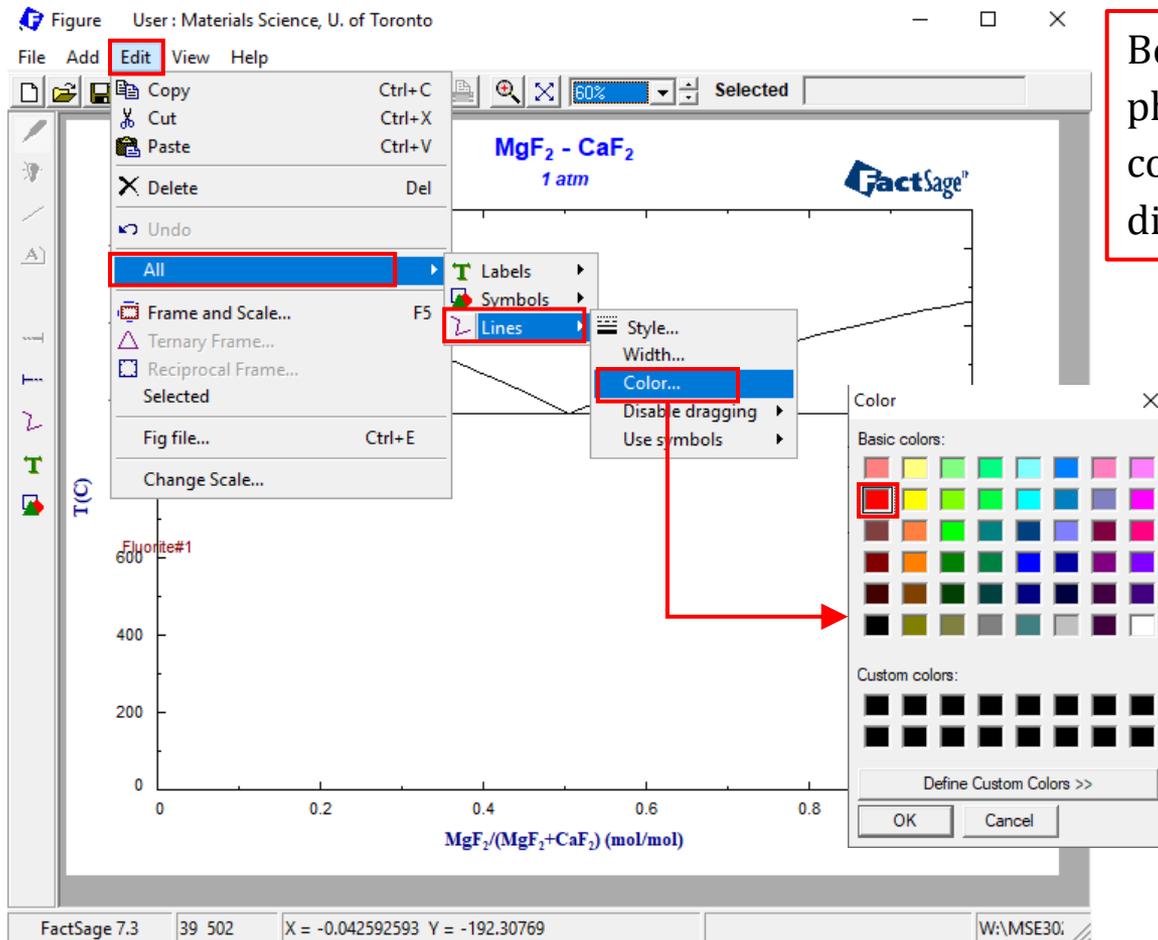
Phase Diagram Module: MgF₂-CaF₂ System

Comparison: Open the first phase diagram



Phase Diagram Module: $\text{MgF}_2\text{-CaF}_2$ System

Comparison: Open the first phase diagram



Before we superimpose the second phase diagram, let us change the color of lines on the first phase diagram (FTsalt-SALTA) to red.

Phase Diagram Module: $\text{MgF}_2\text{-CaF}_2$ System

Comparison: Superimpose the second phase diagram

The screenshot displays the FactSage 7.3 interface. The main window shows a phase diagram for the $\text{MgF}_2\text{-CaF}_2$ system at 1 atm. The y-axis is Temperature (T) in degrees Celsius, ranging from 0 to 1400. The x-axis is the mole fraction of MgF_2 in the $\text{MgF}_2\text{-(MgF}_2\text{+CaF}_2)$ system, ranging from 0 to 0.4. The diagram shows a liquid phase region and a solid phase region (Salt-liquid). Key features include the Cotunnite phase at approximately 1150°C and the Fluorite#1 phase at approximately 600°C. A red box highlights the 'Superimpose...' option in the File menu. An 'Open File' dialog box is open, showing the file 'MgF2-CaF2_Ideal Liquid.fig' selected. Red arrows indicate the workflow: from the 'Superimpose...' menu option to the 'Open File' dialog, and from the selected file back to the main phase diagram window.

Figure User: Materials Science, U. of Toronto

File Add Edit View Help

MgF₂ - CaF₂
1 atm

FactSage[®]

1400
1200
1000
800
600
0

Cotunnite
Salt-liquid
Fluorite#1

T (C)

MgF₂ / (MgF₂ + CaF₂) (mole)

Open File

Look in: Exercise

Name	Date modified	Type
Fe-Cr_FTlite.fig	7/8/2022 4:25 PM	M
MgF2-CaF2_FTsalt.fig	7/21/2022 8:05 AM	M
MgF2-CaF2_Ideal Liquid.fig	7/21/2022 8:06 AM	M

File name: MgF2-CaF2_Ideal Liquid.fig

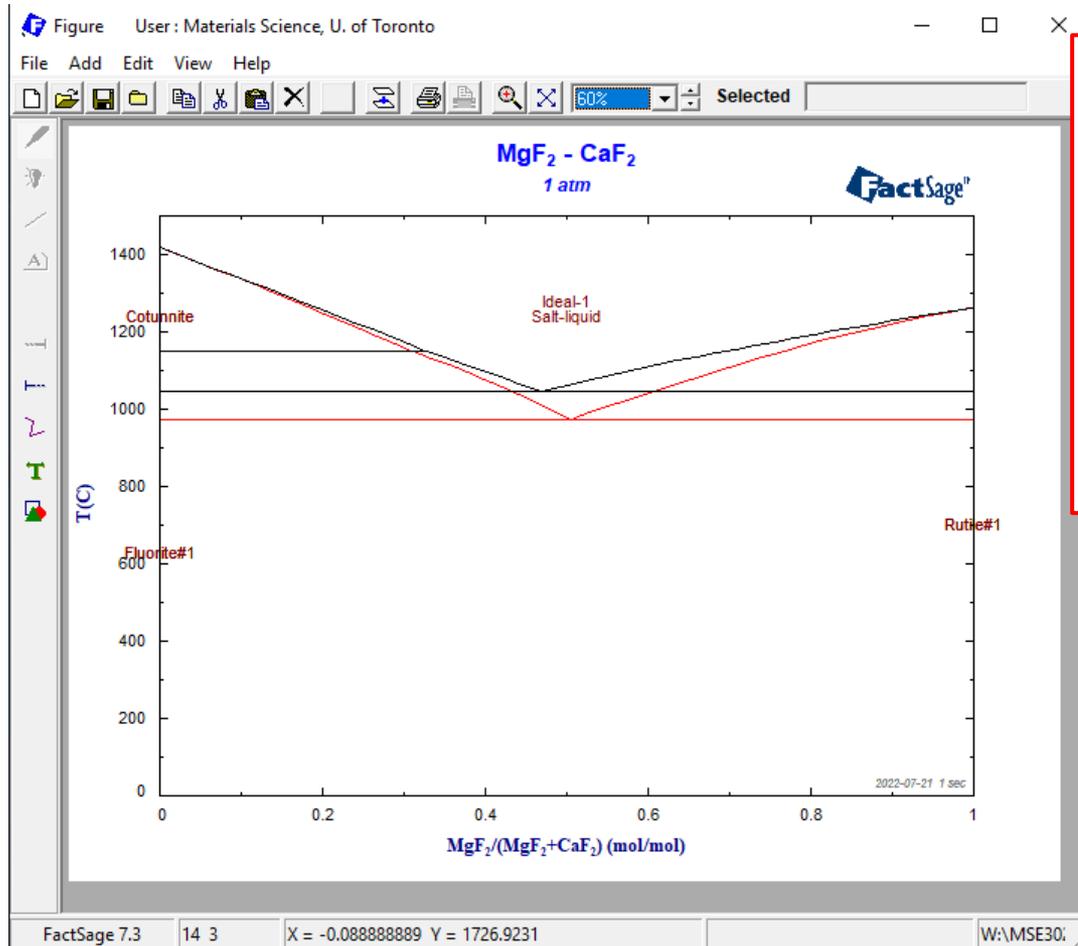
Files of type: FACT figures (*.fig)

Open Cancel

FactSage 7.3 370 423 X = 0.57037037 Y = 111.53846 W:\MSE30

Phase Diagram Module: $\text{MgF}_2\text{-CaF}_2$ System

Comparison: Superimpose the second phase diagram



It is seen that the real liquid solution model (FTsalt-SALTA, labeled as red) gives lower liquidus lines and eutectic temperature than if ideal liquid solution model is used. This means that liquid MgF_2 and liquid CaF_2 exhibit negative deviation from ideality. (Reason?)

In-Class Exercise

Question 1.

Calculate the predominance diagram of the Mo-C-O system at 1400 K. Use $\log_{10}(P_{\text{CO}_2}/1 \text{ atm})$ as Y-axis, and $\log_{10}(P_{\text{CO}}/1 \text{ atm})$ as X-axis.

For a total hydrostatic pressure of 1 atm, what are the pressures of CO_2 and CO when metallic Mo is stable with its carbide phase at 1400 K?

In-Class Exercise

Question 2.

Calculate the Al-Mg phase diagram. Label all the liquid and all solid phases. Then answer the following questions:

- (a) What is the lowest melting point in the system?
- (b) What is the maximum solubility of Mg in solid FCC Al?
- (c) What is the maximum solubility of Al in solid HCP Mg?
- (d) At 350 °C, what is the solubility limit of Mg in solid FCC Al? What is the solubility limit Al in solid HCP Mg?
- (e) Over what range of temperature is the $\text{Al}_{30}\text{Mg}_{23}$ phase stable?
- (f) What is the non-stoichiometric range of the gamma phase (CBCC-A12)?

In-Class Exercise

Question 3.

Calculate the phase diagram for the Fe-Cr-O₂ system at 1300 °C.

Use $\log_{10}(P_{O_2}/1 \text{ atm})$ as the Y-axis which varies from from -20 to 0 , and use the mole fraction of Cr X_{Cr} as the X-axis which varies from 0 to 1 . For an Fe-Cr alloy with the composition of $X_{Cr} = 0.18$, what is the maximum P_{O_2} that will permit this alloy to remain free of oxidation at 1300 °C?

In-Class Exercise

Question 4.

Calculate the “**quasi-**” binary phase diagram of the MgO-Al₂O₃ system. Find the temperature and specify the co-existing phases and reactions at all the invariant points.

In-Class Exercise

Question 5.

Choose FTlite database to calculate the liquidus projection of the Al-Mg-Si and isothermal sections at 500 and 1000 K (1 bar). Then compare them with the diagrams calculated by SGTE2017 database (available from Documentation).