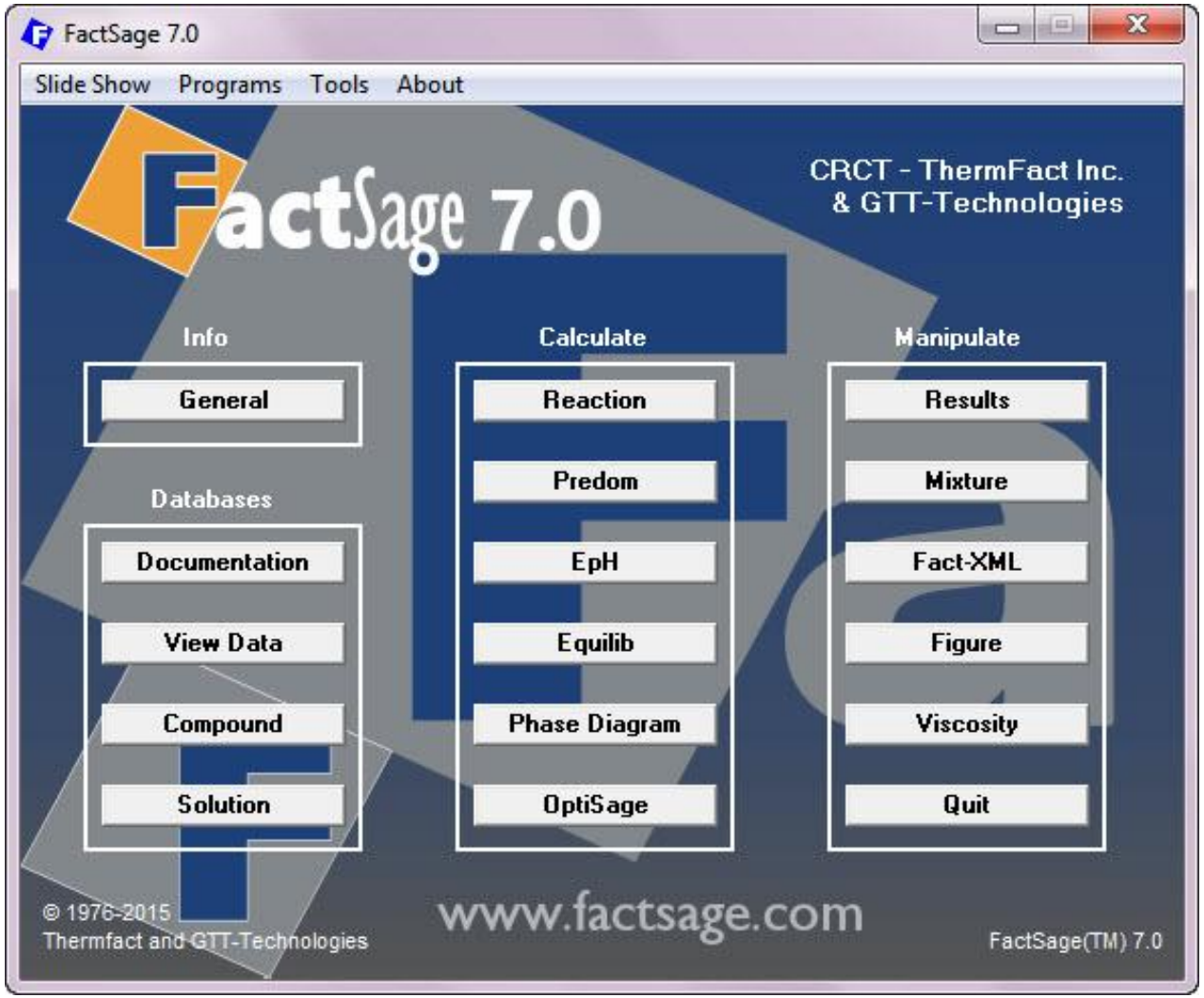
FactSage Overview



Several thermochemical software/database packages with applications in materials science have been developed over the last 40+ years.

These packages all contain large **critically evaluated** databases of **thermochemical properties** for thousands of compounds and hundreds of solution phases, as well as user interfaces of varying degrees of user-friendliness.

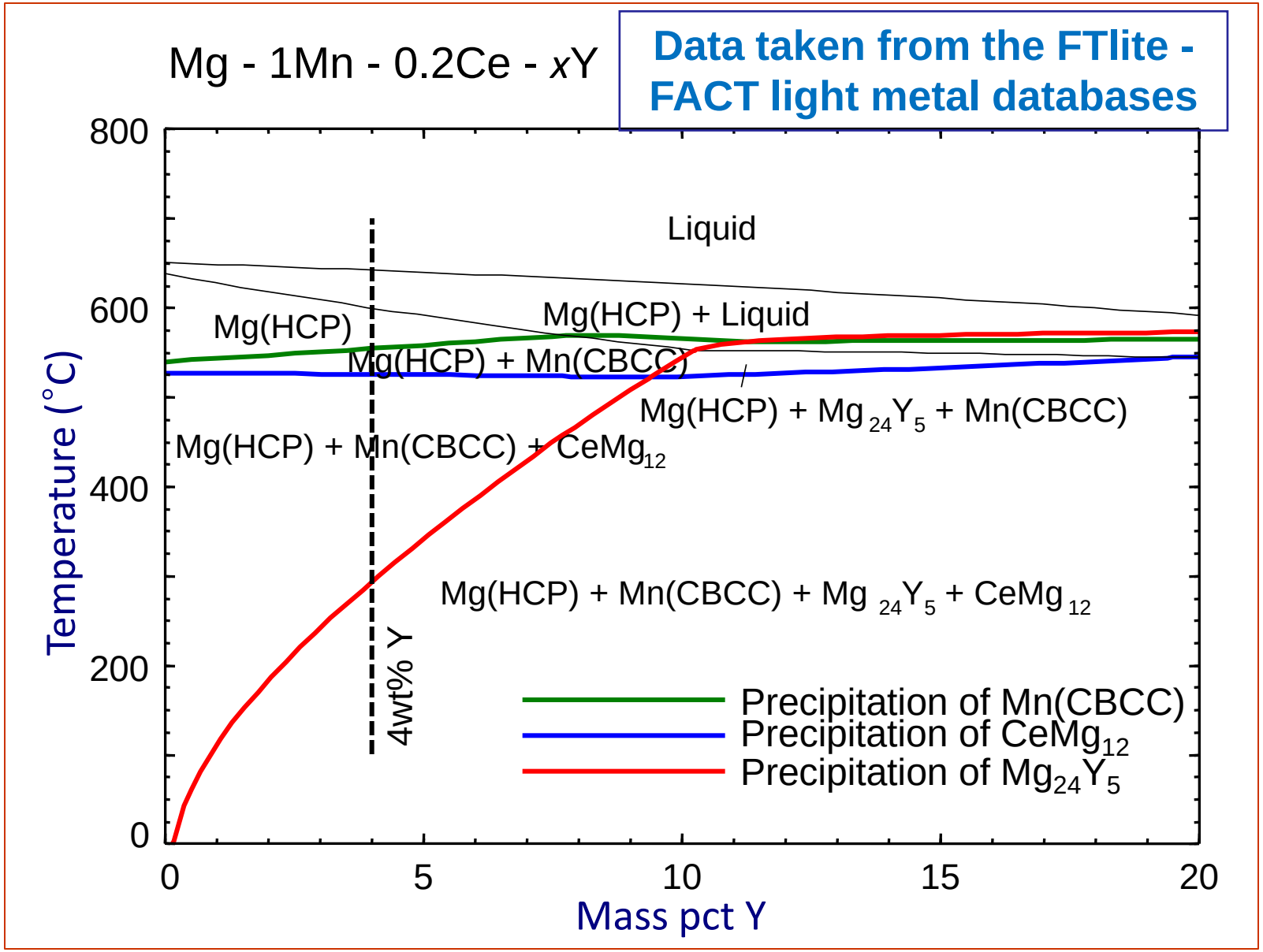
- **HSC Chemistry**
- **MTS-NPL**
- **Thermo-Calc**
- **Thermodata**
- **FactSage**

- **Thermochemical databases** contain parameters giving the **Gibbs energy**, **G**, of all compounds as functions of T (and P) and of all solutions as functions of T, (P) and composition. This is a complete database because all the other thermodynamic properties (H, C_p, μ, etc.) can be calculated by taking the appropriate derivatives of the G functions.

- **For a given set of constraints** (such as temperature, total pressure, total mass of each element) the ***software*** calculates the equilibrium conditions by **minimizing the total Gibbs energy** of the system. This is mathematically equivalent to solving all the equilibrium constant equations simultaneously.

- Data are automatically extracted as required from the databases.

Calculated Phase Diagram Section in a 4-component System

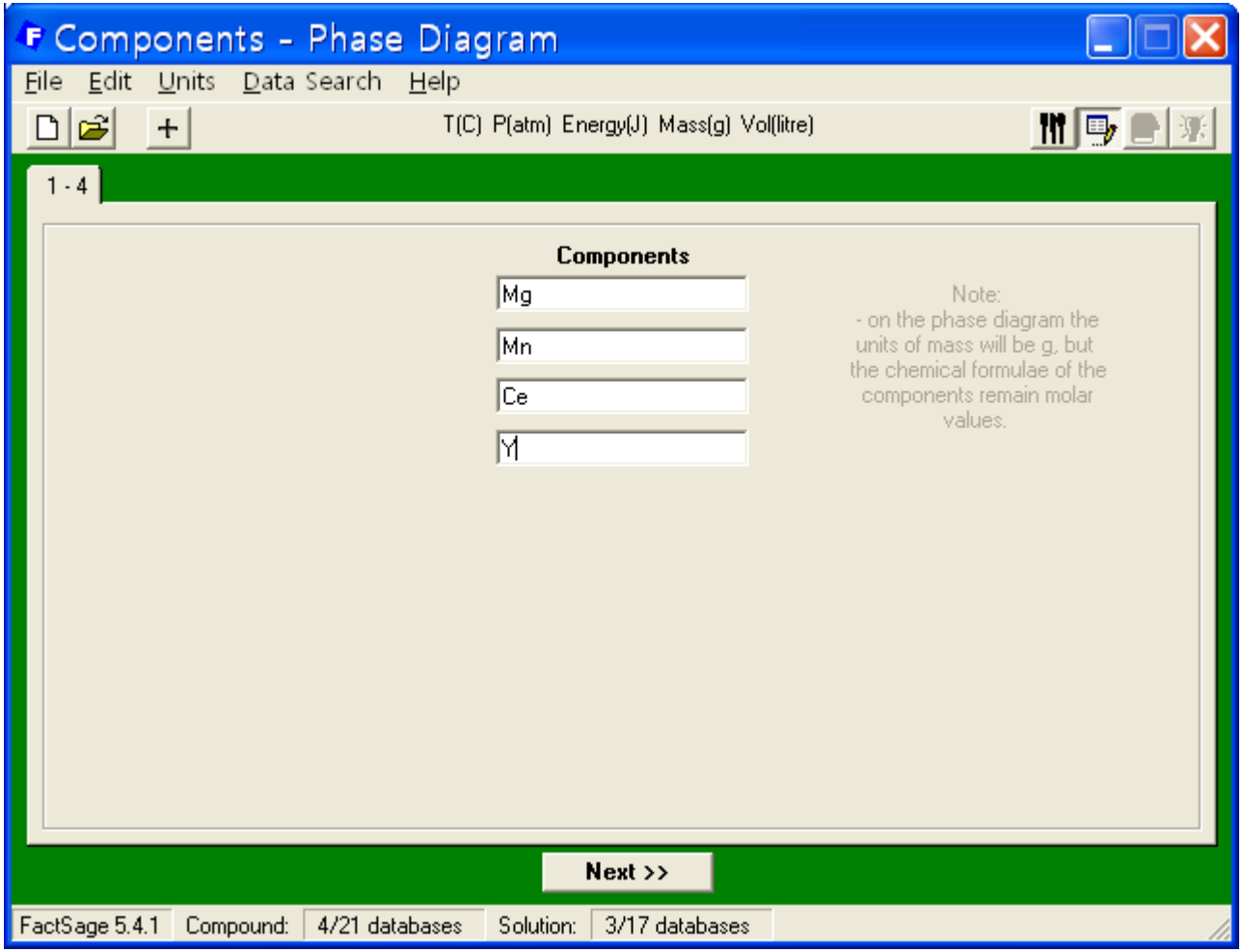


Calculating the Previous Phase Diagram using *FactSage*

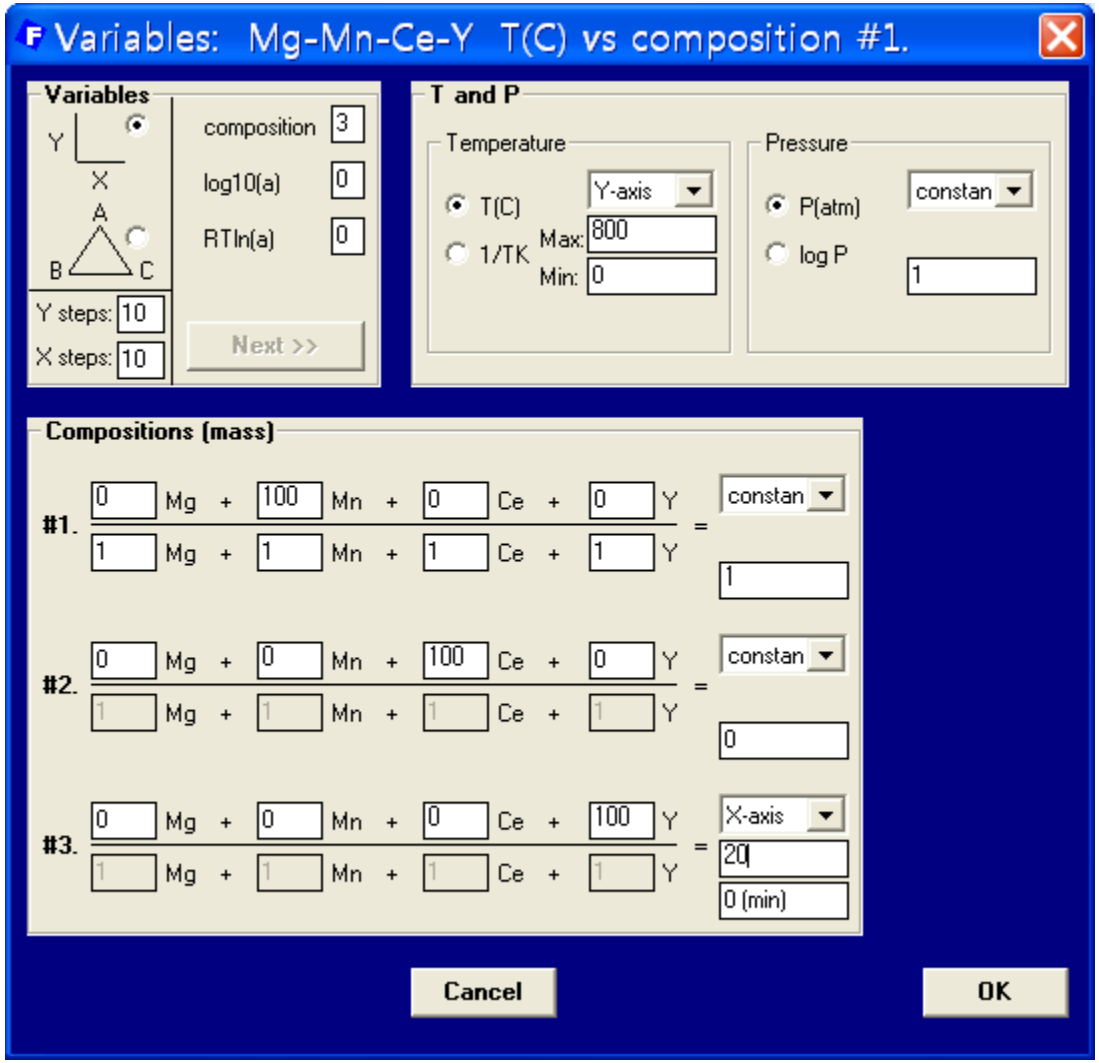
Click on ***Phase Diagram*** in the main ***FactSage*** window.

Input to calculate the previous phase diagram in **FactSage**

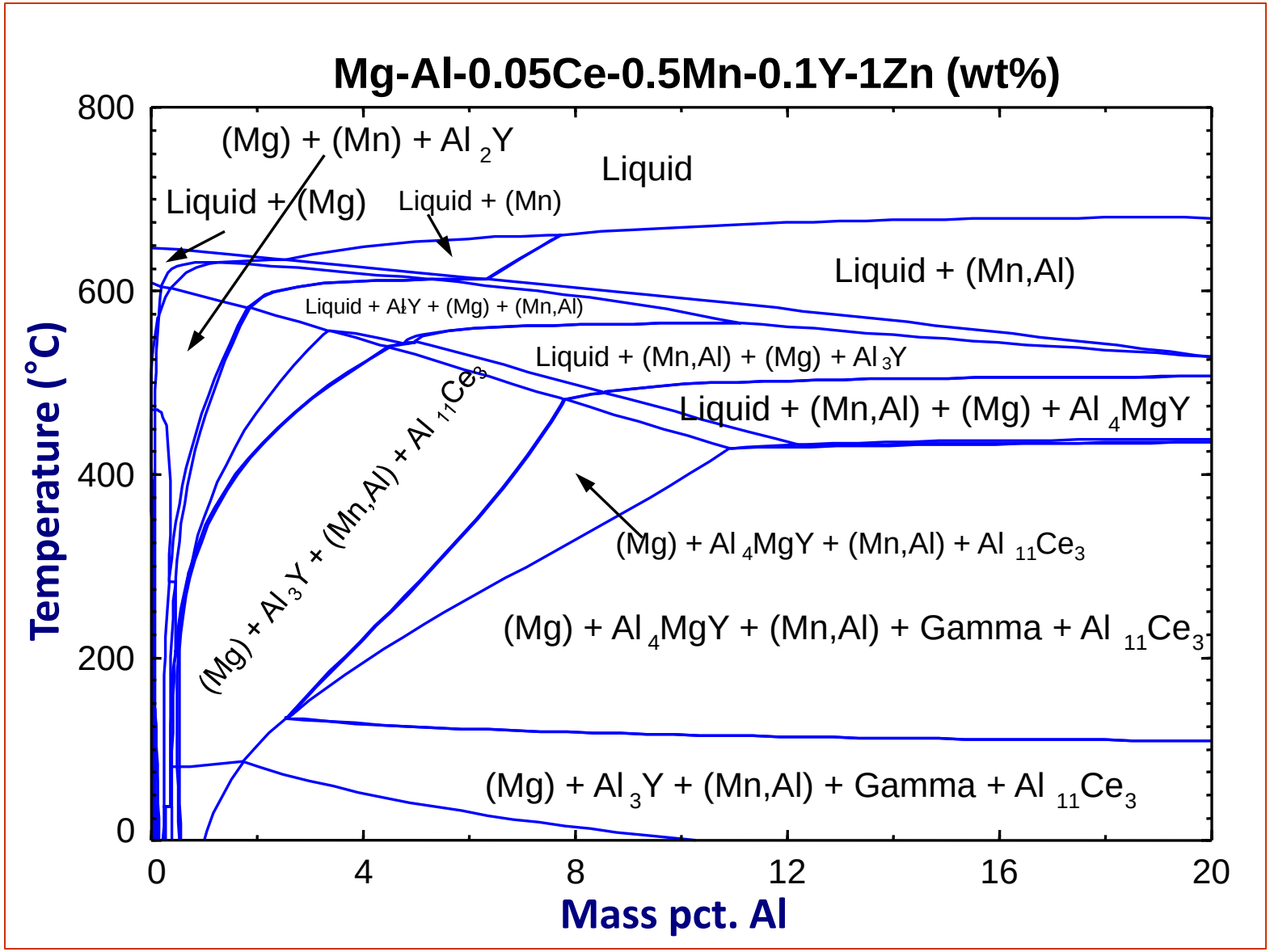
Definition of the components:



Definition of the axes:



Phase Diagram of a 6-component System Calculated from FTlite Thermodynamic Database



The thermodynamic database can be used along with the Gibbs energy minimization software of ***FactSage*** to

- calculate any phase diagram section

  (isothermal, isoplethal, etc.)

- calculate cooling paths of alloys

  (Equilibrium, Scheil-Gulliver, etc.)

- calculate amounts of each phase

  (→ estimation of amounts and composition of microstructural constituents)

- calculate heat evolution during cooling, etc.

(the thermodynamic database permits calculation of the driving force for diffusion, precipitation kinetics, etc. and can be coupled to software for phase field and kinetic modeling)

How ***FactSage*** Thermodynamic Databases are Developed

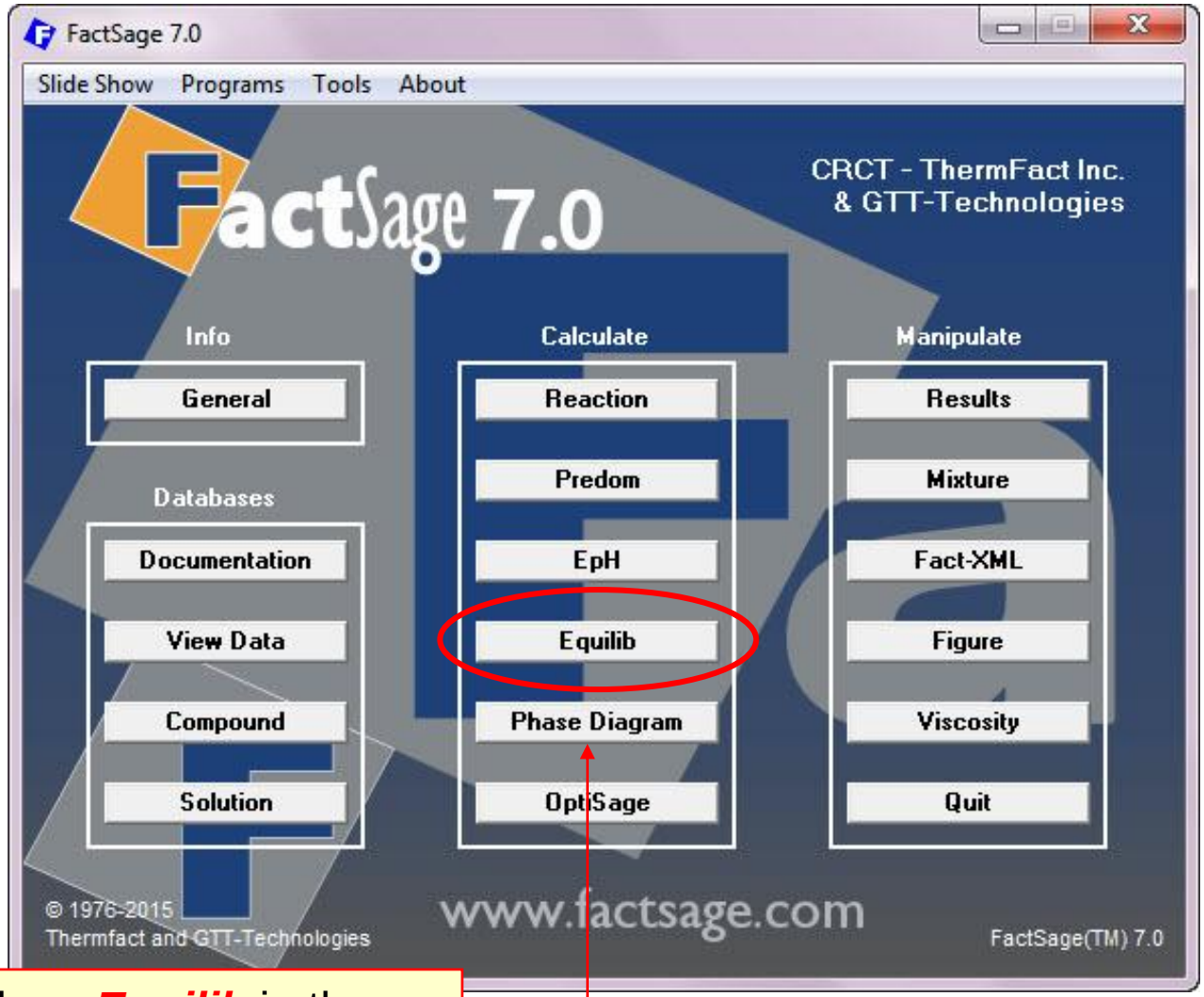
1. Develop a mathematical model for G(T, P, Composition) for each phase (oxide, alloy, salt, matte, aqueous, gas …)
2. Optimize model parameters simultaneously using all available thermodynamic and phase equilibrium data from the literature (activities, solubilities, pressures, heats, …)
3. Use models and database to estimate properties of multicomponent systems (ternaries, quaternaries, …)
4. Calculate thermodynamic properties and phase equilibria by Gibbs energy minimization (**Equilib** & **Phase Diagram**).
5. Dissemination to academic and industrial communities via the ***FactSage*** system (**www.factsage.com**).

The ***Equilib*** module

- ***Equilib*** calculates the conditions for multiphase, multicomponent equilibria, with a wide variety of tabular and graphical output modes, under a large range of constraints through Gibbs energy minimization.

(continued)

The *Equilib* module



Click on ***Equilib*** in the ***FactSage*** Menu Window

Desulfurizing a steel by **CaSi** addition. *Definition of the reactants:*

Starting composition of the steel melt

Note the use of the variable amount <A> for the slag.

Calcium silicide addition

Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 10 | 11 - 13

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100	Fe	solid-1 bcc	1000	1.0	1	FACT
0.1	C	solid-1 graphite	1000	1.0	1	FACT
0.2	Si	solid	1000	1.0	1	FACT
1.5	Mn	solid-1	1000	1.0	1	FACT
0.02	S	solid-1 orthorhombic	1000	1.0	1	FACT
0.05	Al	solid	1000	1.0	1	FACT
<40A>	CaO	solid lime	1000	1.0	1	FACT
<10A>	SiO2	solid-1 quartz(l)	1000	1.0	1	FACT
<20A>	Al2O3	solid-1 gamma	1000	1.0	1	FACT
<10A>	MnO	solid	1000	1.0	1	FACT

initial conditions

Next >>

FactSage 5.0 | Compound: 1/6 database(s) | Solution: 1/5 database(s)

1 - 10 | 11 - 13

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
<5A>	FeO	solid wustite	1000	1.0	1	FACT
0.2	CaSi	solid	1000	1.0	1	FACT
0.04	Ar	gas	1000	1.0	1	FACT

Desulfurizing a steel by **CaSi** addition.

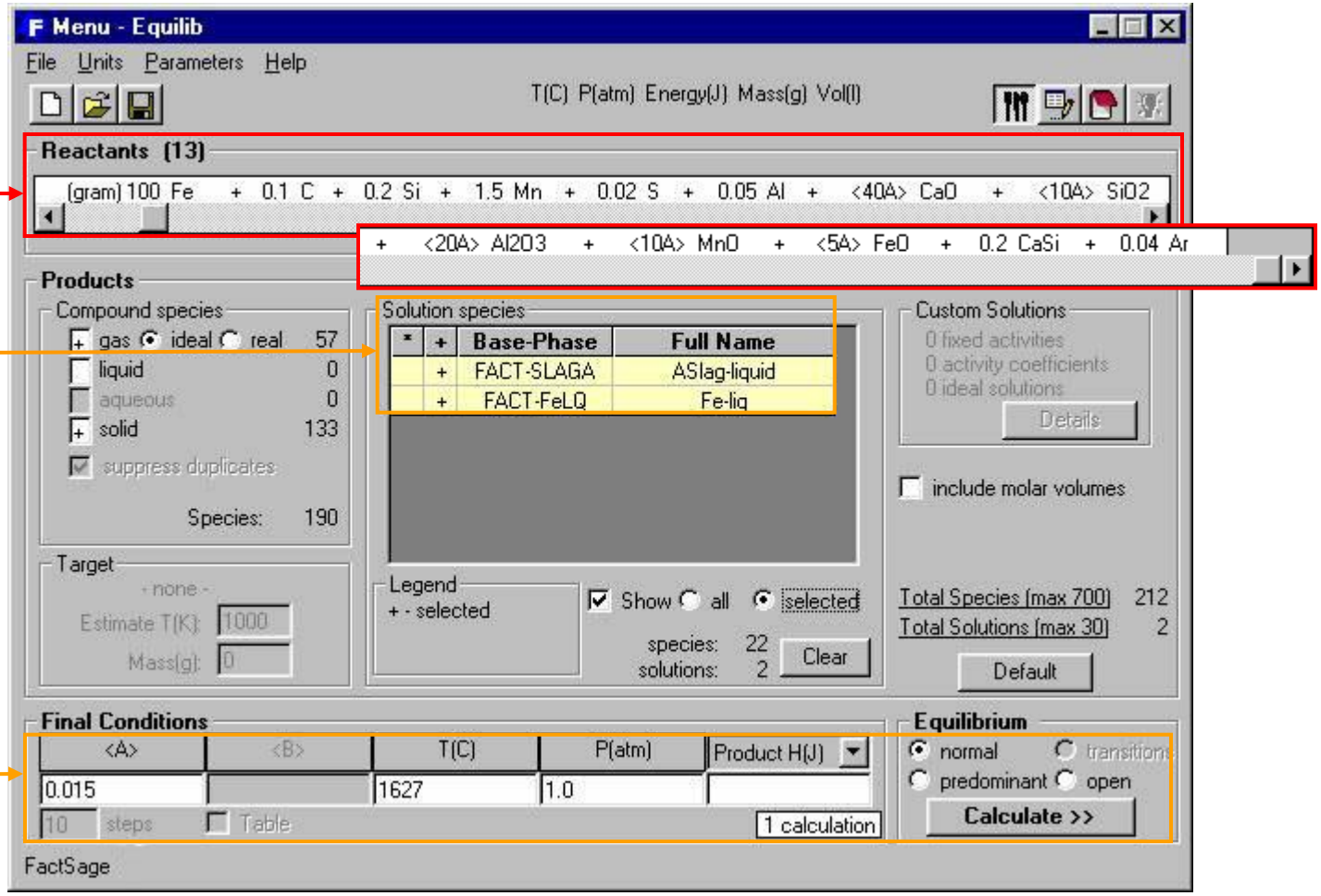
Selection of product phases and final conditions:

Summary of the **Reactants** window

Solution species selected

Final conditions:
- <A> = 0.015
- T = 1627°C
- P = 1 atm

and **Calculate >>**



Desulfurizing a steel by **CaSi** addition. *Results Window:*

```
(gram) 100 Fe +  0.1 C +  0.2 Si +  1.5 Mn +

(gram) 0.02 S +  0.05 Al +  <40A> CaO +  <10A> SiO2 +

(gram) <20A> Al2O3 +  <10A> MnO +  <5A> FeO +  0.2 CaSi +

(gram) 0.04 Ar =

  1.0069E-03 mol   gas_ideal
  (4.0188E-02 gram, 1.0069E-03 mol, 0.15699 litre, 2.5599E-04 g/ml)
          (1627.00 C, 1 atm,     a=1.0000)
          ( 0.99448          Ar
          + 4.3098E-03       CO
          + 1.0377E-03       Mn
          + 1.1361E-04       Fe)

+ 102.09     gram  Fe-liq
  (102.09 gram, 1.8407 mol)
          (1627.00 C, 1 atm,     a=1.0000)
          ( 98.008     wt.% Fe
          + 2.0738E-02 wt.% Al
          + 9.7900E-02 wt.% C
          + 1.5825     wt.% Mn
          + 1.1478E-04 wt.% O
          + 9.2123E-04 wt.% S
          + 0.28770    wt.% Si
          + 2.1753E-03 wt.% CaO
          + 1.2349E-04 wt.% AlO)

+ 1.2528     gram  ASlag-liquid
  (1.2528 gram, 1.9174E-02 mol)
          (1627.00 C, 1 atm,     a=1.0000)
          ( 1.5496E-02 wt.% FeO
          + 4.7420E-02 wt.% MnO
          + 10.041     wt.% SiO2
          + 58.191     wt.% CaO
          + 28.282     wt.% Al2O3
          + 3.4200     wt.% CaS
          + 8.6622E-04 wt.% FeS
          + 2.6569E-03 wt.% MnS)

+ 0.00000    gram  Fe_bcc                                          T
          (1627.00 C, 1 atm, S1, a=0.93200)

+ 0.00000    gram  Fe_fcc                                          T
          (1627.00 C, 1 atm, S2, a=0.92352)
```

Gas phase, mainly **Ar**

Two liquid solutions:

- **liquid steel**
- slag containing **sulfur**

No **solid** phases (activity<1)

The *Phase Diagram* module

Click on ***Phase Diagram*** in the main ***FactSage*** window.

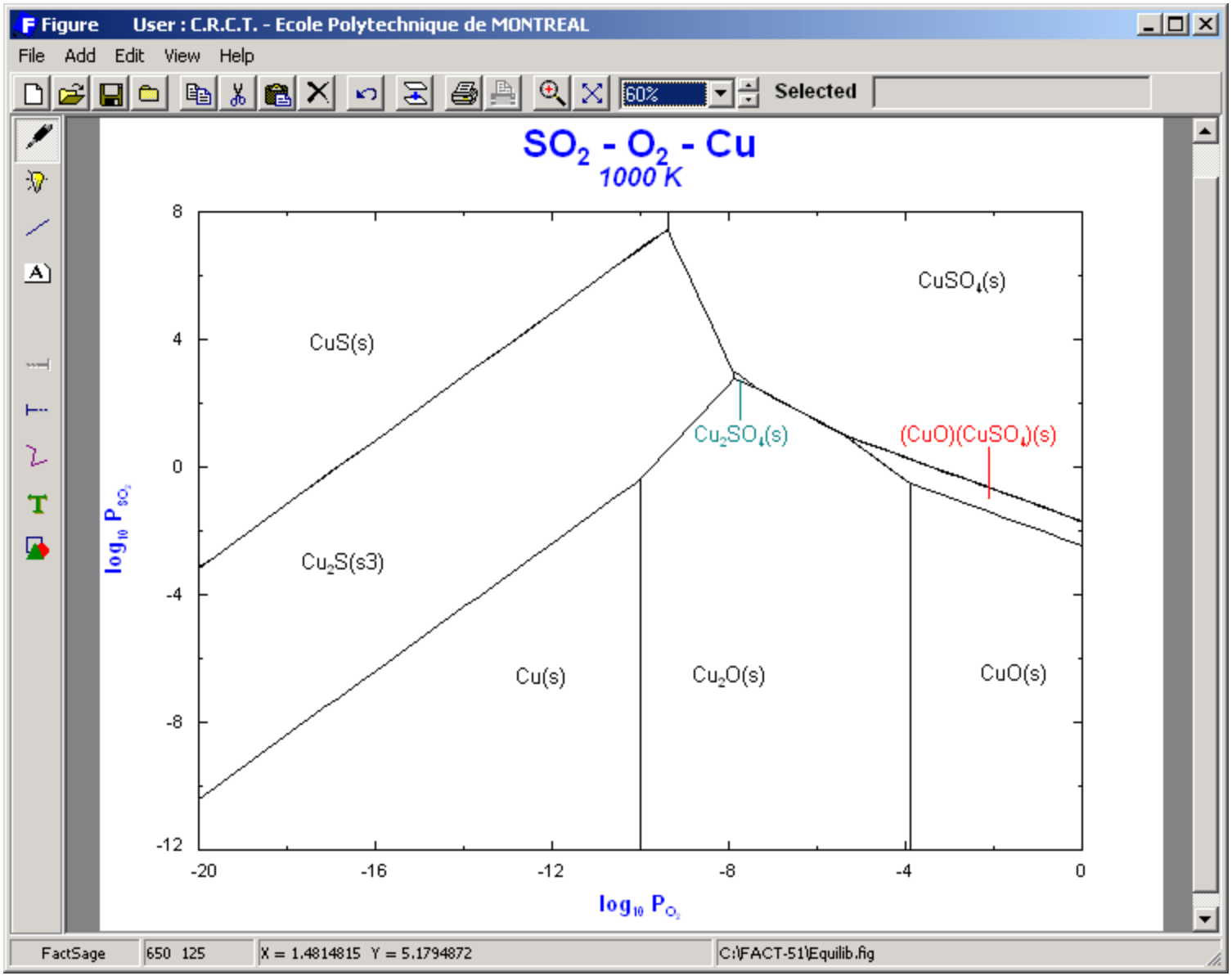
Many Types of Phase Diagrams

For phase diagram calculations the axes and constants are various combinations of the variables T, 1/TK, P, log(P), RTln(P), V, log(V), log(a), Eh, pH, H and X.

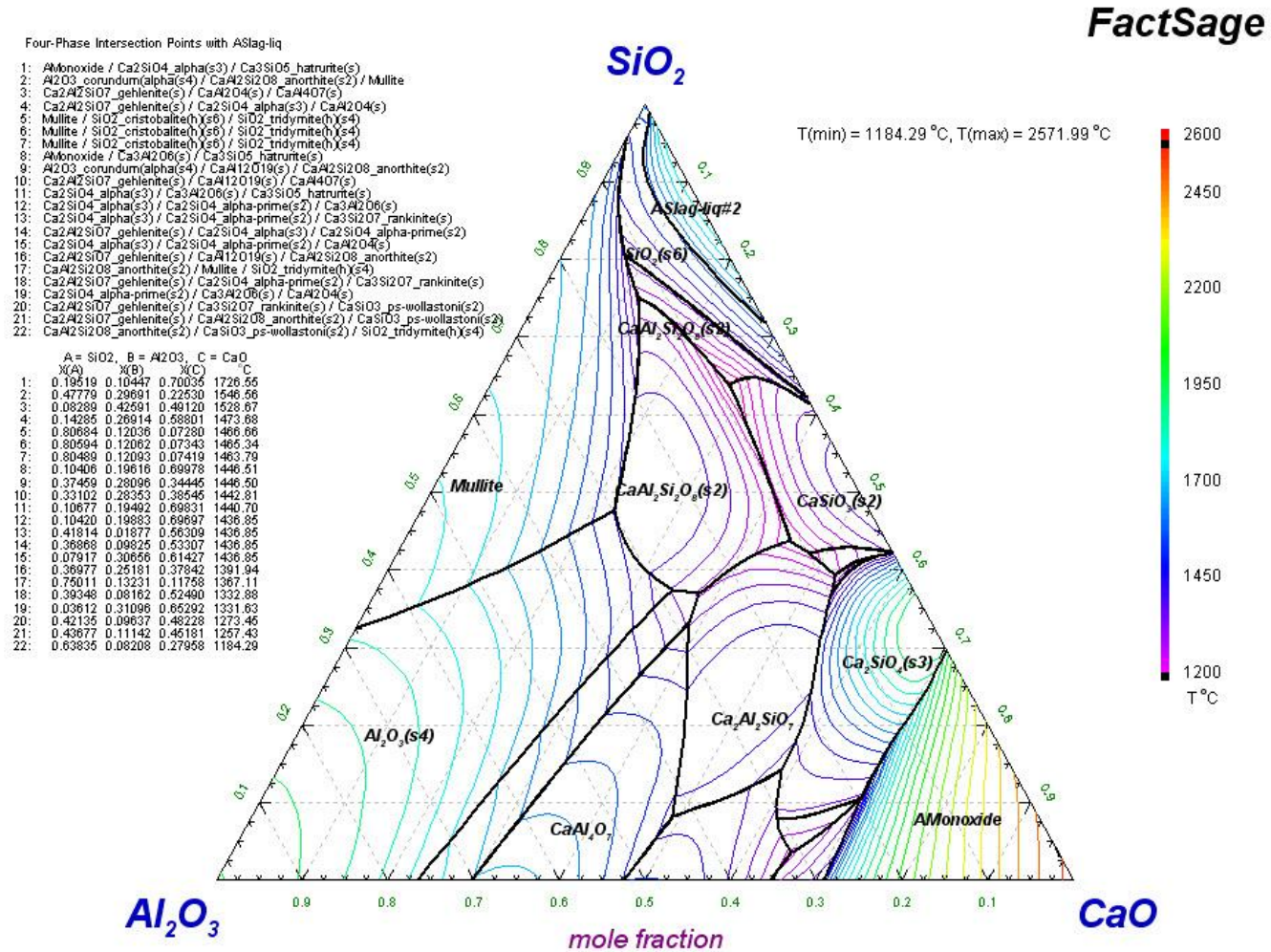
Type	Y-axis	X-axis	
1	T	P, log P, V, log V	
2	P, log P, V, log V	T	
3	RTln(a), log(a)	P, log(P)	
4	P, log(P)	RTln(a), log(a)	
5	RTln(a), log(a)	T	
6	T	RTln(a), log(a)	
7	RTln(a), log(a)	T	
8	Eh	pH	(Pourbaix diagram)
9	V, log(V)	X	
10	H	X	
11	P, log(P)	X	
12	T	X	(classical temperature vs. composition)
13	RTln(a)	X	
14	X	X	(isothermal X vs Y section)
15	X	X	(isothermal Gibbs ternary)
16	X	X	(polythermal X vs Y projection)
17	X	X	(polythermal Gibbs ternary)

T = temperature (or 1/TK), P = total pressure, V = total volume, H = enthalpy, a = activity (or fugacity), X = composition (mole fraction, weight fraction)

Predominance area diagram: $Cu\text{-}SO_2\text{-}O_2$



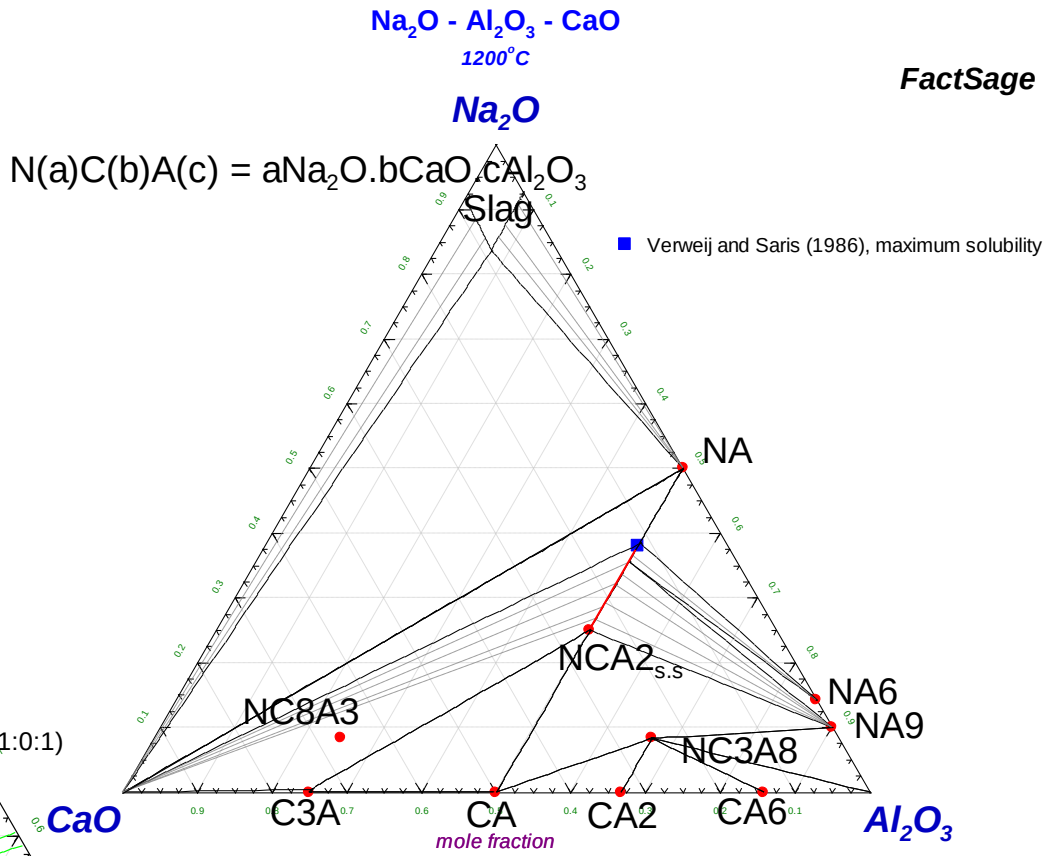
Al_2O_3-CaO-SiO_2 polythermal projection



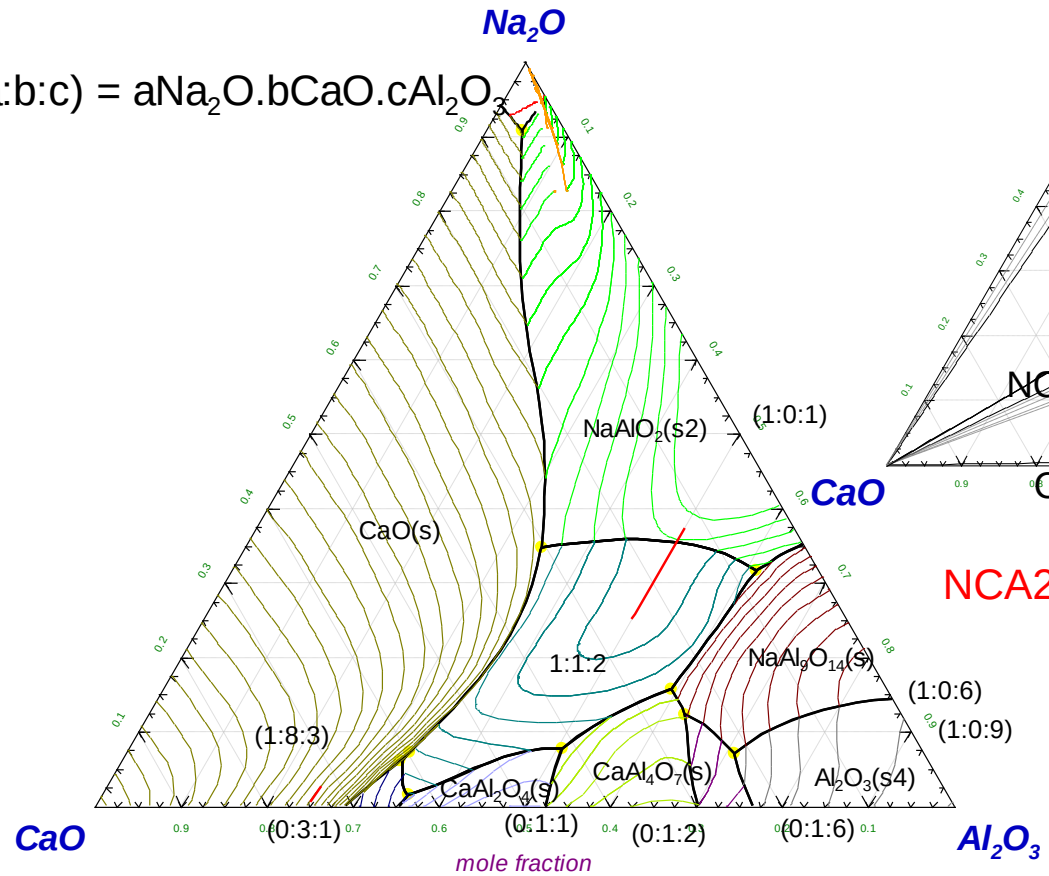
Data taken from the FToxid - FACT oxide databases

Phases and Phase diagrams: Na_2O-Al_2O_3-CaO System

Data taken from FToxid
- FACT oxide databases



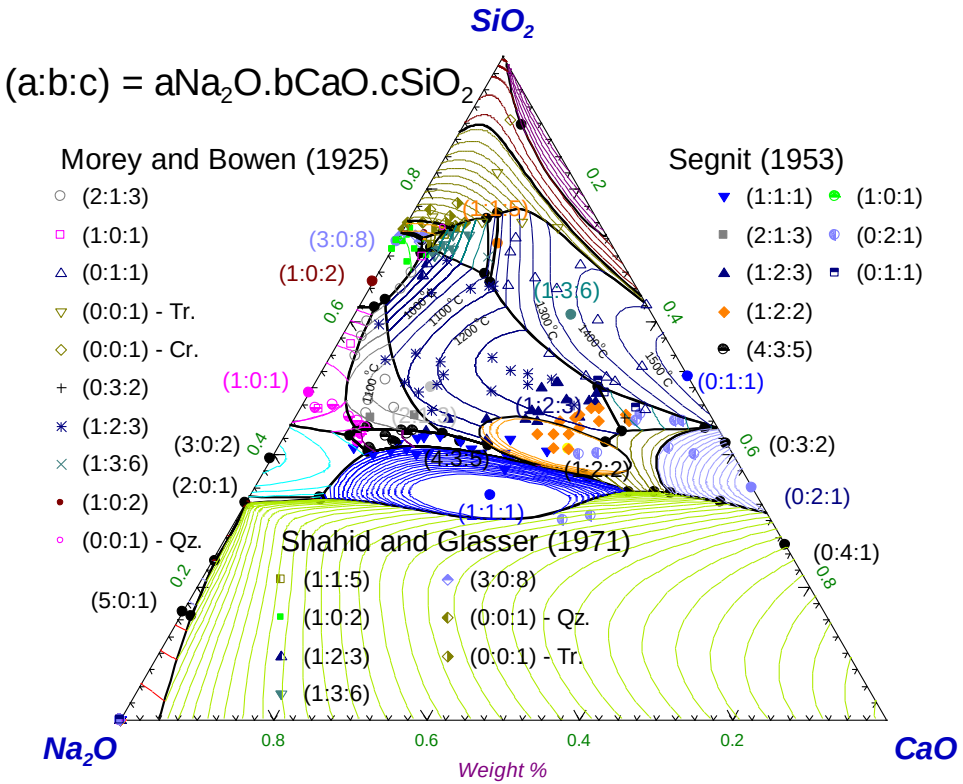
NCA2: $(Na_2,Ca)O \cdot Na_2O \cdot 2Al_2O_3$ solid solution

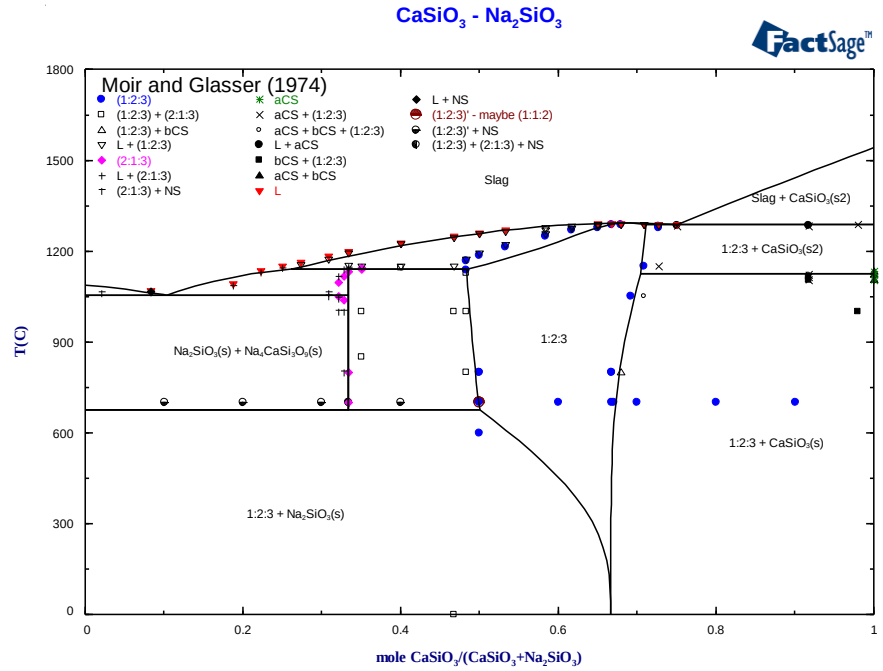


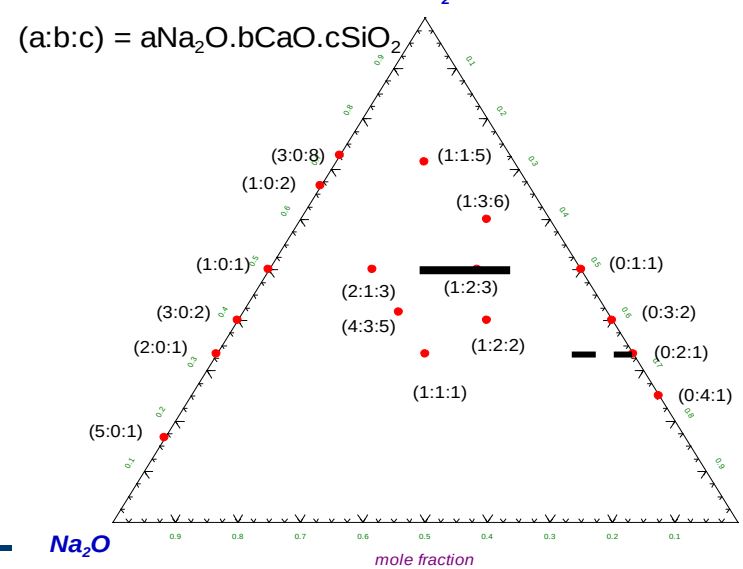
Phases and Phase diagrams: Na_2O-CaO-SiO_2 system

Data taken from FToxid
- FACT oxide databases

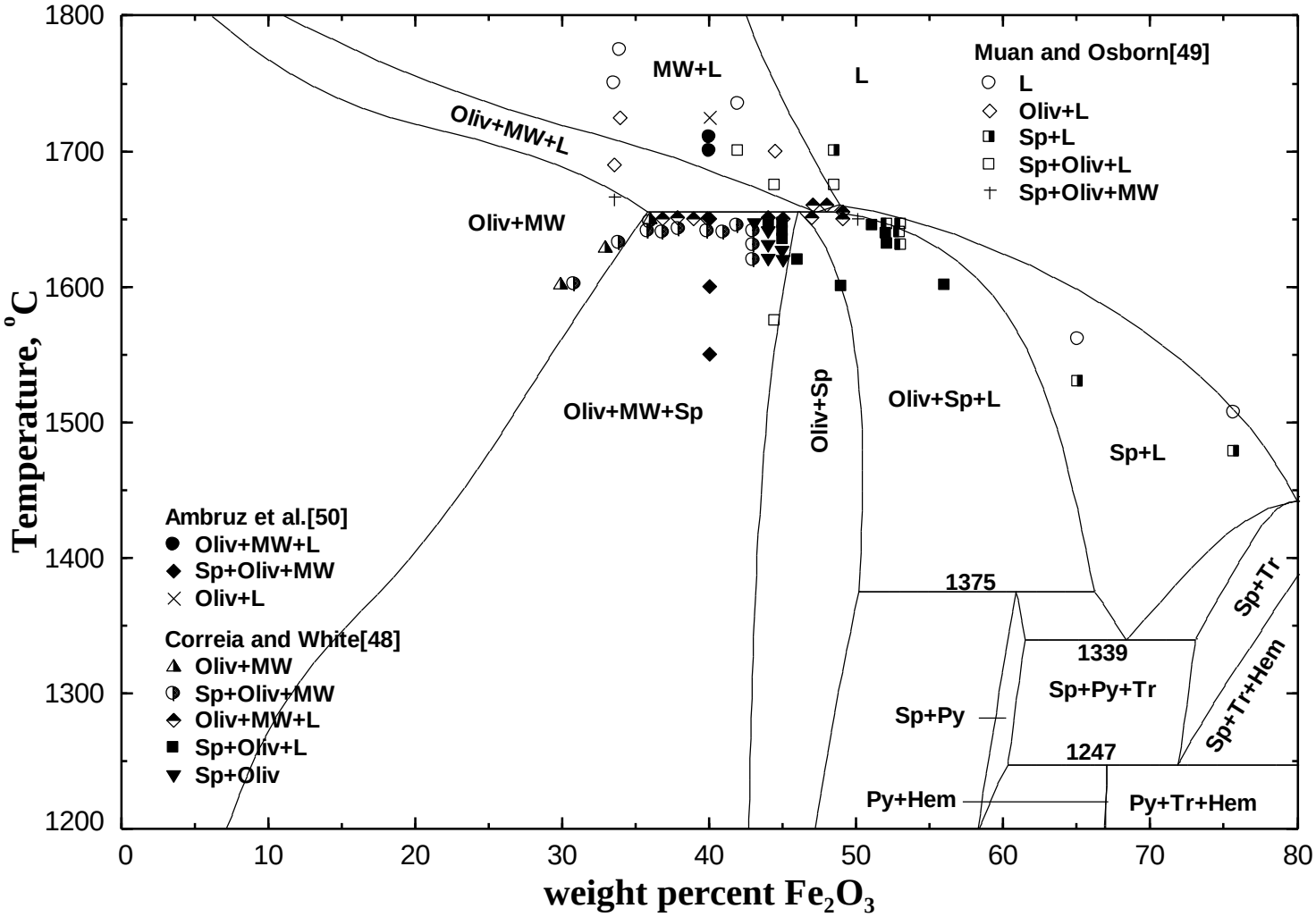
NCSO: 1:2:3 solid solution







Calculated section of the Fe_2O_3-MgO-SiO_2-O_2 phase diagram in air at $SiO_2/(MgO+Fe_2O_3+SiO_2)$ = 20 weight %



Data taken from FToxid - FACT oxide databases

Many Types of Calculations

- **Equilibrium**
- **Scheil-Gulliver** and **Equilibrium Cooling**
- **Casting** software
- **Open** calculations
- **Viscosities** of slags and glasses
- **Streams** and recycling
- **Fact-XML** customized output – tables, spreadsheets, graphs
- **Fact-Function-Builder –** customized functions
- **FactOptimal** – identify the optimal conditions for alloy and process design using thermodynamic and property databases (maximum adiabatic T, minimum liquidus T, density, cost, …)
- Etc.

Scheil-Gulliver cooling of AZ91

i.e. no diffusion in solid phases;

full diffusion in the liquid solution

AZ91 alloy - Al, Zn, Mn, Si

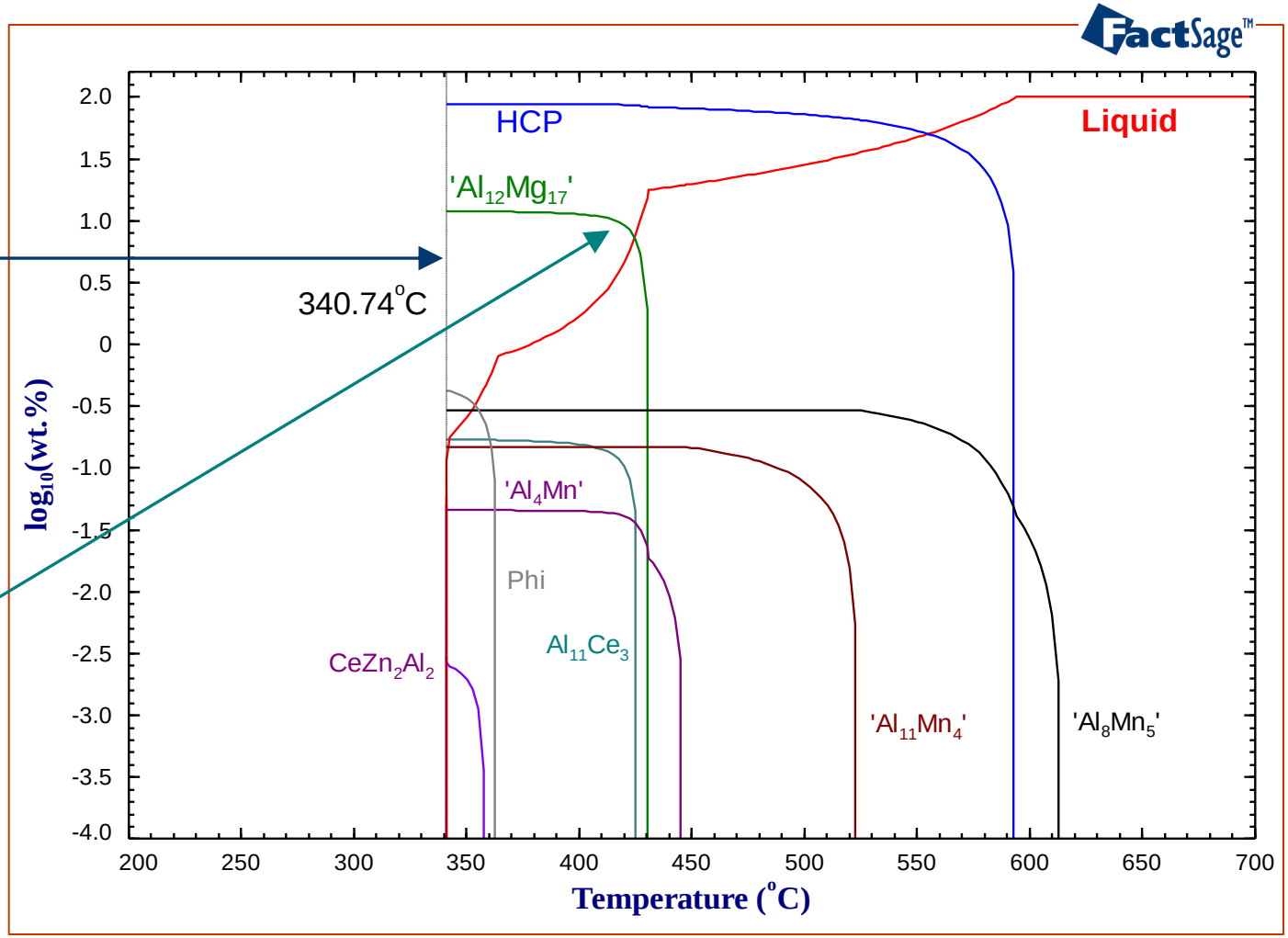
(0.25 wt.% Mn + 50 ppm Fe + 0.1 wt.% Ce)

Data taken from FTlite

- FACT light alloy databases

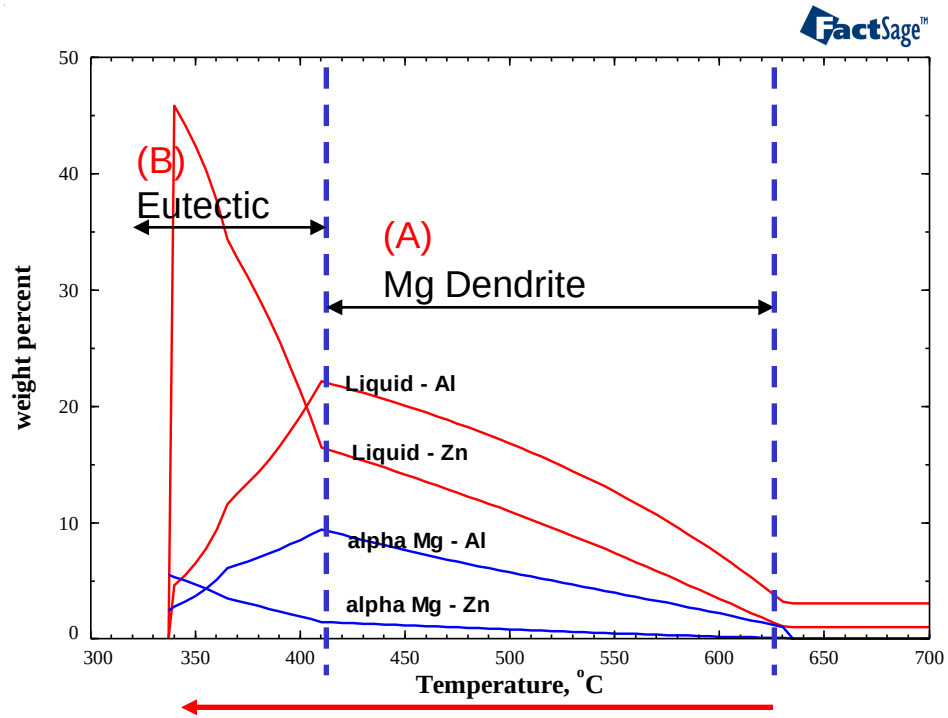
Final solidification at 340.74°C (102°C lower than equilibrium cooling!)

'$Al_{12}Mg_{17}$' forms at higher T and in larger proportion

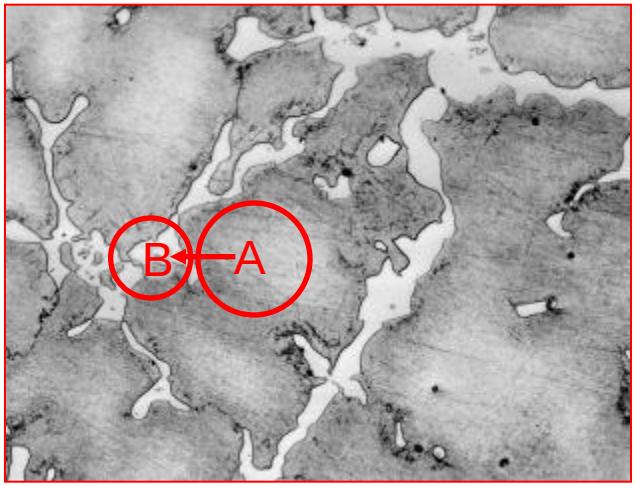


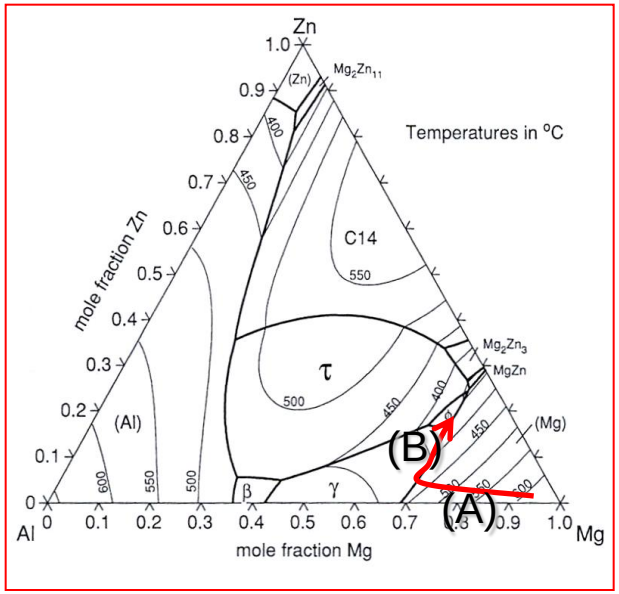
Scheil-Gulliver cooling of AZ31 alloy

-solidification path calculation



Compositional change of dendrites & eutectic area





Solidification software - extended Scheil-Guilliver cooling - casting and post equilibration of Scheil microstructure AZ91 alloy (0.25 wt.% Mn)

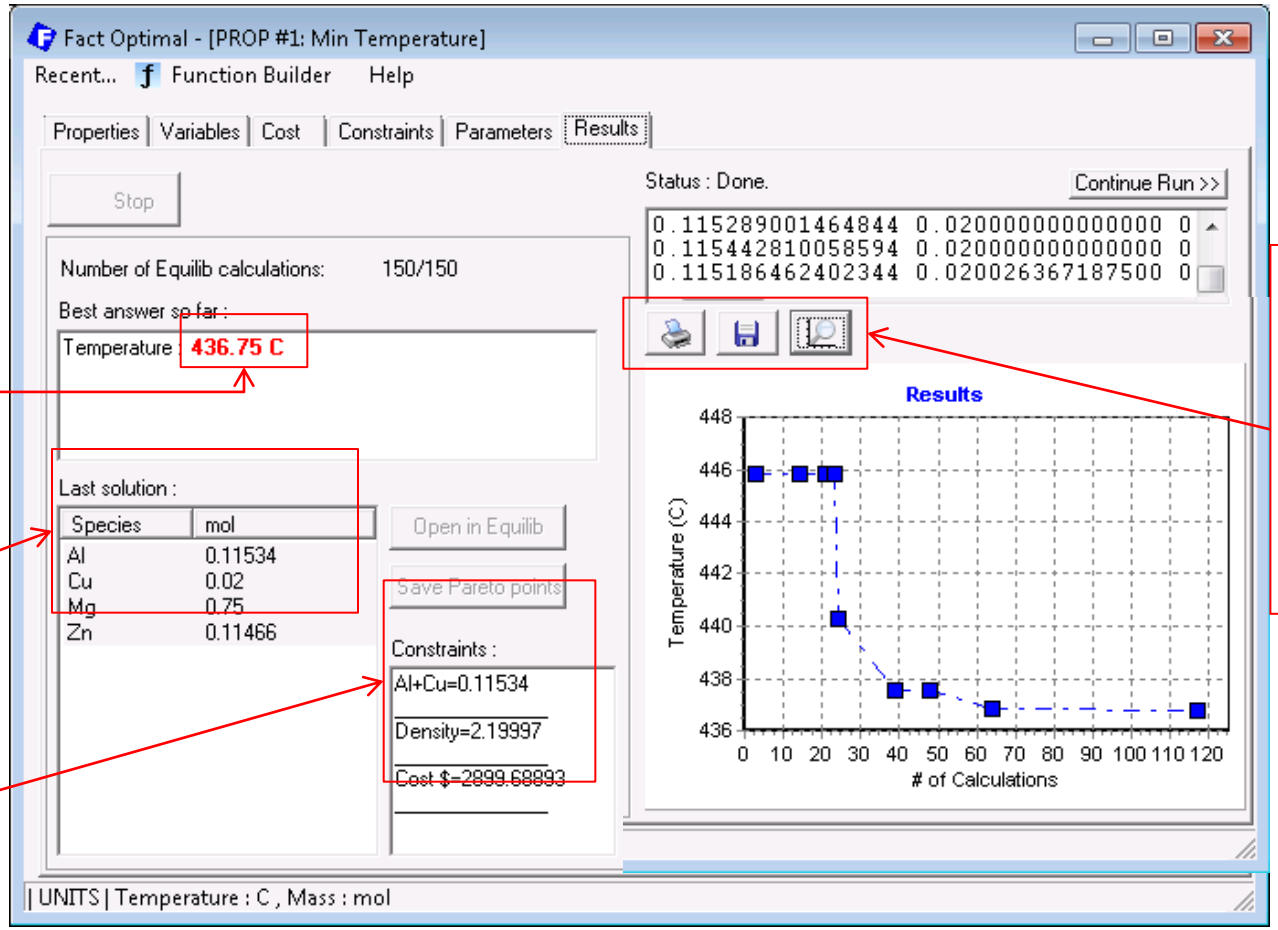
Tracking microstructure constituents

Output : Solidification temperature of 340.89°C

CONS.	PHASE	TOTAL AMT/gram	
1	1 'Al8Mn5'	5.2241E-04	Constituent 1 594.16 to 594.06 C Liq. -> 'Al8Mn5'
2	1 HCP	6.4599E+01	Constituent 2 594.06 to 524.15 C
2	2 'Al8Mn5'	2.8231E-01	Liq. -> HCP + 'Al8Mn5'
3	1 HCP	1.5644E+01	Constituent 3 524.15 to 447.46 C
3	2 Al11Mn4	1.4638E-01	Liq. -> HCP + Al11Mn4
4	1 HCP	1.7084E+00	Constituent 4 447.46 to 431.74 C
4	2 'Al4Mn'	1.7892E-02	Liq. -> HCP + 'Al4Mn'
5	1 HCP	4.9213E+00	Constituent 5 431.74 to 364.34 C
5	2 'Al12Mg17'	1.1878E+01	Liq. -> HCP + 'Al12Mg17' + 'Al4Mn'
5	3 'Al4Mn'	2.6558E-02	
6	1 HCP	1.9669E-01	Constituent 6 364.34 to 342.66 C
6	2 Phi	4.0423E-01	Liq. -> HCP + Phi + 'Al4Mn' + Al11Mn4
6	3 'Al4Mn'	1.7904E-05	
6	4 Al11Mn4	3.8196E-05	
7	1 HCP	2.4177E-02	Constituent 7 342.66 to 340.89 C
7	2 Tau	3.5706E-02	Liq. -> HCP + Tau + Al11Mn4
7	3 Al11Mn4	1.4894E-06	
8	1 HCP	4.2084E-02	Constituent 8 340.89 C (isothermal)
8	2 MgZn	5.1501E-02	Liq. -> HCP + MgZn + Tau + Al11Mn4
8	3 Tau	2.1364E-02	
8	4 Al11Mn4	2.3786E-06	

FactOptimal - identifies the optimal conditions for alloy and process design using thermodynamic and property databases, FactSage software and the Mesh Adaptive Direct Search Algorithm.

Example: locate the minimum liquidus temperature under constraints



Minimum

Composition at the minimum

Values of the chosen constraints

Save and print the graph or change the axis scale

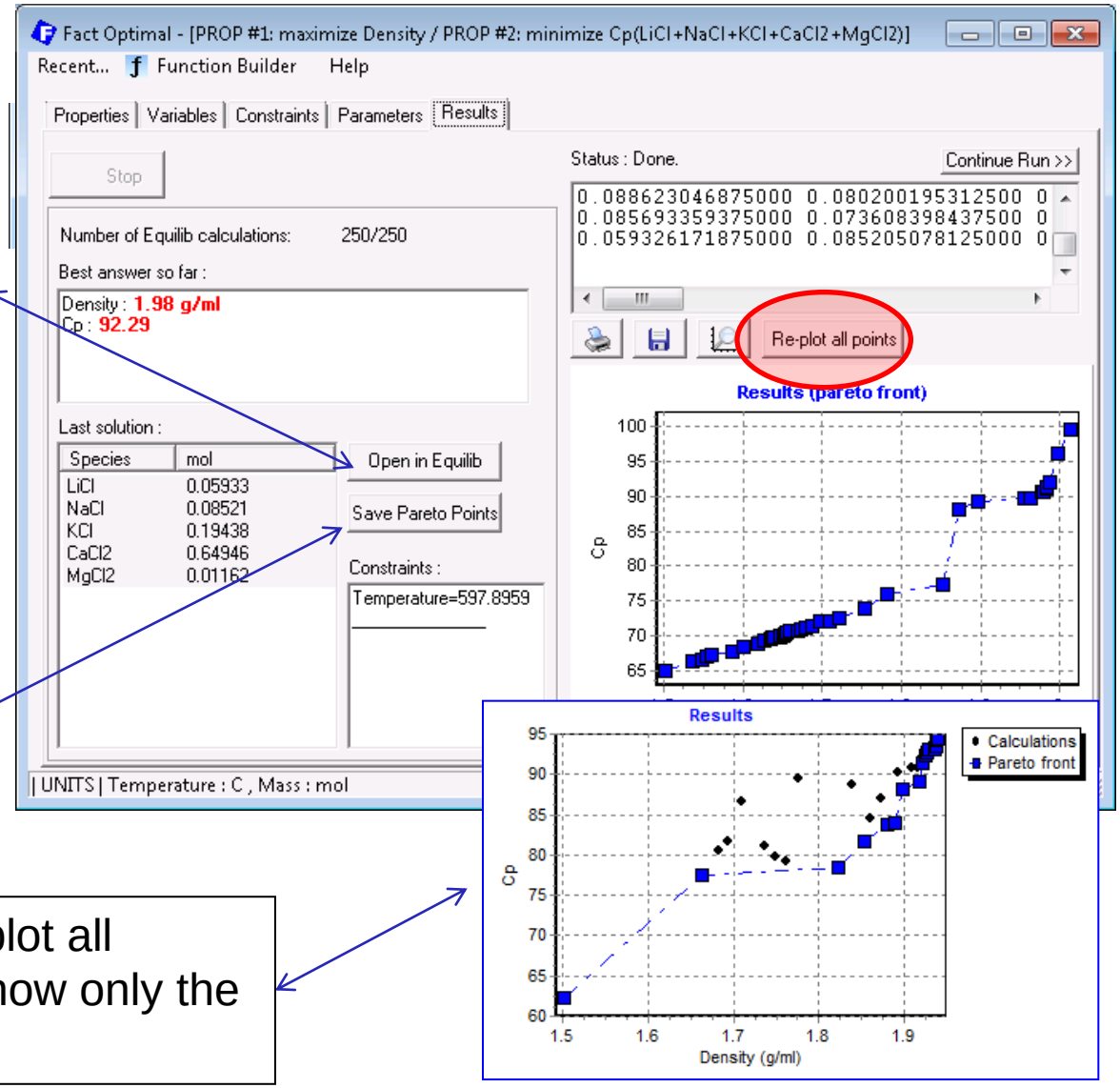
FactOptimal and the Pareto Concept - the simultaneous minimum and/or maximum of more than one function.

Example - minimize the density and maximize Cp under constraints on T-liquidus

One can choose any point on the *Pareto Front* by clicking on it in the graph and and opening it in the **Equilib** module.

The compositions on the *Pareto Front* can be saved and opened in Text, Excel,.....

One can chose to re-plot all calculated points or show only the *Pareto front.*



Many Types of Databases

The FactPS Compound Database

- The FactSage compound (pure substances) database **FactPS** contains data (ΔH^o_{298}, S^o_{298} , Cp(T), ..) for over 4750 compounds taken from standard compilations (such as JANAF) as well as most of the data for those compounds which have been evaluated / optimized.

Many Types of Databases

FToxid - the FACT Oxide Database

- contains data for all pure oxides and oxide solutions (solid and liquid) formed among **Al_2O_3, CaO, FeO, Fe_2O_3, MgO, SiO_2**.

- includes various combinations of the above oxides with oxides of **As_2O_3, B_2O_3, CoO, CrO, Cr_2O_3, Cu_2O, GeO_2, K_2O, Na_2O, MnO, Mn_2O_3, NiO, PbO, SnO, TiO_2, Ti_2O_3, ZnO, ZrO_2**.

- includes data for **Al_2O_3-Re_2O_3** systems, where Re = **La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu**.

The liquid/glass solution phase is called **FToxid-Slag. FToxid-Slag** includes dilute solutions of **S, SO_4, PO_4, H_2O/OH, CO_3, F, Cl, I, C, N, CN**.

FToxid - the FACT Oxide Database

Major Oxide Solid Solutions

- **Spinel:** $(Al, Co^{2+}, Co^{3+}, Cr^{2+}, Cr^{3+}, Fe^{2+}, Fe^{3+}, Mg, Ni^{2+}, Zn)$
  $[Al, Co^{2+}, Co^{3+}, Cr^{3+}, Fe^{2+}, Fe^{3+}, Mg, Ni^{2+}, Zn, \square]_2 O_4$
- **Pyroxenes:** $(Ca, Fe^{2+}, Mg)^{M2} (Fe^{2+}, Fe^{3+}, Mg, Al)^{M1} (Fe^{3+}, Al, Si)^{B} Si^{A} O_6$
- **Olivine:** $(Ca, Fe^{2+}, Mg, Mn, Ni, Co, Zn) [Ca, Fe^{2+}, Mg, Mn, Ni, Co, Zn] SiO_4$
- **Melilite:** $(Ca)_2 [Mg, Fe^{2+}, Fe^{3+}, Al, Zn] \{Fe^{3+}, Al, Si\}_2 O_7$
- **Monoxide:** $CaO - MgO - MnO - CoO - NiO - FeO$
  $(+ Fe_2O_3 - Al_2O_3 - ZnO - Cr_2O_3)$
- **α-Ca_2SiO_4:** α-Ca_2SiO_4 (+ Fe_2SiO_4, Mg_2SiO_4, Mn_2SiO_4)
- **α'-Ca_2SiO_4:** α'-Ca_2SiO_4 (+ Fe_2SiO_4, Mg_2SiO_4, Mn_2SiO_4 , Pb_2SiO_4 , Zn_2SiO_4)
- **Wollastonite:** $CaSiO_3$ (+ $FeSiO_3$, $MgSiO_3$, $MnSiO_3$)
- **Corundum:** $Al_2O_3 - Cr_2O_3 - Fe_2O_3$
- **Ilmenite:** $(Fe^{2+}, Mg, Mn, Ti^{3+}) (Ti^{4+}, Ti^{3+})O_3$
- **Pseudobrookite:** $(Fe^{2+}, Mg, Mn, Ti^{3+}) (Ti^{4+}, Ti^{3+})_2 O_5$
- **26 other solid solutions**

Summary of Databases

Fact *Package:*

FToxid - oxide database for slags, glasses, ceramics, refractories
FTsalt - salt database
FThall - Hall aluminum database
FThelg - aqueous (Helgeson) database
FTmisc - miscellaneous database for sulfides, alloys, etc.
FTpulp - pulp and paper database (also for corrosion and combustion)
FTfrtz - fertilizer database (also for explosives)
FTOxCN - oxycarbonitride high temperature database

Fact *Other databases :*

FTlite - light metal database (formerly FSlite)

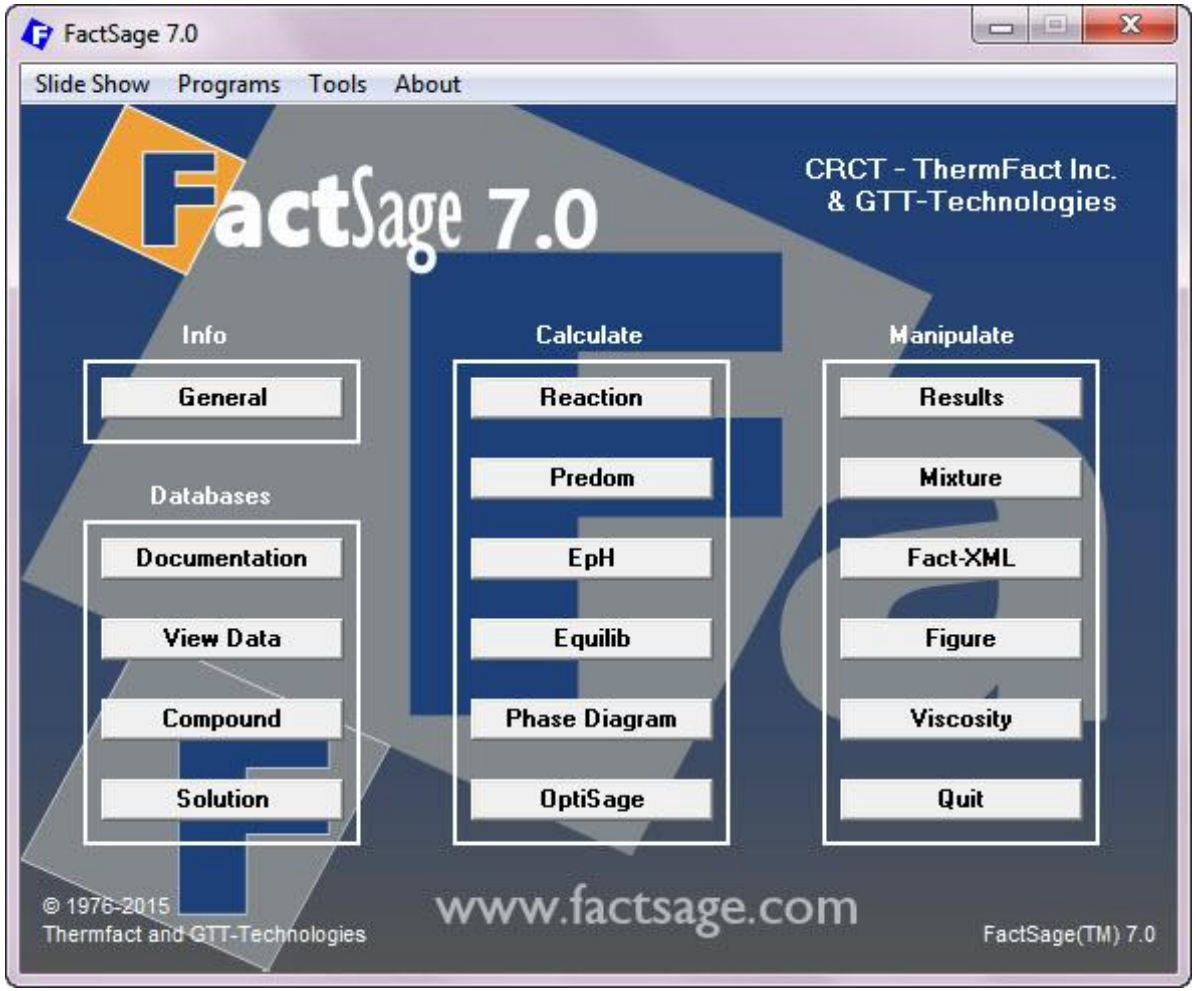
FactSage™ *Databases:*

FScopp - copper alloy database
FSlead - lead alloy database
FSstel - steel database
FSupsi - ultrapure silicon database

SGTE *Databases :*

SGnobl - noble metal database (formerly FSnobl)
SGnucl - nuclear database
SGTE(2011) - alloy database (formerly SGTE (2007))
SGsold - solders database
BINARY - (2004) free alloy database

FactSage Overview



For information visit www.factsage.com