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FactSage thermochemical software and databases, 2010–2016

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ABSTRACT

The FactSage computer package consists of a series of information, calculation and manipulation modules that enable one to access and manipulate compound and solution databases. With the various modules running under Microsoft Windows® one can perform a wide variety of thermochemical calculations and generate tables, graphs and figures of interest to chemical and physical metallurgists, chemical engineers, corrosion engineers, inorganic chemists, geochemists, ceramists, electrochemists, environmentalists, etc. This paper presents a summary of the developments in the FactSage thermochemical software and databases during the last six years. Particular emphasis is placed on the new databases and developments in calculating and manipulating phase diagrams.

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1. Introduction

FactSage began in 1976 as F*A*C*T – *Facility for the Analysis of Chemical Thermodynamics* – a joint research project between McGill University and École Polytechnique de Montréal (Université de Montréal Campus). In 1984 the CRCT – Centre for Research in Computational Thermochemistry/Centre de Recherche en Calcul Thermochimique – was founded at École Polytechnique de Montréal. A principal activity of the CRCT was, and still remains, the promotion and development of the F*A*C*T thermochemical databases and software.

During the 1990s F*A*C*T migrated to personal computers running in a Windows environment. In 2001 there was a fusion between F*A*C*T / FACT-Win and ChemSage (formerly *SOLGASMIX* [1]) resulting in FactSage®. Since then FactSage has expanded into a fully integrated thermochemical software and database package that is used worldwide at over 800 sites in universities, governmental and non-governmental research laboratories and industry.

The original F*A*C*T package was designed to simulate the thermochemistry of pyrometallurgical processing and plot classical binary and ternary phase diagrams. Today FactSage applications include hydrometallurgy, electrometallurgy, corrosion, glass technology, combustion, ceramics, geology, environmental studies, etc. and it can calculate and plot binary, ternary and multicomponent phase diagrams with a wide variety of axes. Forty years ago the turnaround time using a mainframe computer to calculate and print thermochemical tables was measured in hours. Using today's personal computers one can calculate and plot phase diagrams within seconds.

While an understanding of chemical thermodynamics is useful in order to run the modules, it is not essential for a user to be an expert in the field. With practice and the assistance of extensive documentation, one can acquire a practical understanding of the principles of thermochemistry, especially as these relate to complex phase equilibria. Articles on *FactSage Thermochemical Software and Databases* (2002) and *FactSage Thermochemical Software and Databases – Recent Developments* (2009) have been published in the Calphad Journal [2,3]. The reader who is unfamiliar with FactSage is encouraged to consult these original publications. The present article outlines the new databases and developments in calculating and manipulating phase diagrams that have been introduced since the last publication (2009) and briefly describes developments in the programs.

The FactSage main menu (Fig. 1) offers access to the various modules of the package. The modules are grouped into four categories: 1. Info, 2. Databases, 3. Calculate and 4. Manipulate.

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2. Info

The general option gives the user access to the latest slide shows, documentation on FactSage, Macro Processing, FactSage-Teach, What is New in FactSage 7.0, FAQ – Frequently Asked Questions, Information, List of references, FactSage family of products and services, etc. All topics are updated with each release of FactSage.

3. Databases

FactSage provides access to both solution databases and compound databases. The former contain optimized model parameters for the Gibbs energy of solution phases as functions of composition and temperature. The latter contain the properties of stoichiometric compounds (pure substances), either obtained from published experimental data and phase diagram optimizations or taken from standard compilations.

During the past six years most of the databases have been revised and updated and some new ones have been added. The modifications to databases are outlined in the following sections.

3.1. FACT Databases – FactPS, FToxid, FTsalt, FTmisc, FTOxCN, FTfrtz, FTlite, FTnucl, FThall, FThelg, FTpulp

The **FACT** (FT) databases are the result of evaluations/optimizations performed by the FACT CRCT groups in Montreal.

FactPS – (formerly FACT53) now contains pure substances data for 4777 compounds (was 4538 in 2009). It contains data from standard compilations as well as most of the data for those compounds that have been evaluated/optimized to be thermodynamically consistent with the FACT FToxid, FTsalt,… etc. solution databases.

FToxid – is the FACT oxide database for slags, glasses, minerals, ceramics, refractories, etc. It has been extensively updated and now contains data for 374 stoichiometric oxides (was 264) and 87 oxide solutions (was 46). The data are for all pure oxides and oxide solutions (solid and liquid) formed among Al_2O_3, CaO, FeO, Fe_2O_3, MgO, SiO_2 and includes various combinations of the above oxides with As_2O_3, B_2O_3, BaO, CoO, CrO, Cr_2O_3, Cu_2O, GeO_2, K_2O, Na_2O, MnO, Mn_2O_3, NiO, P_2O_5, PbO, SnO, TiO_2, Ti_2O_3, ZnO and ZrO_2. The database also 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 and Lu. The liquid/glass solution phase is called FToxid-Slag and includes dilute solutions of S, SO_4, H_2O/OH, CO_3, F, Cl and I.

For systems containing Ca, Mn, Fe, Mg, Al and Si, FToxid-Slag covers the entire oxysulfide phase from pure oxide to pure sulfide. One such oxysulfide system is CaO–Al_2O_3–CaS(–Al_2S_3), which is a core inclusion system of Al-killed steel followed by Ca injection. Fig. 2 shows the liquidus projection of the CaO–Al_2O_3–CaS system, calculated by the Phase Diagram module. Inclusions found in the

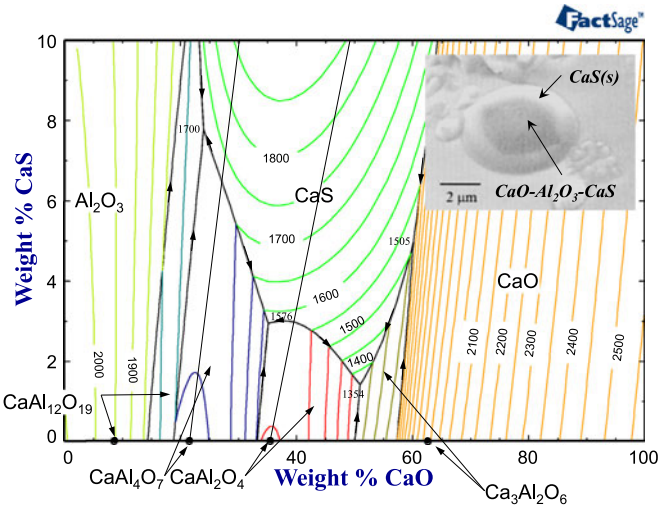


Fig. 2. FTOxid database – calculated liquidus projection of CaO–Al_2O_3–CaS oxysulfide system (FTOxid database) and inclusions found in Al-killed steel followed by Ca injection (inset [4]).

Fig. 1. FactSage 7.0 Main Menu Window.

steel are generally a mixture of liquid oxysulfide and solid CaS as shown by an inset [4] in the same figure. FTOxid-Slag now allows for the calculation not only of the sulfide capacity (dilute S content in liquid oxide slag) but also of the evolution of such oxysulfide inclusions (high S content up to solid sulfide saturation or pure sulfide).

Oxyfluoride systems Ca, Mg, Na, Al, Si//O, F are new additions. The database is reliable for compositions up to 50 mol% fluoride. The database is particularly useful for calculations involving mold fluxes of the continuous steel casting processes and refining slags. For example, the phase diagram of the $CaO–SiO_2–Na_2O–CaF_2$ system is shown in Fig. 3.

Solid and liquid phases of unary, binary and many ternary P_2O_5-containing systems in the $P_2O_5–CaO–MgO–Al_2O_3–SiO_2–BaO–FeO–Fe_2O_3–MnO–Na_2O$ system have been recently updated. The thermodynamic behavior of P in a slag is important for the refining of molten metals and also recycling phosphorus. For example, FactSage can be employed to calculate the equilibrium phosphorus distribution between molten slag and liquid Fe as depicted in Fig. 4. The calculations are in good agreement with experimental data.

FTsalt is the FACT salt database. It has been extensively updated

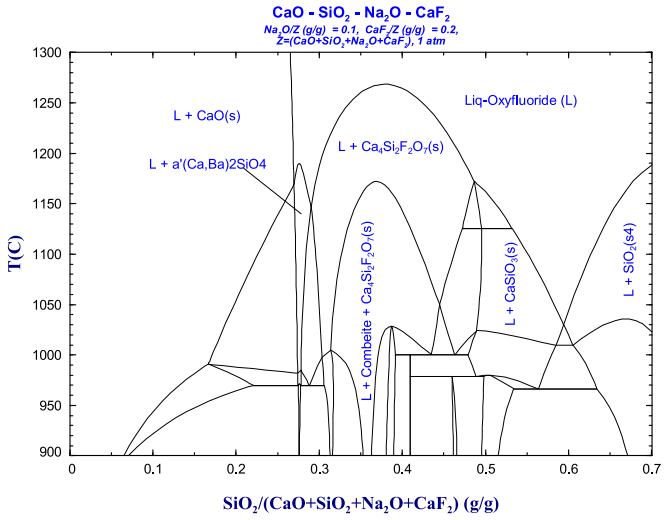


Fig. 3. FTOxid database – calculated phase diagram of the $CaO–SiO_2–Na_2O–CaF_2$ system.

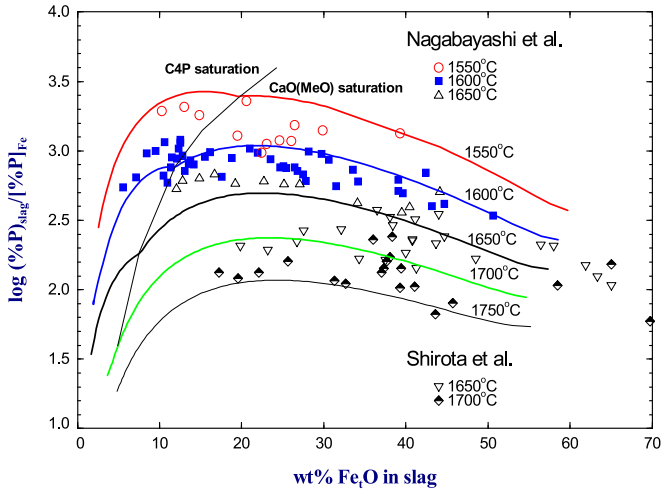


Fig. 4. FTOxid database – employed with the FTmisc database to calculate the equilibrium phosphorus distribution between molten slag and liquid Fe as depicted.

and now contains data for 221 pure salts (was 191) and 79 salt solutions (was 72) formed among various combinations of the 26 cations Li, Na, K, Rb, Cs, Mg, Ca, Sr, Ba, NH_4, Mn, Al, Fe(II), Fe(III), Co, Ni, Zn, Pb, La, Ce, Nd, U, Pu, Th, Cr, Mo and 8 anions F, Cl, Br, I, NO_3, OH, CO_3, SO_4. In particular, it includes the chloro-fluoride system Li, Na, K, Mg, Ca//Cl, F as well as the chloride systems $LiCl–NaCl–KCl–RbCl–CsCl–MgCl_2–CaCl_2–SrCl_2–BaCl_2$ and $LiCl–NaCl–KCl–MgCl_2–CaCl_2–MnCl_2–FeCl_2–FeCl_3–CoCl_2–NiCl_2–AlCl_3$, which may be used as fluxes for metal treatment. The molten salt phase is called FTsalt-Salt and includes dilute solutions of O^{2-} and OH^-. A density model (taking into account excess volume upon mixing) [5] is now available for the $NaCl–KCl–MgCl_2–CaCl_2$, $LiF–NaF–KF–MgF_2–CaF_2$ and $NaCl–KCl–ZnCl_2$ molten salt systems. Approximate density calculations may be performed for larger systems such as Li, Na, K, Mg, Ca//Cl, F. FTsalt is by far the most extensive thermodynamic database on salt systems available.

FTmisc – is the FACT miscellaneous database for sulfides, alloys, etc. All compounds and solutions of the former *Light Metals* subsection of FTmisc have been removed and some minor changes have been carried out. The database includes the following systems: the S–Cu–Fe–Mn–Ni–Co–Cr system; the matte smelting system S–Cu–Fe–Ni–Co–Pb–Zn–As; liquid Fe with dilute solutes Al, B, Bi, C, Ca, Ce, Co, Cr, Mg, Mn, Mo, N, Nb, Ni, O, P, Pb, S, Sb, Si, Te, Ti, V, W, Zn and Zr; liquid Sn with dilute solutes Al, Ca, Ce, Co, Cr, Cu, Fe, H, Mg, Mo, Na, Ni, O, P, S, Se, Si and Ti; liquid Pb with dilute solutes Ag, As, Au, Bi, Cu, Fe, Na, O, S, Sb, Sn, Zn; the Hg–Cd–Zn–Te system; alloy solutions FTmisc–ZnLQ, –CdLQ, –TeLQ, –SbLQ, –SeLQ, –SeTe, –SbPb and –PbSb which are alloy solutions of a limited number of components, valid over limited composition ranges; and non-ideal aqueous solutions of 96 solutes with Pitzer parameters.

FTOxCN – is a new FACT database for oxycarbonitride systems and contains data for performing equilibrium calculations in the Al–(Si–Ca–Mg–Fe–Na)–C–O–N–S system at very high temperatures. Carbonates, cyanides, nitrates, oxidized states of sulfur (e.g. SO_4^{2-}, $S_2O_7^{2-}$, etc.) and polysulfides (e.g. S_2^{2-}, S_3^{2-}, S_4^{2-}, etc.) are assumed not to be stable under high-temperature relatively reducing conditions and are neglected. When Fe is present the database is only valid for reducing conditions. The FTOxCN solution database contains oxycarbonitride solutions and a compatible liquid metallic solution. In particular, the liquid "Slag" phase is treated as a single solution phase containing all 10 elements, valid at all temperatures and over all composition ranges of interest. This phase thus incorporates the high-temperature oxycarbide slag, sulfide-rich liquid and oxide slags which might appear at lower temperatures, oxynitride liquids, etc., all in one solution (with possible miscibility gaps, of course). The FTOxCN compound database contains all stoichiometric solid and liquid oxycarbonitride, sulfide and oxysulfide compounds evaluated/optimized to be thermodynamically consistent with the FTOxCN solution database.

FTfrtz – is a new FACT database used for the production of nitrate-based fertilizers, from hydrous to anhydrous conditions. It can also be used for calculating the thermodynamic properties and phase equilibria in the fertilizer products, and for some explosives. The FTfrtz compound and solution databases contain data for 26 pure salts and 14 salt solutions based on the family of ammonium nitrate (NH_4NO_3), ammonium di-hydrogen phosphate ($NH_4H_2PO_4$), ammonium chloride (NH_4Cl) and ammonium sulfate ($(NH_4)_2SO_4$), fertilizers with additions of their corresponding potassium salts (and in some cases sodium salts). The model covers the addition of up to roughly 50 wt% water.

FTlite – is a new FACT database designed for thermodynamic and phase equilibrium calculations involving Al alloys and Mg alloys. Calculations involving Ti alloys and Li–Na–K mixtures can also be performed but not to the same extent as for Al– and Mg–alloys.

Al Alloys: Ag, Al, As, Au, B, Ba, Be, Bi, C, Ca, Ce, Co, Cr, Cu, Dy, Er, Eu, Fe, Ga, Gd, Ge, H, Hf, Hg, Ho, In, K, La, Li, Lu, Mg, Mn, N, Na,

Nb, Nd, Ni, O, P, Pb, Pr, S, Sb, Sc, Si, Sm, Sn, Sr, Ta, Tb, Ti, Tm, V, W, Y, Yb, Zn and Zr.
Mg Alloys: Ag, Al, B, Ba, Be, Bi, C, Ca, Ce, Cr, Cu, Dy, Er, Eu, Fe, Gd, Ge, H, Ho, In, K, La, Li, Lu, Mg, Mn, Na, Nd, Ni, Pb, Pr, Sb, Sc, Si, Sm, Sn, Sr, Tb, Ti, Tm, V, Y, Yb, Zn and Zr.

A total of 622 binary systems have been evaluated, for most of them over the entire range of composition and for all stable phases. For around 120 of these binary systems only the liquid phase mixing parameters are stored. Several dozen ternary systems have been assessed, and important quaternary systems have also been evaluated. The database contains 200 solution phases and over 1400 pure compounds (with more than 1700 stoichiometric phases counting allotropic forms).

FTnucl – is a new FACT database that has been developed for the nuclear industry. It contains data for pure substances and solutions containing the following elements**: (**Th, U, Np, Pu, Am)+(Zr, Fe, Ru, Ba)+(Li, Na, K, Rb, Cs)+(C, N, O, I)+(He, Ne, Ar, Kr, Xe, Rn). The database can be used for the development of advanced nuclear fuels based on: Th, U, Np, Pu and Am; oxides; carbides, nitrides and carbo-nitrides; metals. It can also be used for estimating the thermodynamic behavior and phase relationships involving fission products based on Cs. I, Zr, Ru, Ba and Rb, and including noble gases and metallic claddings (Fe, Zr, C).

FThall – FACT Hall-Héroult aluminum database remains essentially unchanged. However, a density model, taking into account excess volume upon mixing [6]**,** and a viscosity model [7] are now available for the $NaF–AlF_3–CaF_2–Al_2O_3–LiF–MgF_2$ electrolyte as a function of temperature and composition. Shortly, an electrical (ionic) conductivity model for the same electrolyte will be implemented in the database.

FThelg, FTpulp remain essentially unchanged since 2009. These FACT databases contain, respectively, the Helgeson [8] aqueous database (including solid precipitates and gases) and systems of interest primarily to the pulp and paper industry.

3.2. FactSage alloy databases–FScopp, FSlead, FSstel, FSupsi

FactSage (FS) databases for metallic alloys are the result of evaluations/optimizations by the FactSage groups (FACT, Montreal; GTT Technologies, Aachen; The Spencer Group, Trumansburg NY). For each group of systems there is a corresponding pair of databases – a solution database and a compound database – containing data for solutions and compounds which have been evaluated and optimized together.

FScopp – copper alloy database is directed primarily to the liquid state of Cu-rich alloys and includes the elements: Ag, Al, As, Au, Ba, Be, Bi, C, Ca, Cd, Ce, Co, Cr, Fe, Ga, Ge, In, Li, Mg, Mn, Nb, Nd, Ni, O, P, Pb, Pd, Pt, Pr, S, Sb, Se, Si, Sm, Sn, Sr, Te, Ti, Tl, V, Y, Zn, Zr and also includes data for Cu-rich solid phases. The database is generally valid for the temperature range of approximately 400–1600 °C. Minor revisions have been performed and modifications have been carried out that simplify solution phase selection.

FSlead – lead alloy database is directed primarily to the liquid state of Pb-rich alloys and includes the elements: Ag, Al, As, Au, Bi, C, Ca, Cd, Cu, Fe, Ga, Ge, Hg, In, Mn, Ni, O, Pd, S, Sb, Se, Si, Sn, Sr, Te, Tl, Zn, and Zr. It also includes data for Pb-rich solid phases. It permits the calculation of the complete Pb binary systems with all the above elements with the exception of the Pb–Fe, –Mn, –S, –Se and –Sr binary systems. It is intended to provide a sound basis for calculations relating to lead production and refining. Minor revisions have been performed (Cd–Pb system) and modifications have been carried out that simplify solution phase selection.

FSstel – steel database has been extensively updated and now contains data for 140 (was 115) completely assessed binary alloy systems, 100 (was 85) ternary and 17 quaternary systems that include the elements: Al, B, Bi, C, Ca, Ce, Co, Cr, Cu, Fe, La, Mg, Mn, Mo, N, O, Nb, Ni, P, Pb, S, Sb, Si, Sn, Ti, V, W and Zr. It is intended to provide a sound basis for calculations covering a wide range of steelmaking processes, e.g. reduction of oxygen and sulfur concentration levels through deoxidation and desulphurization of the melt; constitution of a wide range of steels, including austenitic, ferritic and duplex stainless steels and including carbide and nitride formation; conditions for heat treatment operations to produce a desired constitution; conditions for scrap remelting to maintain as low concentrations as possible of undesirable “tramp elements”; melt-crucible interactions, etc.

FSupsi database for ultrapure silicon remains essentially unchanged.

3.3. SGTE databases – SGPS, SGTE, SGnobl, SGnucl, SGsold, BINARY

The following **SGTE** (SG) databases were prepared by the **SGTE International Consortium** (http://www.sgte.org) and are available in **FactSage**.

SGTE 2014 – alloy database is new and represents a significant update and revision of the previous SGTE 2007 and SGTE 2011 databases. The 78 elements included in the database are: Ag, Al, Am, As, Au, B, Ba, Be, Bi, C, Ca, Cd, Ce, Co, Cr, Cs, Cu, Dy, Er, Eu, Fe, Ga, Gd, Ge, Hf, Hg, Ho, In, Ir, K, La, Li, Lu, Mg, Mn, Mo, N, Na, Nb, Nd, Ni, Np, O, Os, P, Pa, Pb, Pd, Pr, Pt, Pu, Rb, Re, Rh, Ru, S, Sb, Sc, Se, Si, Sm, Sn, Sr, Ta, Tb, Tc, Te, Th, Ti, Tl, Tm, U, V, W, Y, Yb, Zn and Zr. From among these elements, there are some 577 completely assessed binary alloy systems, of which over 32 are newly assessed systems and many others have been revised or amended on the basis of newly published experimental information. The database also includes about 141 ternary and 15 higher-order systems for which assessed parameters are available for phases of practical relevance. The systems now incorporate approximately 317 different solution phases and 1166 stoichiometric intermetallic compound phases. The database is intended to provide a sound basis for calculations relating to the production, heat treatment, constitution, and application of a wide range of alloy types.

SGnobl – noble metal database has been extensively updated and now contains 124 solutions (was 53) and 362 compounds (was 105). The database contains evaluated thermodynamic parameters for 223 binary and 130 ternary alloys of Ag, Au, Ir, Os, Pd, Pt, Rh, Ru alloyed amongst themselves and also in alloys with the metals Al, As, B, Ba, Be, Bi, C, Ca, Cd, Ce, Co, Cr, Cu, Dy, Fe, Ge, Hf, In, Mg, Mo, Nb, Ni, Pb, Re, Sb, Si, Sn, Ta, Tc, Te, Ti, Tl, V, W, Zn and Zr. Noble metals and their alloys have a wide variety of applications, and calculations of relevant phase equilibria in a particular case are important e.g. for optimizing suitable alloy compositions or predicting reaction products in chemically aggressive environments.

BINARY 2014 – free alloy database is the new SGTE free binary alloy database and comprises some 115 of the binary systems taken from the SGTE 2014 alloy databases.

SGPS, the SGTE pure substance database, **SGnucl**, the database for applications in the nuclear industry, and **SGsold**, the solder database, remain essentially unchanged since 2009.

3.4. Other Databases – SpMCBN, TDmeph, TDnucl

SpMCBN - the Spencer Group Non-Oxide Refractories Database, is new and contains assessed thermodynamic parameters for binary and ternary alloys of high-temperature materials containing carbon, nitrogen, boron, and silicon. The alloys include Me1–Me2–C, Me1–Me2–N, Me1–Me2–B, Me1–Me2–Si, Me–C–N, Me–C–B, Me–C–Si, Me–N–B, Me–N–Si and Me–B–Si systems. It includes the elements B, C, N, **Si** with Al, Ca, Co, Cr, Fe, Hf, Mg, Mn, Mo, Nb, Ni, Re, Sc, Ta, Tc, Ti, V, W, Y and Zr. While no data for oxide systems have been included in the database, a number of the elements

listed above are important in refractory oxide materials. Reactions of the carbide, nitride, boride and silicide systems with such refractory oxides and with oxygen-containing gas atmospheres can be calculated using FactSage by selecting the SpMCBN database together with appropriate combinations of the FToxid, FactPS and SGPS databases for the materials in question. Some application examples are in furnace construction, high-temperature coatings, cutting tools, abrasives, aircraft brake linings, rockets, jets, turbines, and nuclear power plants.

TDmeph – the MEPHISTA database for a new generation of nuclear fuels from IRSN in Cadarache, France. MEPHISTA–*Multiphase Equilibria in Fuels via Standard Thermodynamic Analysis* – is a

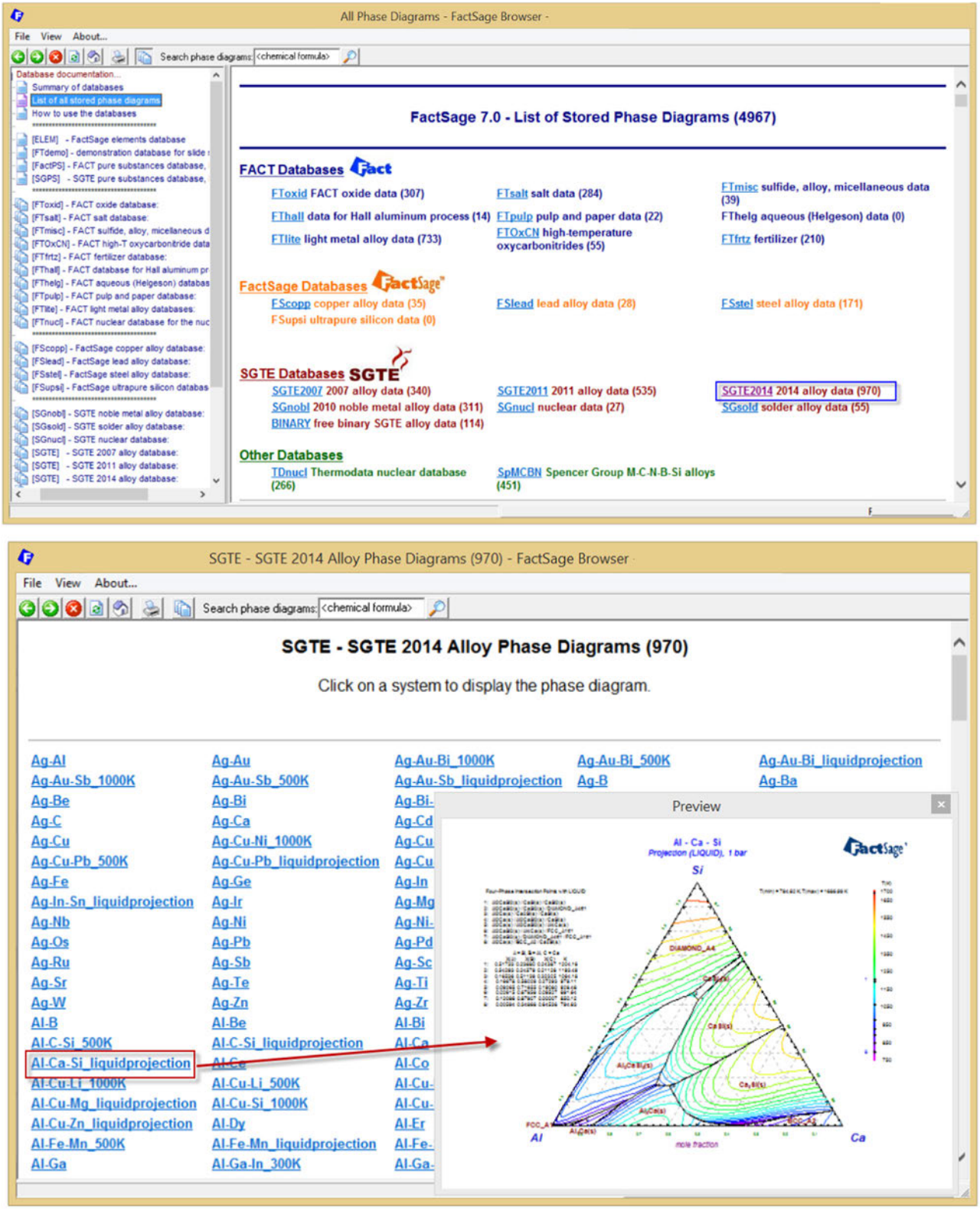


Fig. 5. FactSage Browser module – list of stored phase diagrams; summary of figures and display of the Al–Ca–Si liquidus polythermal projection taken from the **SGTE 2014** database.

self-consistent database designed for thermochemical equilibria calculation codes. It contains 14+2 elements: Ba–C–Ce–Cs–Fe–La–Mo–O–Pu–Ru–Si–Sr–U–Zr+Ar–H (Ar and H are only taken into account in the gas phase). This database covers the entire field from metal to oxide domains, and the temperature range up to 3500 K. 78 binary, 34 quasi-binary, 18 ternary, 2 quasi-ternary systems, 219 condensed stoichiometric compounds and 151 gaseous species are included in the database.

TDNucl – another database for the nuclear industry remains essentially unchanged.

3.5. Documentation

The **Documentation** opens the **FactSage Browser** and enables one to manipulate the database help files and display the phase diagram previews. The *List of stored phase diagrams* posted in the **FactSage Browser** has been updated to 4967. For example, Fig. 5 lists the calculated phase diagrams in the **SGTE 2014** database and shows the calculated Al–Ca–Si liquidus polythermal projection.

3.6. Compound and Solution Modules

Thermodynamic data can be stored in private compound and solution databases via the **Compound** and **Solution** modules.

In **FactSage 7.0** the solution file structures have been completely reformatted. The old solution files (***.dat**, ***.sdb**, ***.sda**) have been replaced by two new files (***.sln**, ***.sdc**). The **Solution** module has been completely rewritten and replaces the old module that was programmed over a decade ago.

With the new **Solution** module, data can be entered and stored using the following solution models: One-sublattice polynomial model (simple, Redlich-Kister or Legendre polynomials with interpolations to multicomponent systems using Muggianu, Kohler or Toop methods), Compound Energy Formalism with up to 5 sublattices [9], Two-sublattice polynomial model with or without short-range-ordering [10], One-sublattice Modified Quasichemical Model [11,12], Two-sublattice Modified Quasichemical Model including coupling between first- and second-nearest-neighbor short-range-ordering [13], Ionic Liquid Model [14], Unified Interaction Parameter Formalism (corrected Wagner formalism) [15], and the Pitzer model. Data can also be entered for magnetic and volumetric (density, expansivity, compressibility) properties.

Data are entered by via a highly flexible user interface that offers extensive editing capabilities. For example Fig. 6 displays the expanded tree-views of a private solution database with access to the *Functions* and solution phase *Sublattices*, *End Members* and *Interactions*. Fig. 7 shows the entry of a *ternary Redlich–Kister parameter* in the Al–Sn–Zn system.

The **Solution** module has other new features which include:

- expressions of Gibbs energy for solution end-members can be imported from a compound database and stored as functions within the new solution database. The required expressions are selected using the **Compound** module then imported by *drag and drop* into the **Solution** module.
- stored functions in the database are accessible to all solution phases within that database.

3.7. View Data Module

The **View Data** module displays a summary of the thermochemical data stored in the solution and compound databases. The data may be sorted and displayed in a variety of formats.

Previously it was not possible to list all the phases in a solution database. In **FactSage 7.0** the search option for all elements is now included. With the new *Sort Solutions* dropdown menu it is also possible to display all the solutions and sort the phases: by phase number, alphabetically (see Fig. 8), by number of species, by number of elements, or by solution model number, with restrictions on the output list all species, do not list all species. It is also possible to display

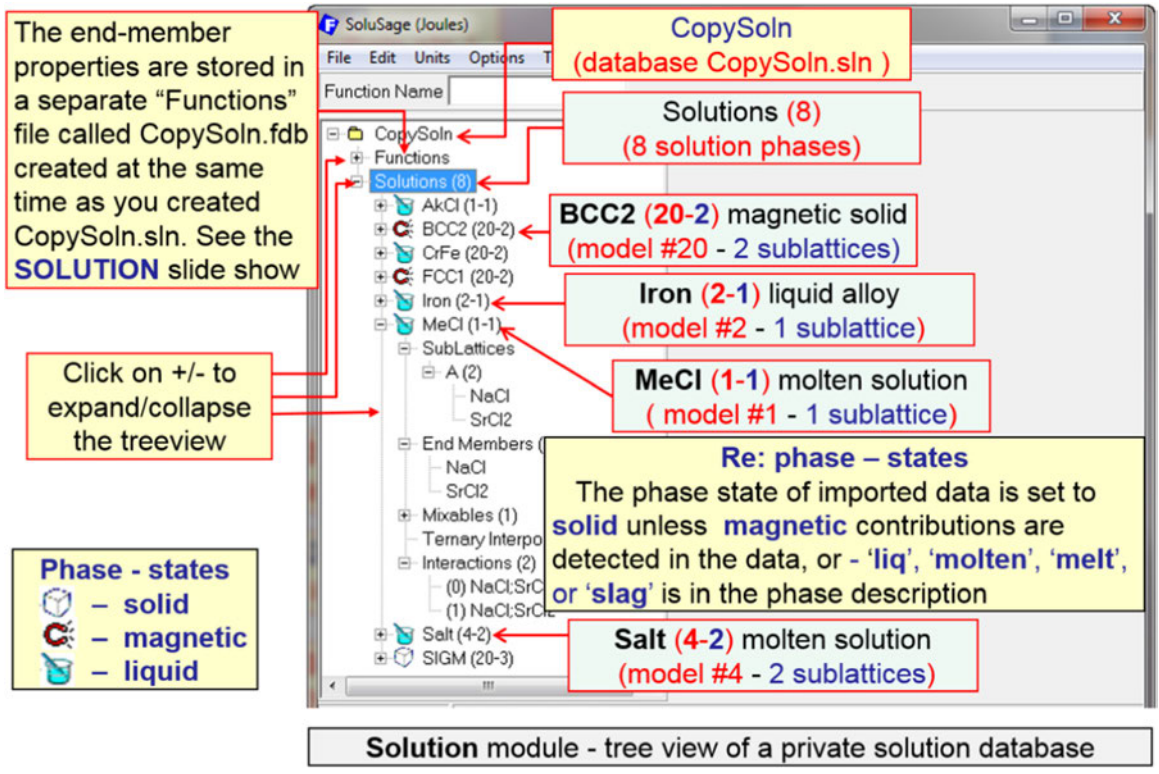
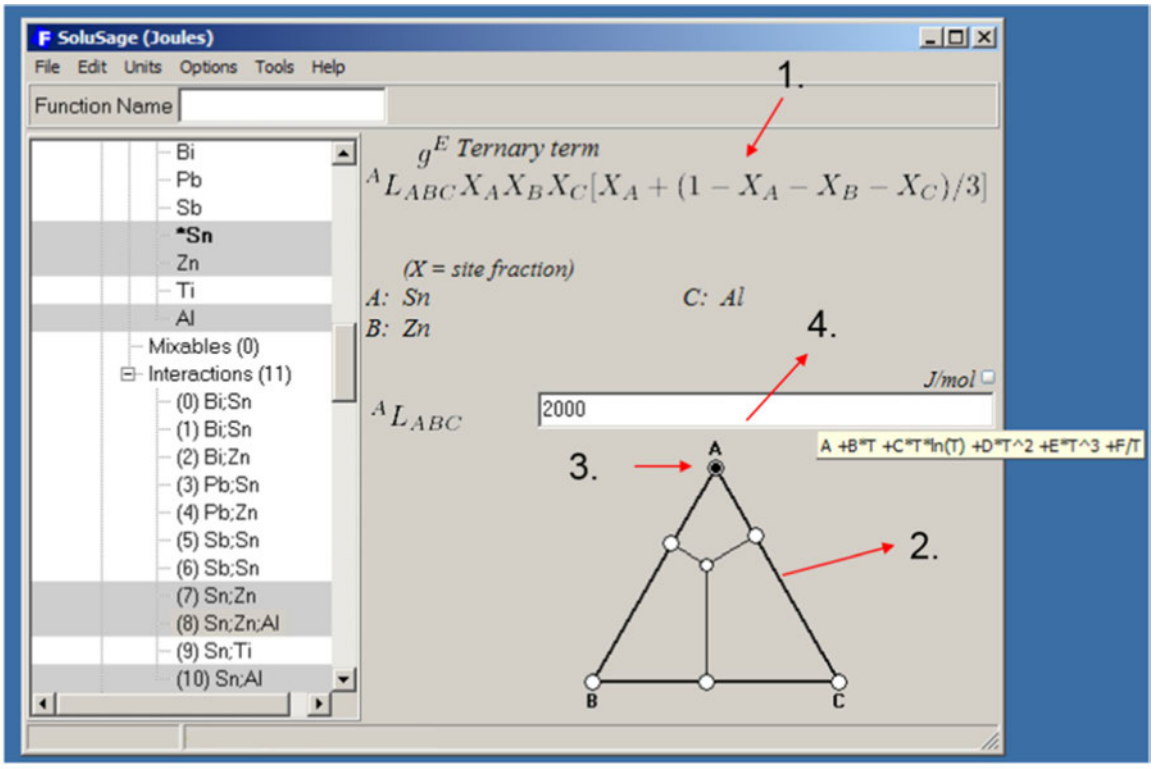


Fig. 6. Solution module – expanded tree-views of data stored in a private solution database.



1. In this model, ternary parameters are expressed by the « Redlich-Kister » equation.
2. The diagram reminds you that the «All Muggianu» configuration is used.
3. Click on the A-corner to enter the $^A L_{ABC}$ term as shown.
4. Enter the parameter (as a function of T in general).

Fig. 7. Solution module – entry of a *ternary Redlich-Kister parameter* in the Al–Sn–Zn system.

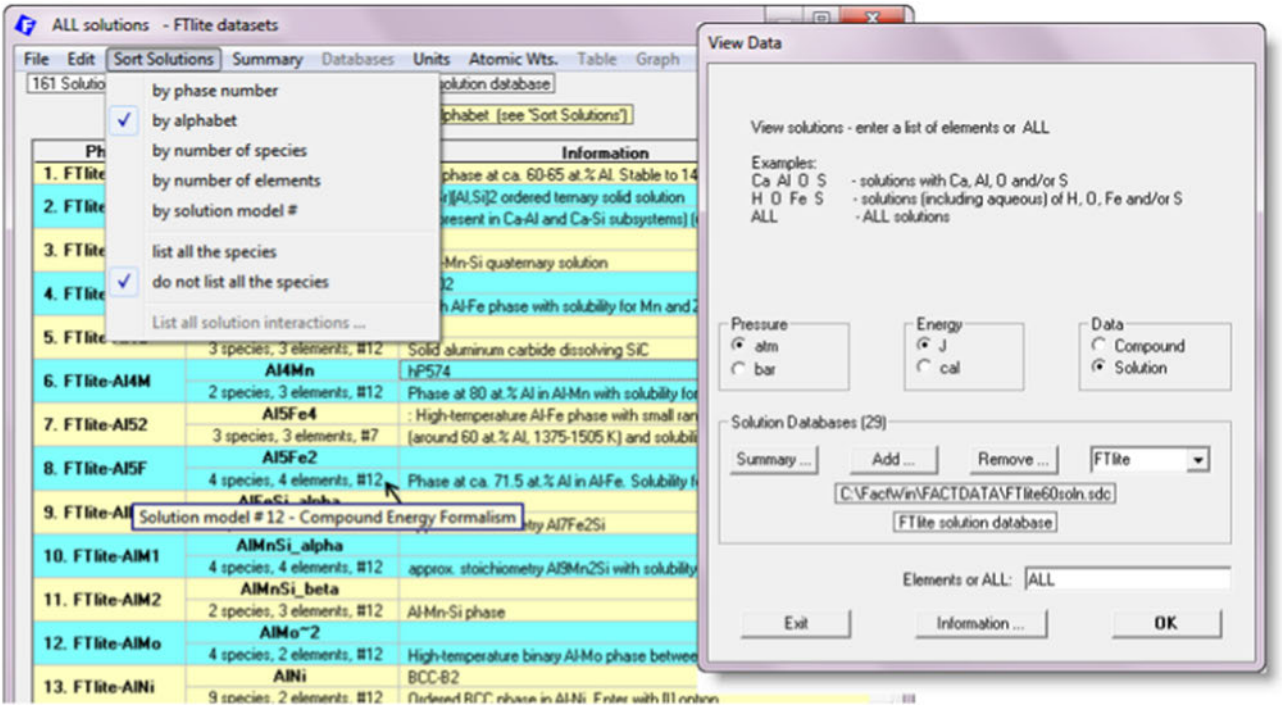


Fig. 8. View Data module – list of all solution phases in the **FTlite** database ordered by alphabet.

the solution data (interactions and expressions) that have been stored in a private database.

4. Calculate

This group of modules is at the heart of FactSage. One can interact with the software and databases in a variety of ways and calculate and display thermochemical equilibria and phase diagrams in a multitude of formats. Major modifications have been carried out on the Equilib and Phase Diagram modules.

4.1. Equilib Module

The **Equilib** module is the Gibbs energy minimization workhorse of FactSage. The **Equilib** module calculates the conditions for multi-phase, multicomponent equilibria, with a wide variety of tabular and graphical output modes, under a large range of possible constraints through Gibbs energy minimization based on the **ChemApp** algorithm [16]. There are many different types of **Equilib** calculations, for example:

- **Equilibrium** using thermochemical data from single or multiple databases
- **Scheil–Gulliver** and **Equilibrium Cooling**
- **Casting** algorithms
- **Open** calculations
- **Simulation** of processes – Macro Processing
- **Streams** and recycling
- **Fact-XML** customized output – tables, spreadsheets, graphs
- **Fact-Function-Builder –** customized functions
- **FactOptimal** – identifying the optimal conditions for alloy and process design using thermodynamic and property databases

4.2. Equilibrium cooling and Scheil–Gulliver cooling

Equilib performs both **Equilibrium cooling** and **Gulliver–Scheil cooling** calculations. In **Equilibrium cooling** the total mass balance remains constant. In **Gulliver–Scheil cooling**, as phases precipitate from the **Scheil target phase**, they are dropped from the total mass balance.

Generally a value for T (the initial temperature) and a cooling step size must be specified in the **Final Conditions** frame. In **Gulliver–Scheil cooling** the *Scheil* calculation is repeated until the *Scheil Target Phase* disappears. However, it is possible to stop the calculation by either specifying a second temperature in the Final Conditions frame, or by specifying a target mass. The *Scheil target phase* must be the gas phase or a real solution.

Fig. 9 shows the **Equilib** setup for a **Scheil cooling** calculation of a AZ91+0.25 wt% Mn alloy **(FTlite-Liqu).** All possible 26 solution phases as well as 42 solid compounds (pure substances) are included in the phase selection as possible products. The 'cooling-step' is 5 K. The results (Fig. 10) give a *Summary* of all the constituents and phases at the final disappearance of the liquid (340.89 °C) as well as a list of the *Transitions* during cooling. A more detailed list of *Microstructure constituents* is given in Fig. 11.

4.3. FactOptimal Module

The **FactOptimal** module [17] is accessed through the **Equilib** module. **FactOptimal** is a new program that computes optimal conditions for material and process design by coupling FactSage with the Mesh Adaptive Direct Search (MADS) [18] algorithm for nonlinear optimization developed by the GERAD research group at the Ecole Polytechnique de Montréal. **FactOptimal** was developed in part to assist industry in optimizing alloy and process design.

FactOptimal minimizes and/or maximizes a set of functions: $\{f1(x1,x2\ldots T,P); f2(x1,x2\ldots T,P)\}$ where

- the functions f (e.g. T, P, V, heat, mass, density, conductivity,…)

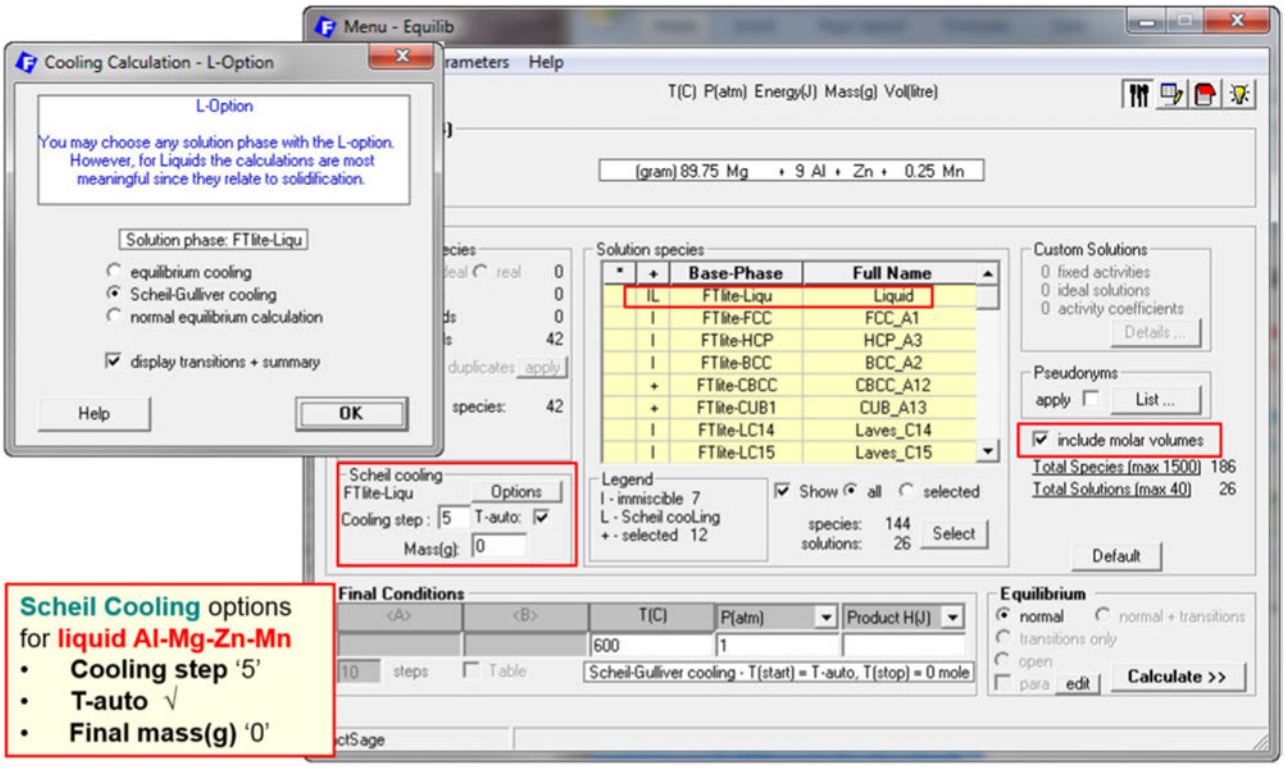


Fig. 9. Equilib module – setup in the Menu Window for a Scheil cooling calculation of a AZ91+0.25 wt% Mn liquid alloy using data from FTlite.

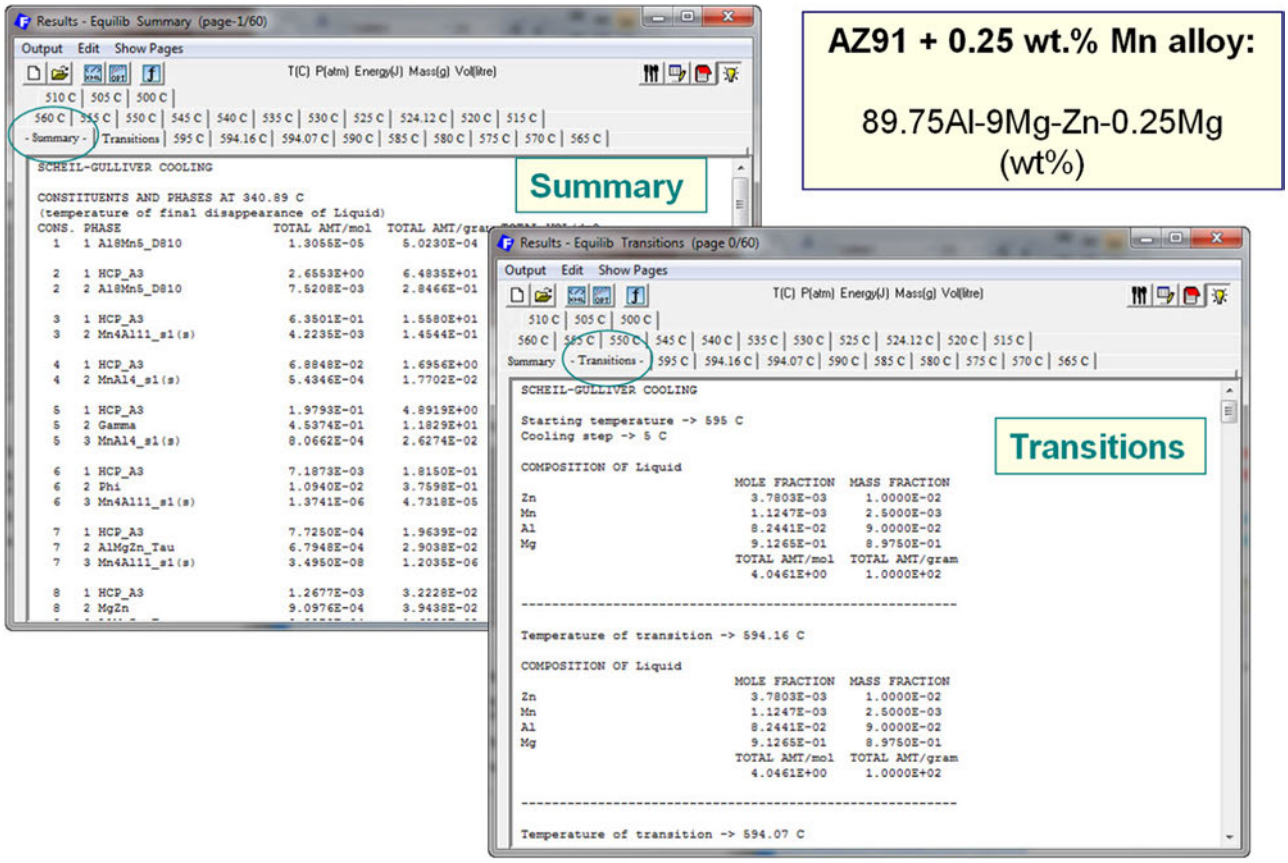


Fig. 10. Equilib module – Results Window summary of all the constituents and phases at the final disappearance of the liquid and list of the Transitions during cooling.

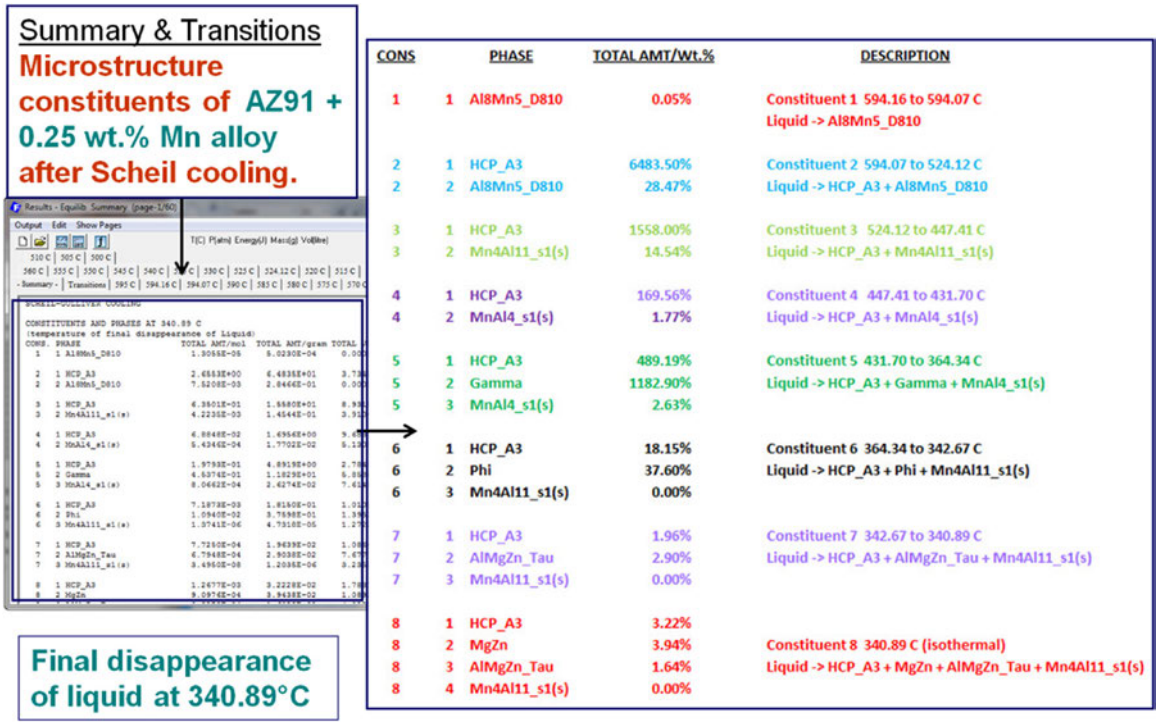


Fig. 11. Equilib module – Results Window and detailed list of Microstructure constituents.

are calculated by **Equilib**
- the functions may be non-smooth (e.g. liquidus temperature)
- the estimation of derivatives may be problematic
- the evaluations of *f* may be time-consuming
- the function calculation may fail unexpectedly at some points
- the constraints may be non-linear, non-smooth or Boolean

4.4. FactOptimal example–minimum liquidus temperature

Fig. 12 shows the *FactOptimal Results Window* for the calculation of the minimum liquidus temperature of the LiCl–NaCl–KCl–LiF–NaF–KF system using data from the FTsalt database. During the calculation various constraints on composition, density, Cp and cost were imposed. After 895 calculations **FactOptimal** determined the minimum liquidus temperature of 577.39 °C at 0.037 wt% LiCl + 41.909 wt% NaCl + 28.505 wt% KCl + 9.963 wt% LiF + 14.156 wt% NaF + 5.430 wt% KF.

The following steps show how **FactOptimal** arrives at this minimum liquidus temperature.

Step 1: Equilib module – Fig. 13 shows the *Equilib Menu Window* for a single equilibrium calculation at an arbitrary composition for the system LiCl–NaCl–KCl–LiF–NaF–KF. A precipitate (P) calculation on the liquid is specified (i.e. liquidus temperature calculation) and "include molar volumes" is checked (for the calculation of the density). The equilibrium results in Fig. 14 show the calculated precipitate (liquidus) temperature 658.73 °C for this arbitrary composition. Although these particular results are unimportant, the *Menu Window* setup is essential for the next stage where **FactOptimal** is opened.
Step 2: in the *FactOptimal Properties Window* (Fig. 15) the following conditions are imposed: (1) one considers one property; (2) one wants to minimize this property; (3) the property is temperature; (4) the cost is included in the optimization.
Step 3: in the *FactOptimal Variables Window* (not shown) the permissible composition range and a set of initial estimates are defined.
Step 4: in the *FactOptimal Constraints Window* (not shown) are defined the *Composition constraints* on properties (1) total amount 1 kg (1000 g); (2) compositions $g(LiCl)+g(LiF) \leq 100$; (3) $g(NaCl)+g(KCl) \geq g(NaF)+g(KF)$.
Step 5: in the *FactOptimal Constraints Window* (not shown) are defined the *Property constraints* (4) density < 1750 kg/m^3; (5) Cp ≥ 1250 J/kg; (6) cost ≤ 5.5 $/kg.
Step 6: in the *FactOptimal Parameters Window* (not shown) are defined the maximum number of Equilib calculations (1000). The results were shown in the *FactOptimal Results Window* (Fig. 12).

4.5. FactOptimal example–characteristic points in a reciprocal system

FactOptimal is able to calculate the compositions of eutectics, temperature minima and congruent melting points of a multicomponent system. These are referred to as the *characteristic points* on the liquidus surface. This option is straightforward to apply and no initial parameters are required. The calculated *characteristic points on the liquidus surface* in the Li^+, Na^+, K^+, Mg^{++}, Ca^{++}/F^-, Cl^- reciprocal salt system (a system with 2 or more cations and 2 or more anions) are shown in Fig. 16. The complete details of equilibrium for any particular point can be obtained by selecting *Open in Equilib.*

4.6. FactOptimal example–optimizing two properties: minimize the liquidus temperature and minimize the solid fraction 200 °C below the liquidus

With the aid of the *FactOptimal Properties Window* (not shown) it is possible to minimize both the liquidus temperature and the solid fraction 200 °C below the liquidus for the oxide system $MgO–Al_2O_3–CaO–PbO–ZnO–SiO_2$. Fig. 17 shows the results and a plot of solid fraction vs. liquidus temperature. When simultaneously optimizing two properties P1 (solid fraction) and P2 (liquidus temperature) there are an infinite number of solutions, that is there is no unique composition where both solid fraction and liquidus temperature are minimized. The calculated **Pareto** front consists of the points shown in Fig. 17. At any selected temperature a point on the Pareto front gives the minimum solid fraction and at any selected solid fraction a point on the Pareto front gives the minimum liquidus temperature. The user must select a value on the **Pareto** front that, in his judgment, is the "best" compromise.

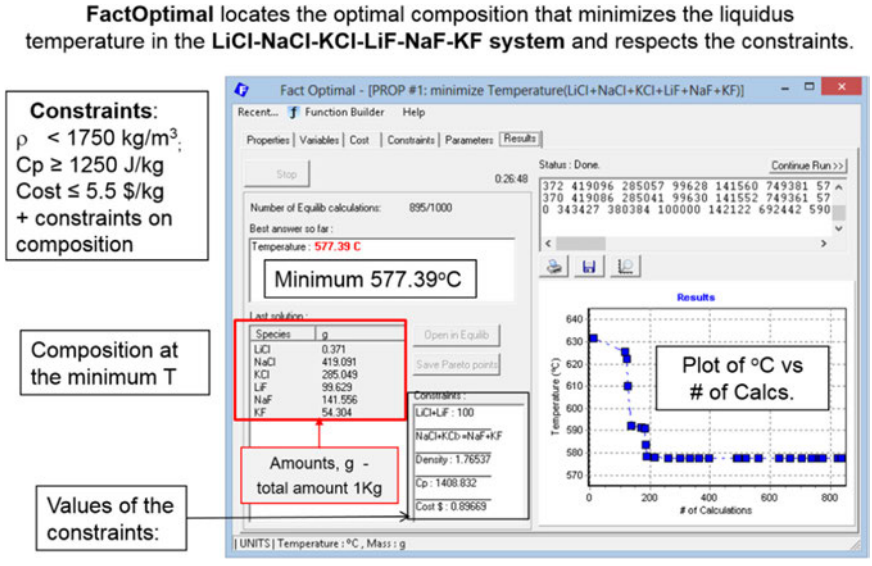


Fig. 12. FactOptimal module – Results Window showing the calculation of the minimum liquidus temperature in the LiCl–NaCl–KCl–LiF–NaF–KF system under constraints of composition, density and cost.

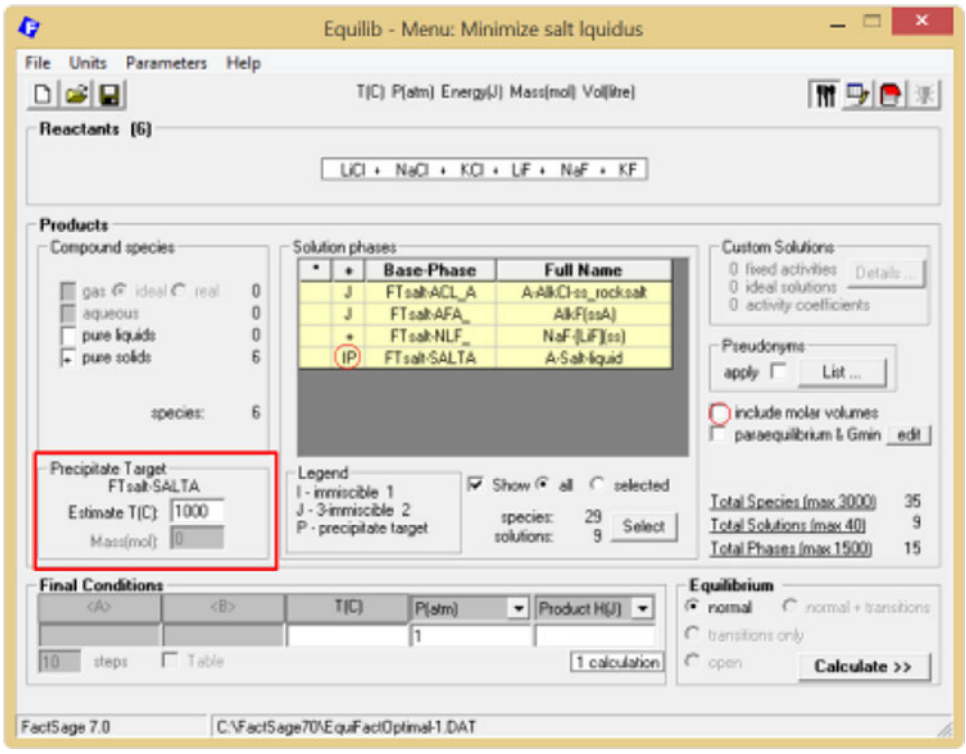


Fig. 13. Equilib module – *Equilib Menu Window* for a single equilibrium liquidus temperature calculation at an arbitrary composition in the LiCl–NaCl–KCl–LiF–NaF–KF system.

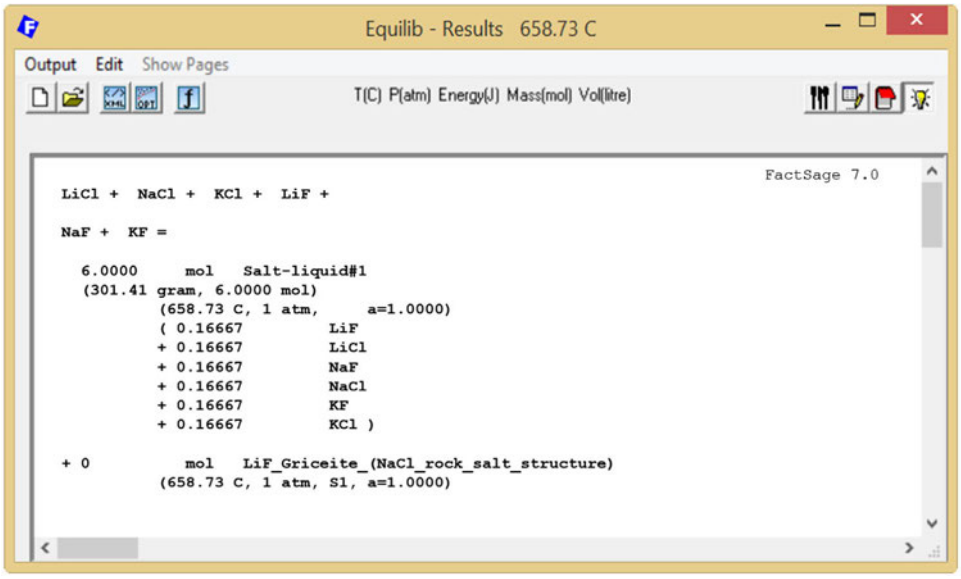


Fig. 14. Equilib module – *Equilib Results Window* for Fig. 11 in the LiCl–NaCl–KCl–LiF–NaF–KF system.

4.7. FactOptimal example–double target optimization

With **FactOptimal** one can calculate the optimal composition to target two properties under constraints of compositions and/or properties. For example, one can calculate the composition of the $MgO–Al_2O_3–CaO–PbO–ZnO–SiO_2$ oxide system while fixing, within a given tolerance, the liquidus temperature and the solid mass fraction 200 °C below the liquidus temperature. Fig. 18 shows the results and a plot of error in mass fraction vs. error in composition.

More *FactOptimal examples* of industrial applications are given in [19,20].

4.8. Viscosities of oxide melts

The viscosity of oxide melts can vary by orders of magnitude depending upon the composition and temperature and it is strongly related to the connectivity of the silica network. The connectivity of the network (which is related to the probability of Si–O–Si bridges) can be calculated from the *Modified Quasichemical Model* [11,12] parameters for FToxid, the FactSage thermodynamic database for molten oxides.

The parameters of the viscosity model are obtained by critical evaluation and optimization of data for pure oxides and selected

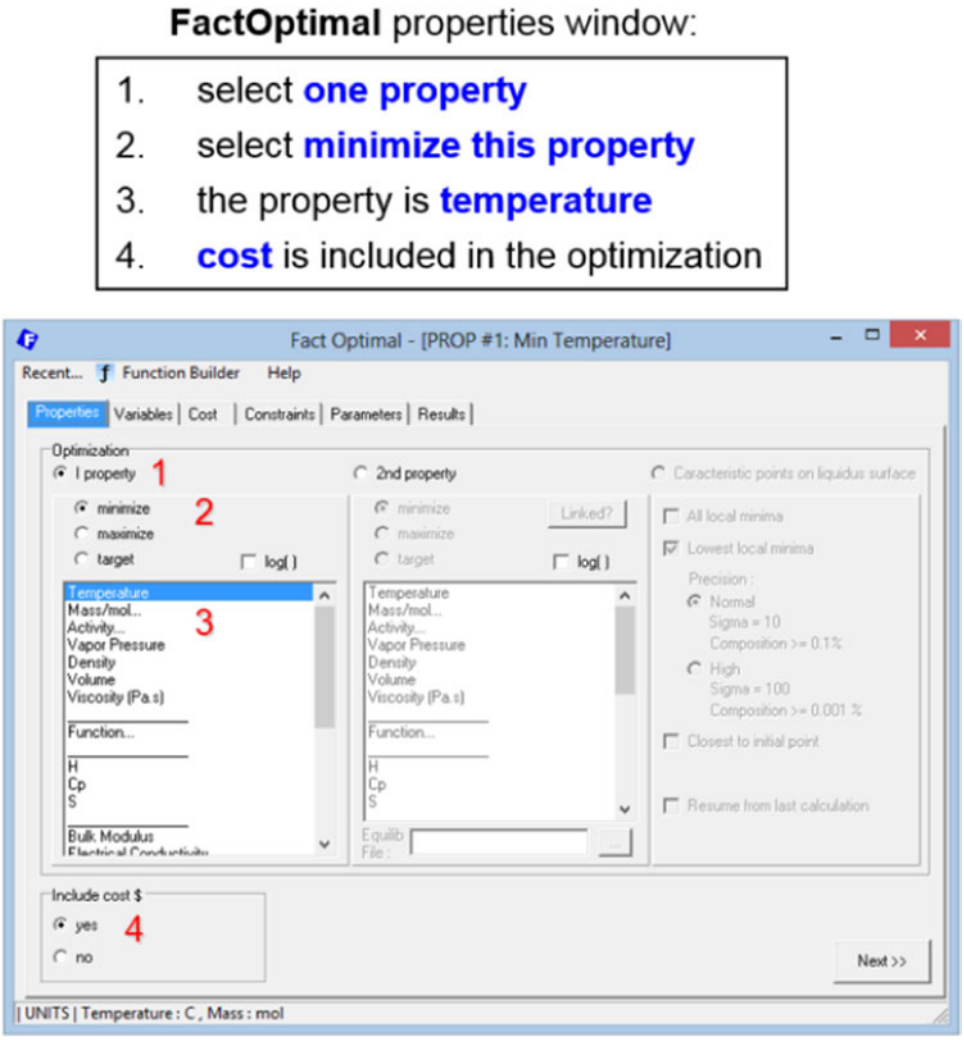


Fig. 15. FactOptimal module – *Properties Window*.

Calculated *Characteristic Points* in the Li^+, Na^+, K^+, Mg^{++}, Ca^{++} / F^-, Cl^- reciprocal system.

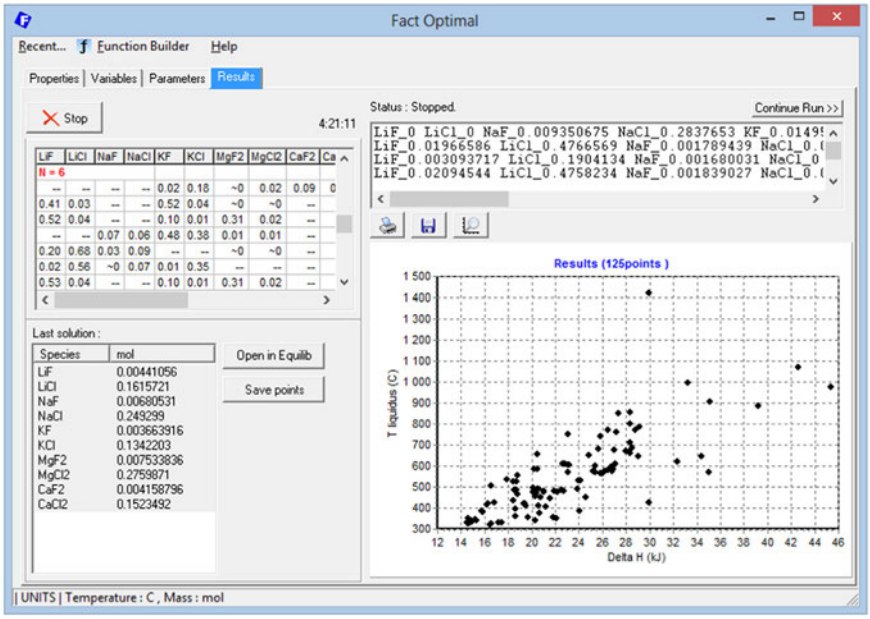


Fig. 16. FactOptimal module **–** calculated of *characteristic points* in the Li^+, Na^+, K^+, Mg^{++}, Ca^{++} / F^-, Cl^- reciprocal system.

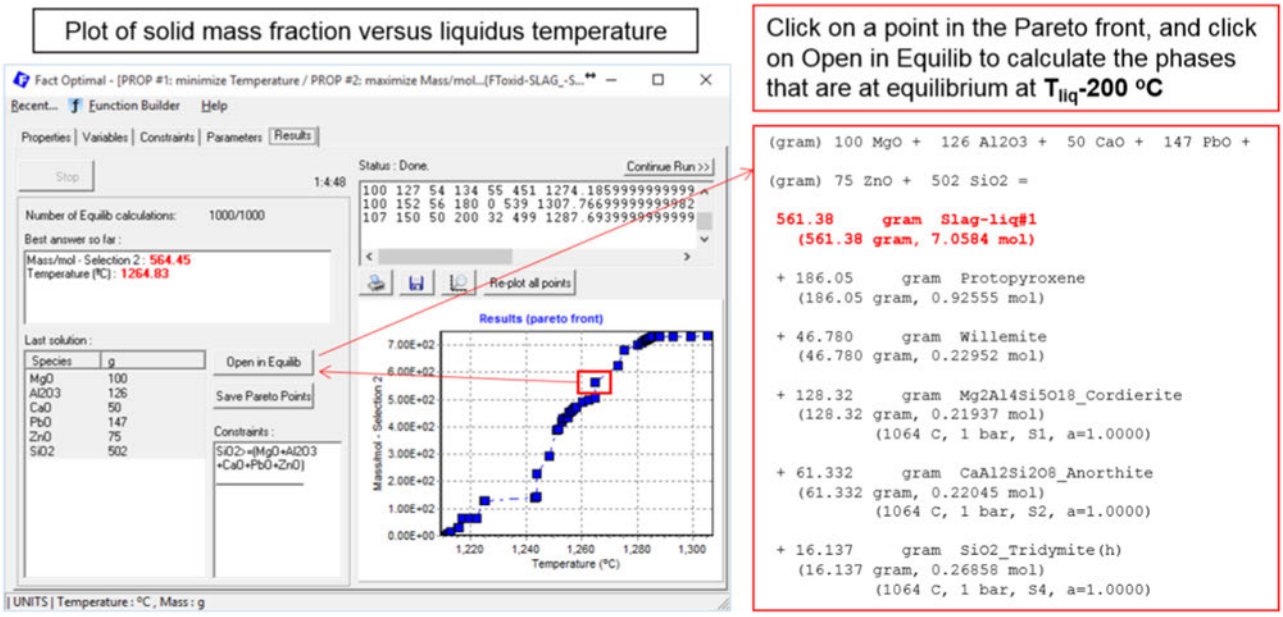


Fig. 17. FactOptimal module – results showing the Pareto front in a plot of solid fraction vs. liquidus temperature in the MgO–Al_2O_3–CaO–PbO–ZnO–SiO_2 oxide system.

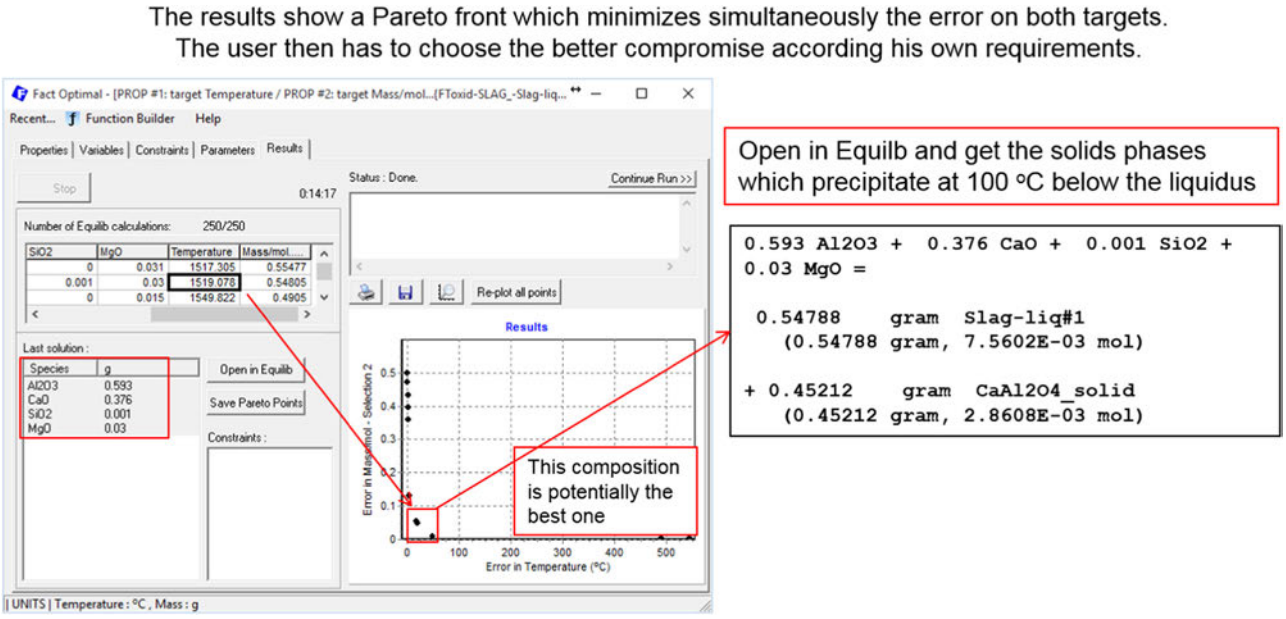


Fig. 18. FactOptimal module – *Results Window* to minimize simultaneously the liquidus temperature and solid mass fraction in the in the Al_2O_3–CaO–SiO_2–MgO oxide system.

binary and ternary systems. The model can then successfully predict viscosities in multicomponent systems [21,22]. There are two viscosity databases:

- database for molten slags: Al_2O_3–B_2O_3–CaO–FeO–Fe_2O_3–K_2O–MgO–MnO–Na_2O–NiO–PbO–SiO_2–TiO_2–Ti_2O_3–ZnO–F
- database for glasses (super-cooled melts): Al_2O_3–B_2O_3–CaO–K_2O–MgO–Na_2O–PbO–SiO_2

Fig. 19 shows a comparison between calculated and experimental viscosities in the Na_2O–Al_2O_3–SiO_2 ternary system with the viscosities calculated using the molten slag database. Note the calculation of the important "charge compensation effect" [21,22]. During the last several years the accuracy of the database for the high iron oxide (FeO and Fe_2O_3) slag systems has been greatly improved due to recent literature data and in-house data by academic and industrial collaborators. The database now gives reliable predictions of the viscosity of mold fluxes in the continuous casting process of steel and of slags in the electro-slag remelting (ESR) processes.

4.9. Phase Diagram and Figure Modules

In the **Phase Diagram** module two thermodynamic properties are plotted on the *X*- and *Y*-axes, while the other properties are held constant. The properties that may be selected as axes or constants are:

T (or **1/*TK*)**–temperature; ***P***–total pressure; ***V***–volume; **Comp**–Composition (mole fractions, molar ratios, weight fractions, weight ratios); **Potl**–Chemical potentials ($RT\ \ln(a_i)$, $RT\ \ln(P_i)$,

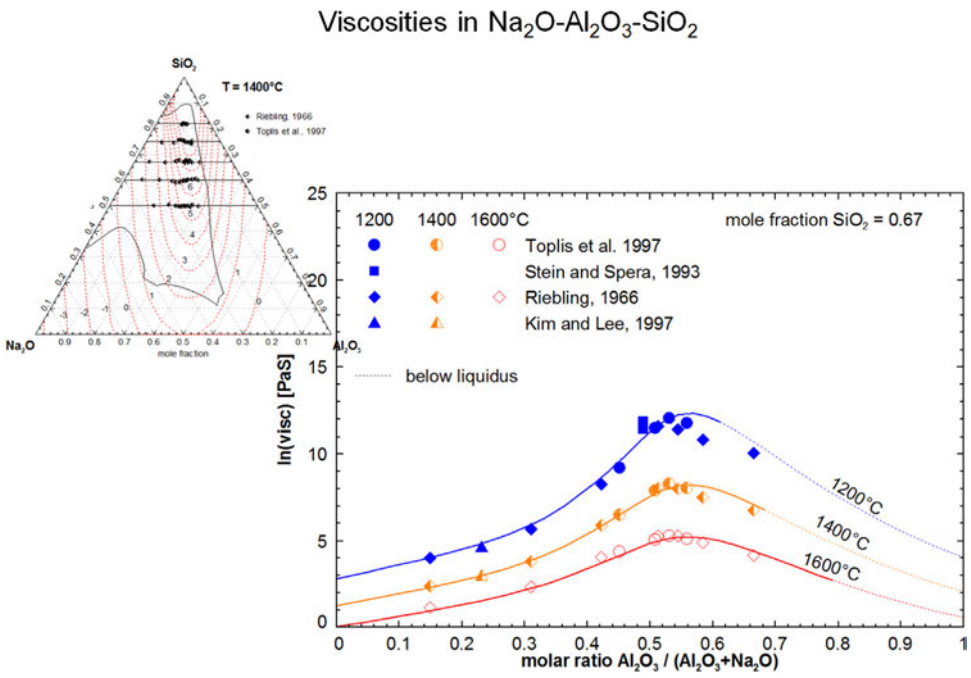


Fig. 19. Viscosity module – viscosities in Na_2O–Al_2O_3–SiO_2.

$\log(a_i)$, $\log(P_i)$ where a_i and P_i=activity or partial pressure of component i); **Delta *H***–Enthalpy relative to a standard state temperature.

As well, various projections (e.g. liquidus surfaces) can be calculated. A unique and very useful feature of FactSage allows the calculation of the amounts and compositions of all phases at equilibrium at any point on the diagram by simply placing the cursor at the point and clicking.

A variety of calculated phase diagrams that are new to FactSage is presented later (Section 5. 'Examples of Phase Diagrams') showing examples of the combined use of the Phase Diagram, Equilib and Figure modules.

5. Manipulate

FactSage offers a variety of ways one can interact with the modules during the calculations (Macro Processing,), and after the calculations through post-processing of the tabular and graphical results of the complex equilibrium calculations in Equilib and Phase Diagram (Streams, Results module, Fact-XML).

6. Calculation of Phase Diagrams

In the following examples all the figures have been calculated by the Phase Diagram module and the domains have been automatically labeled (or tie-lines added) by simply pointing the mouse to the appropriate coordinate and clicking. In some cases text has been edited and symbols added by using the editing features of the Figure module. Some of the calculations also involve private databases only. Only the various types of phase diagrams that are new to FactSage during the period 2010–2016 are presented here.

6.1. Gas polythermal projections

Fig. 20 is the isothermal section of the Zn–Hg–Cd system at 700 °C, 1 bar and shows tie-lines for the two-phase gas-liquid

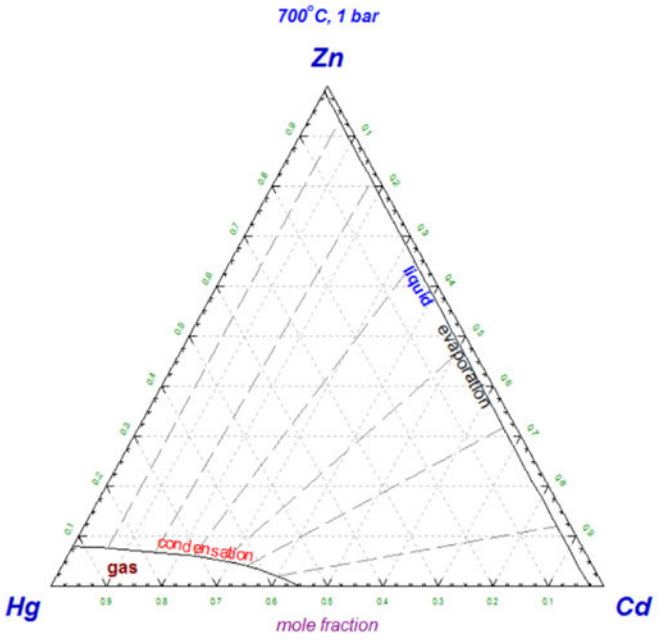


Fig. 20. Phase Diagram module – iso-thermal section of Zn–Hg–Cd at 700 °C, 1 bar.

equilibria (condensation–evaporation). Fig. 21 is the plot of the polythermal projections of condensation (horizontal isotherms of first liquid condensates, precipitate "*P*" target) and of evaporation (vertical isotherms of gas formation, format "*F*" target) in the Zn–Hg–Cd ternary system at 1 bar.

6.2. Enthalpy-Composition Diagrams

In an enthalpy–composition (*H*–*X*) phase diagram the vertical axis is the enthalpy relative to the enthalpy at a specified reference temperature (for example, 25 °C) and the horizontal axis is the composition, either in a binary system or along a constant composition path (isopleth) in a multicomponent system. Fig. 22 is the calculated temperature vs. wt% *Si* phase diagram for Mg–Si–Al–Sr at 0.3 wt% Mg and

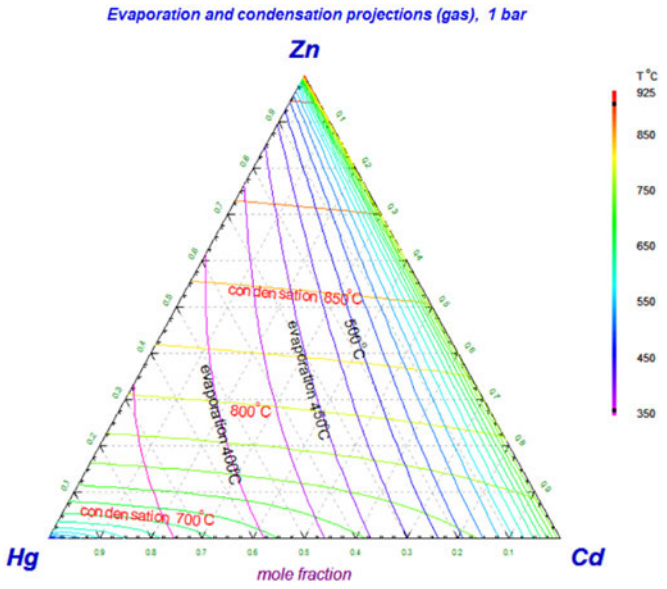


Fig. 21. Phase Diagram module – gas evaporation and condensation polythermal projections of the Zn–Hg–Cd ternary system, 1 bar.

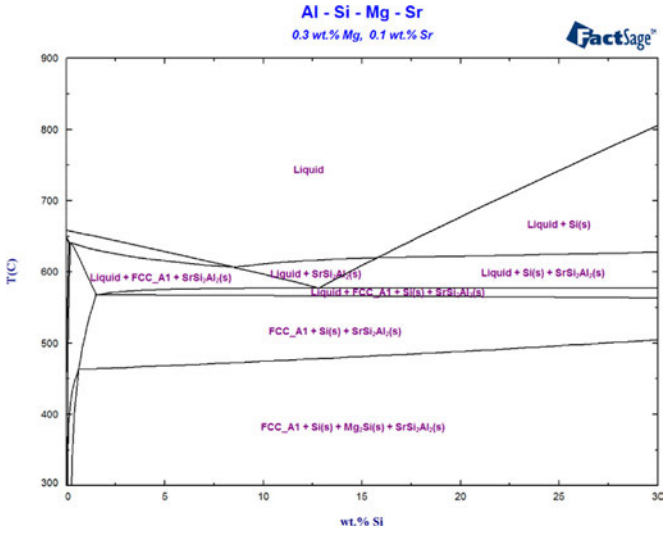


Fig. 22. Phase Diagram module – temperature vs. wt% Si isopleth for Al–Si–Mg–Sr at 0.3 wt% Mg and 0.1 wt% Sr using data from **FTlite**.

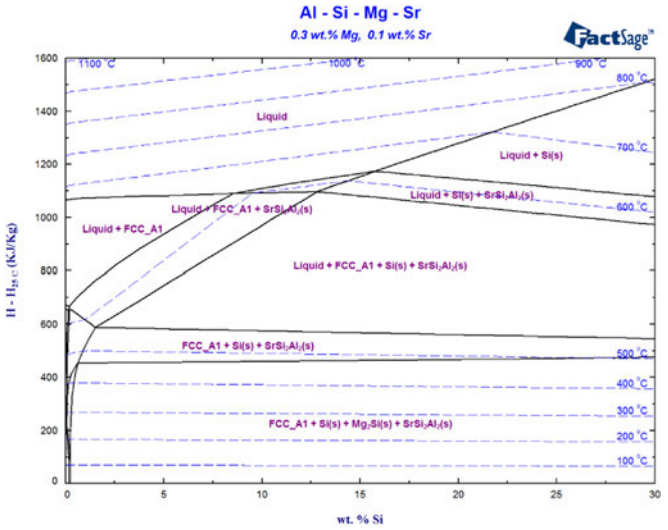


Fig. 23. Phase Diagram module – enthalpy vs. composition diagram for Al–Si–Mg–Sr at 0.3 wt% Mg and 0.1 wt% Sr using data from **FTlite**.

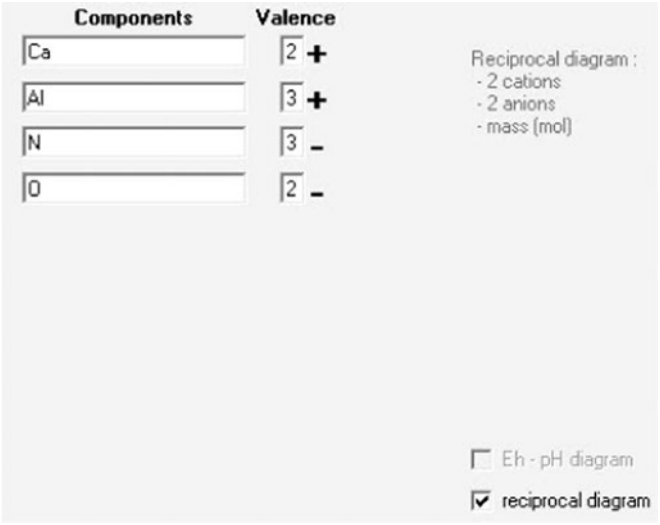


Fig. 24. Phase Diagram – reciprocal phase diagram option and entry of the cationic and anionic components.

0.1 wt% *Sr*. In the enthalpy–composition diagram for the same system (Fig. 23) one can read at a glance the heat change associated with each stage of cooling a Mg–Si–Al–Sr alloy down to 25 °C. The heat change includes the sensible heat during cooling, as well as heat changes during eutectic reactions, etc.

6.3. Reciprocal Diagrams

Ca_3N_2–Al_2O_3–CaO–AlN, or Ca^{2+},Al^{3+}//O^{2-},N^{3-} is a reciprocal oxide-nitride system in which the chemistry can be defined by the following exchange reaction and charge balance:

$$Ca_3N_2 + Al_2O_3 = 3CaO + 2AlN$$

$2n(Ca^{2+}) + 3n(Al^{3+}) = 2n(O^{2-}) + 3n(N^{3-})$ where $n(i)$ = moles of ion i.

The components are Ca, Al, O and N. In a Reciprocal Diagram the *Y*-axis is the "equivalent fraction" 2O/(2O+3N) in the range 0–1 and the *X*-axis is the "equivalent fraction" 2Ca/(2Ca+3Al) in the range 0–1 where (2Ca+3Al)=(2O+3N). Note the corners are not Ca_3N_2–Al_2O_3–CaO–AlN but rather (Ca_3N_2)–(Al_2O_3)–$(CaO)_3$–$(AlN)_2$. This is necessary to ensure the tie-lines are straight lines. A new feature in **Phase Diagram** permits the user to select the reciprocal phase diagram option and then enter the cationic and anionic components (Fig. 24). This results in the calculation of a polythermal projection (Fig. 25) which is labeled with the pertinent information associated with the reciprocal system.

6.4. Volume Diagrams

Volume or log volume may be specified as an *X*- or *Y*-axis. Typical volume diagrams include *V* (or log V) vs. *T* and *V* (or log *V)* vs. X. Fig. 26 shows a *Volume Diagram* of log(*V*) vs. *T*(*K*) in the Si–C–O system when Si/(Si+C+O)=0.1 and C/(Si+C+O)=0.3 (mol/mol).

6.5. First-Melting Projection Diagram

The first-melting projection of the phase diagram of a ternary or higher-order system shows the temperature at which a liquid phase first appears upon heating at any given composition in a

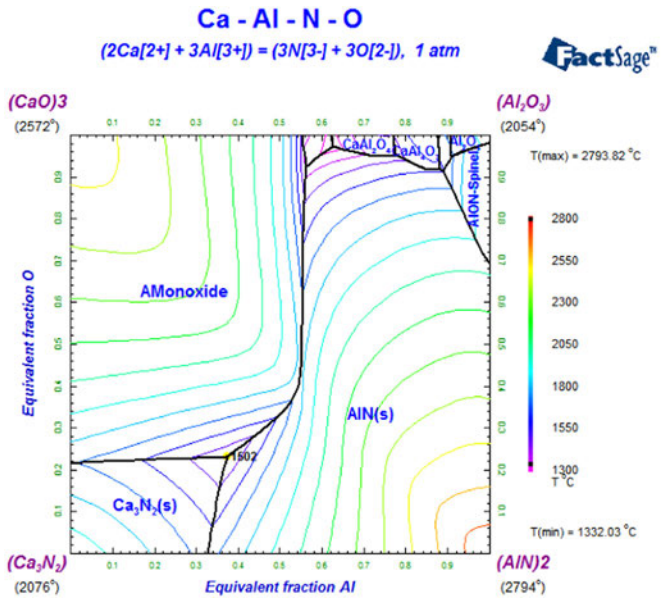


Fig. 25. Phase Diagram – polythermal liquidus projection in the Ca_3N_2–Al_2O_3–CaO–AlN reciprocal system using data from **FTOxCN**.

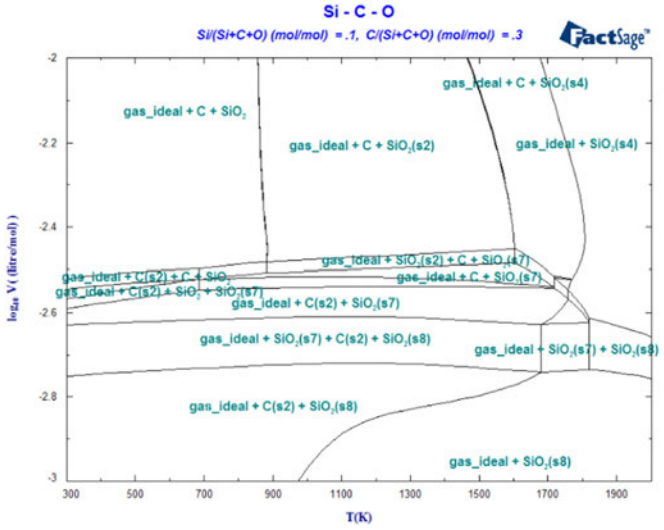


Fig. 26. Phase Diagram – volume diagram of log(V) vs. $T(K)$ in the Si–C–O system when Si/(Si+C+O)=0.1 and C/(Si+C+O)=0.3 (mol/mol).

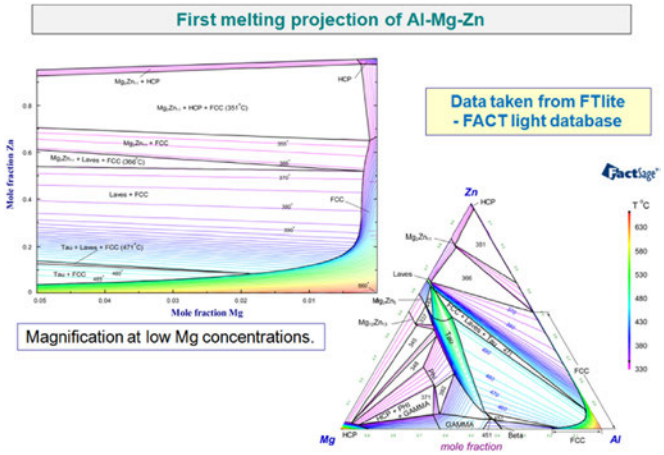


Fig. 27. Phase Diagram –Zn–Mg–Al polythermal first-melting (solidus) projection using data from **FTlite**.

system at thermodynamic equilibrium. In most systems, first-melting projections are identical to solidus projections and they obey the same well-known topological rules as isothermal sections of phase diagrams. Hence, their interpretation is straightforward. Only in systems with catatectic invariants or retrograde solid solubility do exceptions to these rules occur, and then only over limited composition regions. For more details on the algorithm and explanations refer to [23]. For example, Fig. 27 shows a polythermal first-melting (solidus) projection in the ternary Zn–Mg–Al system; Fig. 28 shows a polythermal first-melting (solidus) projection in the quaternary system Zn–Mg–Al–Y.

6.6. *Paraequilibrium phase diagram [24]*

Paraequilibrium refers to the concept that diffusion of interstitial solutes is much faster than that of substitutional atoms. For example, in the Fe–Cr–C–N system carbon and nitrogen diffuse much more rapidly than Fe and Cr. That is, the diffusion of Fe and Cr during relatively rapid cooling can be ignored.

For example, Fig. 29 is the $T(K)$ vs. Cr/(Fe+Cr) (mol/mol) phase diagram of the Fe–Cr–C–N system at C/(Fe+Cr) (mol/mol)=0.02 and N/(Fe+Cr) (mol/mol)=0.02 calculated under normal

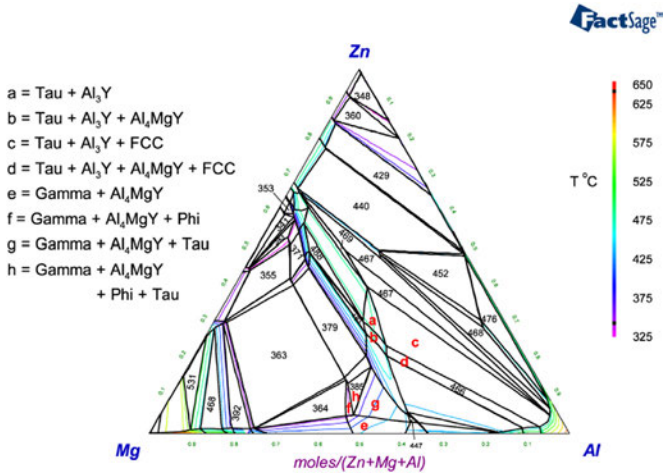


Fig. 28. Phase Diagram –Zn–Mg–Al–Y polythermal first-melting (solidus) projection at X_Y=0.05 using data from **FTlite**.

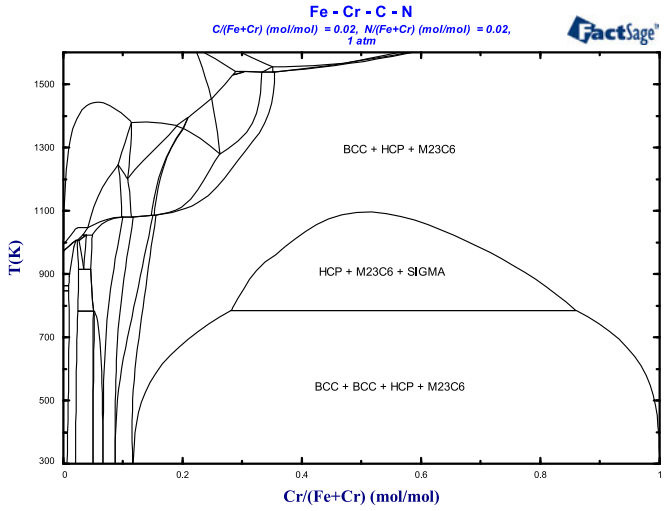


Fig. 29. Phase Diagram – $T(K)$ vs. Cr/(Fe+Cr) phase diagram of the Fe–Cr–C–N system at C/(Fe+Cr)=0.02 and N/(Fe+Cr)=0.02 calculated under normal equilibrium conditions (orthoequilibrium) using data from **FSstel**.

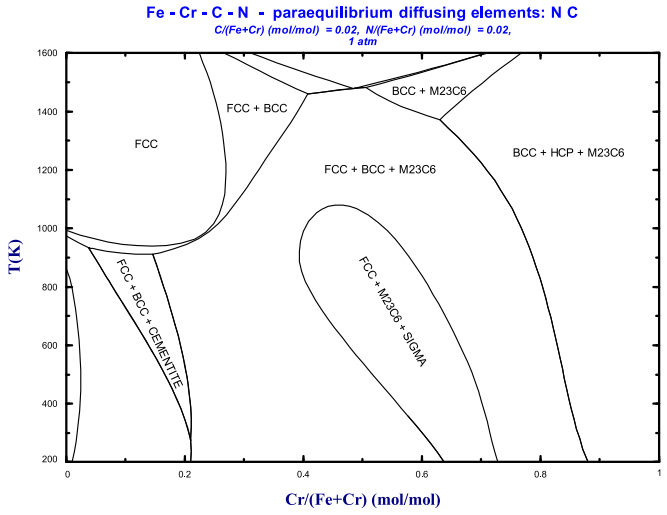


Fig. 30. Phase Diagram module – *paraequilibrium diagram* for the same Fe–Cr–C–N system with only C and N diffusing using data from **FSstel**.

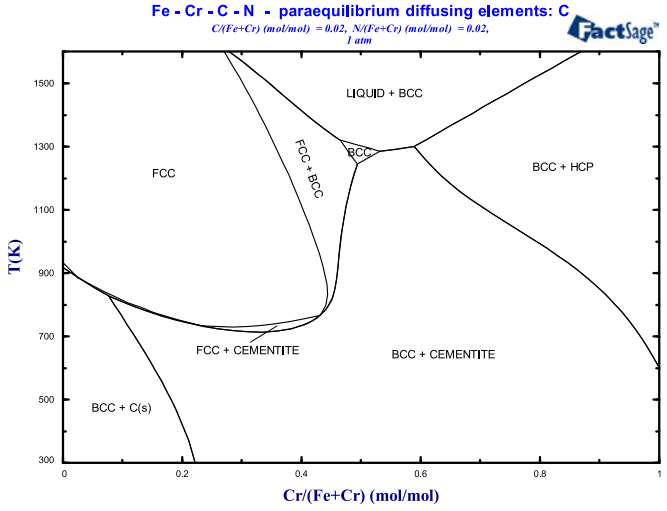


Fig. 31. Phase Diagram module – *paraequilibrium diagram* for the same Fe–Cr–C–N system with only C diffusing using data from **FSstel**.

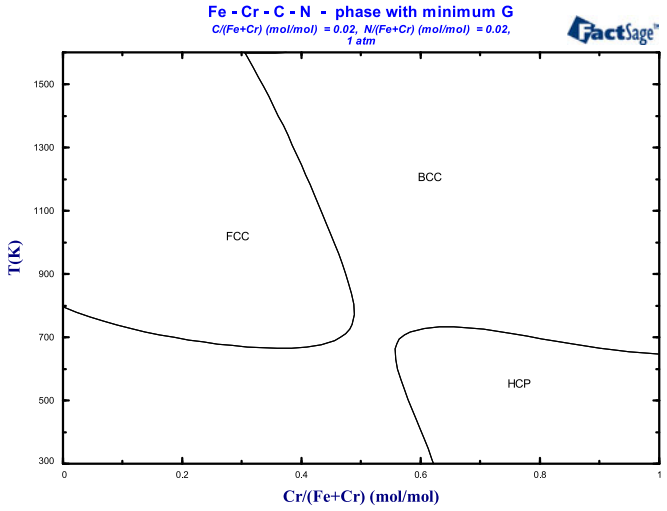


Fig. 32. Phase Diagram module – diagram for the same Fe–Cr–C–N system in which the phase fields show the single phase with the minimum Gibbs energy at any given point on the diagram using data from **FSstel**.

equilibrium conditions (orthoequilibrium). Data are taken from the **SGTE** alloy databases. Fig. 30 is the *paraequilibrium diagram* for the same system with only C and N diffusing. Fig. 31 is a special case when C is the only diffusing component. For more details on paraequilibrium phase diagrams refer to [24].

It is also possible to calculate phase diagrams in which the phase fields show the single phase with the minimum Gibbs energy at any given point on the diagram as shown in Fig. 32. Such calculations may be of practical interest in physical vapour deposition where deposition from the vapour phase is so rapid that phase separation cannot occur, resulting in a single-phase solid deposit.

6.7. *Isobars and iso-activity lines*

On a calculated phase diagram it is now possible to plot *isobars* of a gaseous species or gas phase and *iso-activity lines* of a compound (pure liquid or solid). For compound species, isobars and

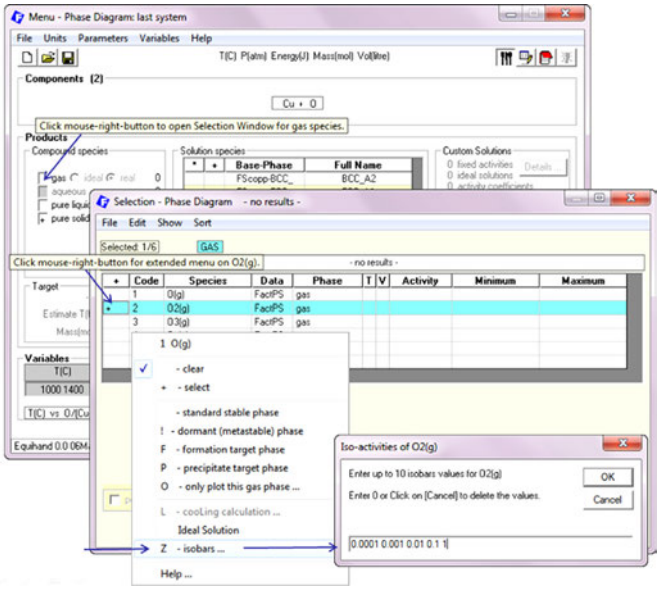


Fig. 33. Phase Diagram module **–** isobars and iso-activity lines for compound species are defined in the *Compound Selection Window*.

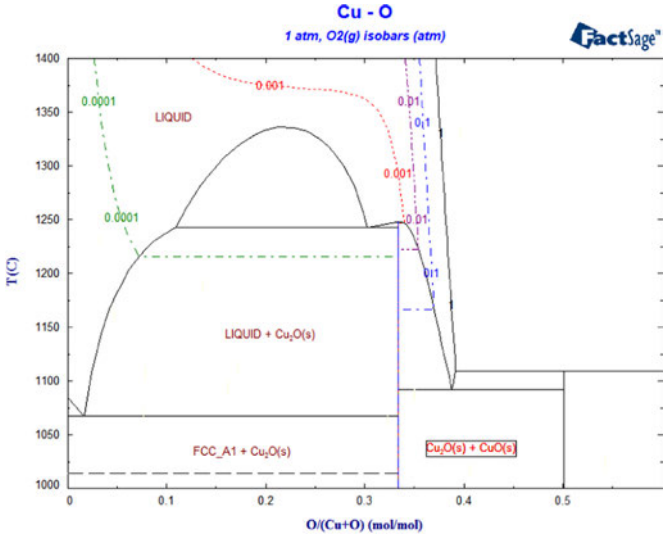


Fig. 34. Phase Diagram module – calculated $O_2(g)$ isobars in the Cu–O binary systems using data from **FScopp**.

iso-activity lines are defined in the *Compound Selection Window* as shown in Fig. 33. The resulting diagram (Fig. 34) shows the calculated O_2(g) isobars in the Cu–O binary system using data from the **FScopp** database. Fig. 35 shows calculated O_2(g) isobars in the FeO–Fe_2O_3–Cr_2O_3 ternary system at 1300 °C using data from the **FToxid** database. Fig. 35 shows calculated C(s) iso-activity lines in the Fe–Cr–C ternary system (Fig. 36).

The basic principles behind the calculation of isobars and iso-activity lines have been discussed by [25]. It involves the introduction of an *auxiliary phase*, and its Gibbs energy function is manipulated in order to plot a specific iso-line as if it were a pseudo-phase boundary (as a zero-phase-fraction-line) of this *auxiliary phase*. This approach can be extended to calculate other iso-lines for other properties (activity coefficients, sulfide capacities, surface tension, etc.) For example, Fig. 37 [26] shows calculated iso-sulfide capacity (C_S) lines of CaO–SiO_2–Al_2O_3 slags at 1400 °C and the calculated liquidus (thin lines).

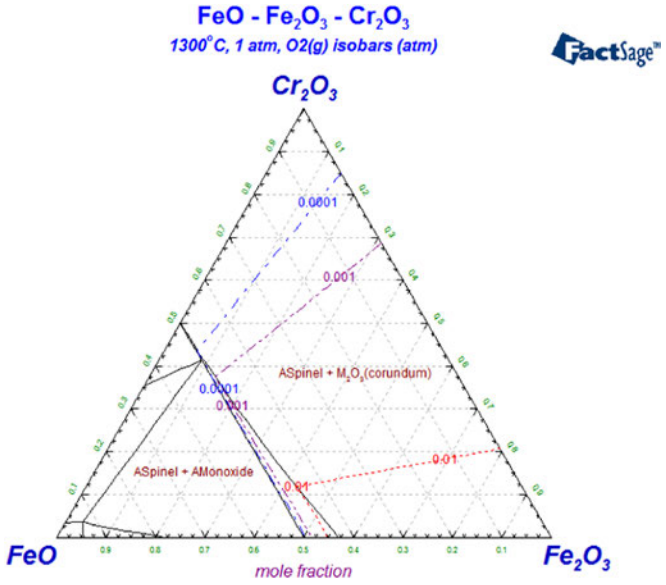


Fig. 35. Phase Diagram module – calculated O_2(g) isobars in the FeO–Fe_2O_3–Cr_2O_3 ternary system at 1300 °C using data from **FToxid**.

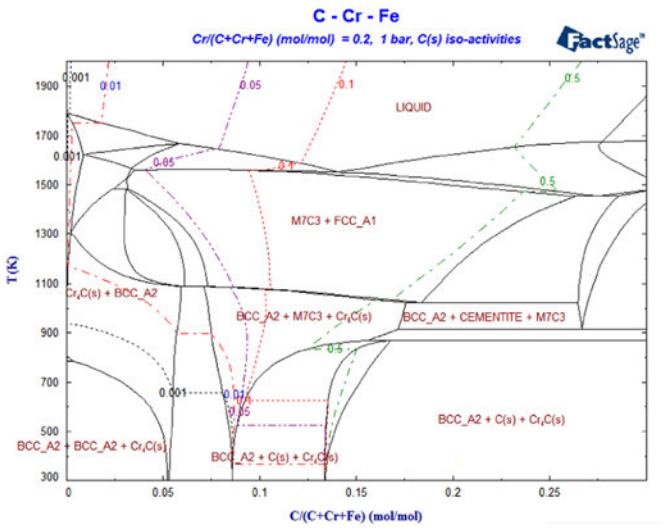


Fig. 36. Phase Diagram – calculated C(s) iso-activity lines in the Fe–Cr–C ternary system.

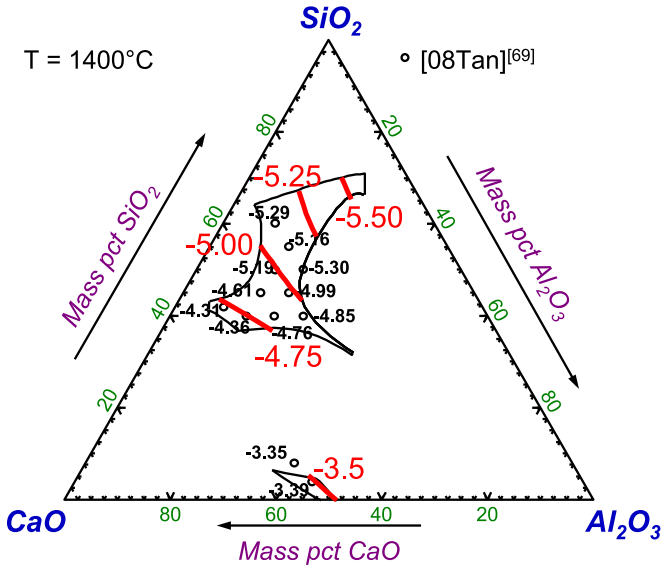


Fig. 37. Phase Diagram – calculated iso-sulfide capacity (C_S) lines of CaO–SiO_2–Al_2O_3 slag at 1400 °C with the calculated liquidus (thin lines) [25] using data from **FToxid**.

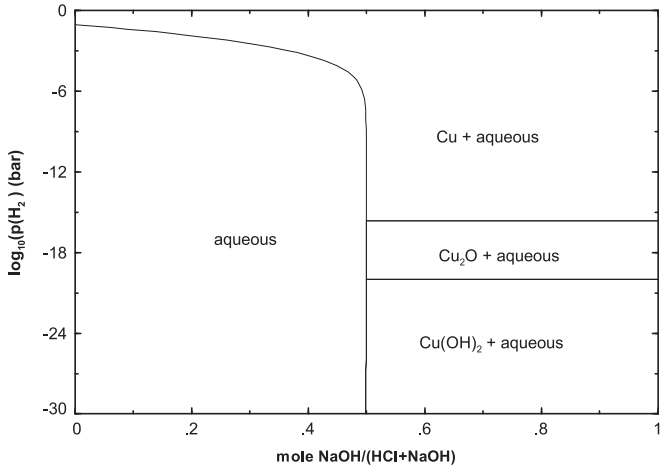


Fig. 38. Phase Diagram – calculated partial pressure of H_2 vs. molar ratio NaOH/(NaOH+HCl) for the the system H_2O–Cu–NaOH–HCl–H_2, molality of Cu = 0.001.

6.8. Miscellaneous

It is should be noted that the **Phase Diagram** module requires no starting values or initial estimates. All phase diagrams shown here were calculated and plotted by simply selecting "Calculate >>". In some cases text and labels were manually added for clarity.

6.9. Current developments

With the release of **FactSage 7.1** it will be possible to calculate *Scheil–Gulliver phase diagrams* showing the phases which result when a system is cooled under Scheil–Gulliver conditions (see *Section 3.2*).

Classical *Eh–pH (Pourbaix) diagrams* are not true phase diagrams inasmuch as (a) the aqueous phase fields show the regions where one aqueous species is predominant, whereas this is actually only one continuous aqueous phase field, (b) they are calculated only at infinite dilution. In Fig. 38 is shown a phase diagram calculated by **Phase Diagram** for the system H_2O–Cu–NaOH–HCl–H_2 in which the *X*-axis is the molar ratio NaOH/(NaOH+HCl), which is related to the pH, and

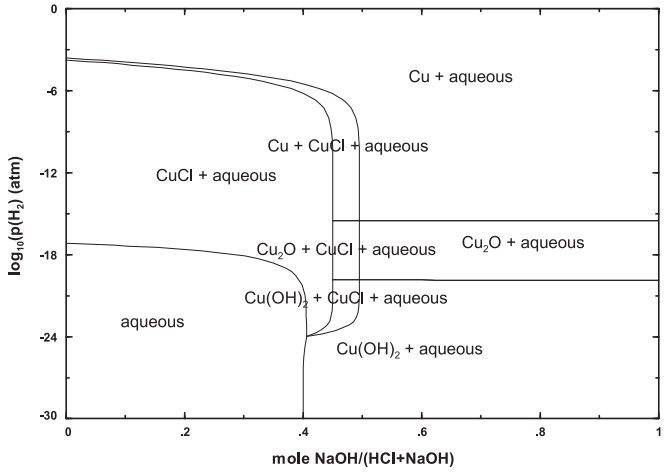


Fig. 39. Phase Diagram – calculated partial pressure of H_2 vs. molar ratio NaOH/(NaOH+HCl) for the system H_2O–Cu–NaOH–HCl–H_2, molality of Cu=0.1.

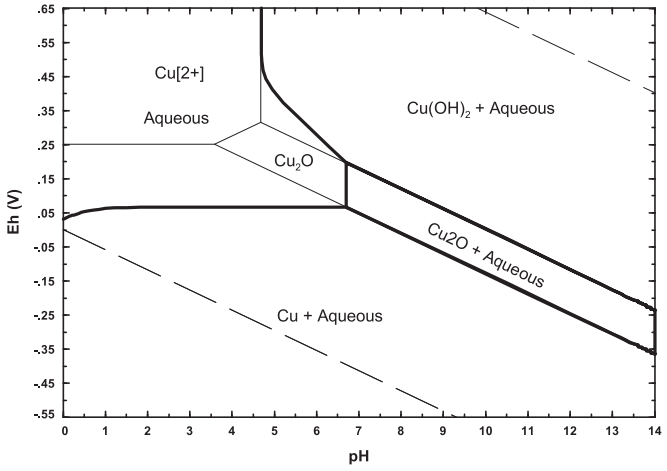


Fig. 40. Phase Diagram – Eh vs. pH true phase diagram derived from Fig.39 with boundaries calculated from FactSage EpH module (classical EpH diagram) overlaid.

the *Y*-axis is the equilibrium partial pressure of H_2, which is related to the redox potential Eh. The figure is calculated on the basis of 1.0 kg H_2O and a total of 1.0 mol (NaOH+HCl) at a constant molality of Cu/(1 kg H_2O)=0.001. Figure shows the effect on changing the Cu molality to 0.01. The composition of the aqueous phase can be calculated by simply placing the cursor at a point on the diagram and clicking. The axes of Figs. 38 and 39 can be converted to Eh and pH as shown in Fig. 40. At present, the conversion involves a good deal of manipulation by the user. In **FactSage 7.1** it is planned to render the conversion automatic.

6.10. Internet

All the calculated phase diagrams and associated database documentation in the **FactSage** package are accessible on the internet through www.factsage.com. In addition, it is possible to display and interact with calculated phase diagrams through the **Fact-Web** suite of interactive programs ⟨www.crct.polymtl.ca/fact web.php⟩. Fact-Web provides limited access to some of the **FactSage** modules (View Compound, Reaction, EpH, Predom, Equilib, Phase Diagram) and access to all the compounds in FactPS – the FACT pure substances database.

7. Summary and conclusions

This article has presented a summary of the most recent developments (2010–2016) in the FactSage thermochemical software and database package with emphasis on the optimization, calculation and manipulation of phase diagrams.

FactSage software and database development is ongoing. Information on the status of FactSage as well as sample phase diagrams of hundreds of alloy, salt, oxide etc. systems is available through the Internet at www.factsage.com.

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