



FactSage Thermochemical Software and Databases

C.W. Bale*, P. Chartrand*, S.A. Degterov*, G. Eriksson**, K. Hack**,
R. Ben Mahfoud*, J. Melançon*, A.D. Pelton* and S. Petersen**

*CRCT - Center for Research in Computational Thermochemistry
École Polytechnique (Université de Montréal), Box 6079, Station Downtown,
Montréal, Québec, CANADA H3C 3A7
<http://www.crct.polymtl.ca>

**GTT-Technologies, Kaiserstrasse 100,
52134 Herzogenrath, GERMANY
<http://gttserv.lth.rwth-aachen.de>

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Abstract This paper presents a summary of the **FactSage** thermochemical software and databases. **FactSage** was introduced in 2001 and is the fusion of the **FACT-Win/F*A*C*T** and **ChemSage/SOLGASMIX** thermochemical packages that were founded over 25 years ago. The **FactSage** package runs on a PC operating under Microsoft Windows® and consists of a series of information, database, calculation and manipulation modules that enable one to access and manipulate pure substances and solution databases. With the various modules 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. In this article emphasis is placed on the calculation and manipulation of phase diagrams. However the reputation of **FactSage** has been established mainly in the field of complex chemical equilibria and process simulation where the software has unique capabilities. Some of these capabilities are also shown in this paper. © 2002 Published by Elsevier Science Ltd.

Introduction

FactSage is the fusion of two well-known software packages in the field of computational thermochemistry: **FACT-Win** (formerly **F*A*C*T**) and **ChemSage** (formerly **SOLGASMIX**).

F*A*C*T - *Facility for the Analysis of Chemical Thermodynamics* - started in 1976 as a joint research project between two universities, McGill University (W.T. Thompson) and the École Polytechnique de Montréal (C.W. Bale and A.D. Pelton). The initial programs [77Pel] were written in FORTRAN on punched cards and performed chemical thermodynamic calculations involving pure substances and ideal gases. In 1979 **F*A*C*T On-Line** was offered as an interactive program through the McGill University MUSIC system (accessed via Datapac and Telenet telephone links) where it was mainly used as a teaching tool [79Tho, 80Tho]. Solution programs and databases were added together with the **POTCOMP** and **TERNFIG** algorithms for optimizing, calculating and plotting binary and ternary phase diagrams [80Lin], [82Bal]. In the 1990's the system evolved into the PC-based program **FACT-DOS** [96Bal] that offered unlimited access to the software

and databases. **FACT-Web** (1996) provided interactive demonstration modules through the Internet at the CRCT [02Crc]. The Windows® version **FACT-Win** was released in 1999 and offered a fully integrated thermochemical database system that coupled proven software with self-consistent critically assessed thermodynamic data. By this time **F*A*C*T** had expanded well beyond chemical metallurgy and was being employed in other fields of chemical thermodynamics by pyrometallurgists, hydrometallurgists, chemical engineers, corrosion engineers, inorganic chemists, geochemists, ceramists, electrochemists, environmentalists, etc. Since 1979 **F*A*C*T** has incorporated the Gibbs Energy minimizer, **SOLGASMIX**.

SOLGASMIX was developed by G. Eriksson. In the early versions [75Eri] it was possible to calculate equilibria in multi-component non-ideal solution phase systems. At that time the user had to be both a thermochemist *and* a programmer since the first code only provided the necessary subroutines for the inclusion of non-ideal Gibbs energy models. Co-operation between G. Eriksson and K. Hack that started in the eighties saw the first editions of an interactive program (**SOLGASALLOY**, 1984) with integrated non-ideal Gibbs energy models (polynomials for substitutional metallic solutions). In time more models were added, for example the Gaye-Kapoor-Froberg cell formalism for non-ideal liquid oxides and the models developed by the **F*A*C*T** group. Further enhancements included the addition of modules for the calculation of thermodynamic properties of phases and a reactor module that permits the calculation of co- and counterflow reactors (**SAGE**, 1988). The combination of these calculational capabilities and access to the full databases of **SGTE** (in co-operation with the MTDS group of NPL, Teddington) led to **ChemSage** [90Eri], an Integrated Thermodynamic Databank System, initially running under DOS. The programs were continually improved, e.g. by the development of a thermodynamic assessment module by the addition of an optimization routine [95Eri] and a graphical post-processor, and finally by the development of a module for two-dimensional phase mapping, i.e. the calculation of generalized phase diagrams (1999). **ChemSage** has found worldwide use in several hundred installations in universities, governmental and non-governmental research laboratories and in industry, where it has been successfully employed to analyze, understand and improve metallurgical processes, materials problems, environmental conditions, etc.

In April 2001, **F*A*C*T** and **ChemSage** were merged into one unified package. **FactSage 5.0** (followed by the **FactSage 5.1** update in 2002) offers more features than those available in the **FACT-Win 3.05** and **ChemSage 4.0** packages. Currently it is installed in well over 100 universities around the world where it is used as a research tool and educational aid. Also approximately 100 industrial users of its predecessors have already upgraded to **FactSage** because of its ease of use, its flexible access to different databases and its powerful calculational modules.

While an understanding of chemical thermodynamics is, of course, necessary in order to run the programs, it is not essential to be an expert in the field. **FactSage** is a powerful self-teaching aid. With regular program usage one can rapidly acquire a practical understanding of the principles of thermochemistry especially as these relate to complex phase equilibria.

This article summarizes the programs and databases offered through **FactSage** with special emphasis placed on the calculation and manipulation of phase diagrams.

Main Menu

The **FactSage** main menu (Fig.1) offers access to the modules of the package. These are grouped into four categories:

1. **Info** – This includes detailed slide shows (Microsoft Power Point® presentations) of most of the program modules and general information with **Frequently Asked Questions** on **FactSage** and its databases.
2. **Databases** – These program modules enable the user to view, manipulate and edit the pure substances and solution databases that may be private (read/write) or public (read only).

3. Calculate – These modules are the central programs of **FactSage**. They permit the calculation of phase diagrams and thermochemical equilibria in various forms with direct access to the databases.

4. Manipulate – This group offers various graphical and tabular program modules for post-processing the results and manipulating the calculated phase diagrams and other figures.

1. Info Modules

The **Slide Shows** are given in the form of Microsoft Power Point® presentations. These introduce the basics of the program modules to a new user and provide extensive examples of industrial applications for advanced users. The files are regularly updated and are also available through the Internet.

The **General** module provides documentation, answers to frequently asked questions (FAQ) and lists of useful addresses and telephone numbers.

2. Databases Modules

In **FactSage** there are two types of thermochemical databases – compound (pure substances) databases and solution databases. The **View Data**, **Compound** and **Solution** modules permit one to list and manipulate the contents of these databases.

Compound databases are for stoichiometric solid, liquid and gaseous species such as CaO(s), FeS(liq), SO₂(g). Compound data may include allotropes, for example graphite C(s1) and diamond C(s2), and isomers, for example ethylene C₂H₄O(liq1) and acetylene C₂H₄O (liq2). Data on a few compounds with non-integer stoichiometry such as FeO_x (x = 0.947) are also stored. Depending upon the type of phase (solid, liquid, gas) and data availability, the stored properties include ΔH°(298.15 K), S°(298.15 K), Cp(T), magnetic data (Curie or Néel temperature and average magnetic moment per atom), molar volumes (298.15 K) coupled with expansivities, compressibilities and pressure derivatives of bulk moduli as functions of T. Infinitely dilute aqueous solution data and non-ideal gas properties (T_{crit.}, P_{crit.}, V_{crit.}, the acentric factor, omega, and the dipole moment from which the first virial coefficient can be calculated by the Tsonopoulos equation) are also stored in the compound databases, as are bibliographical references.

Solution databases are for solid and liquid alloys, carbides, nitrides and carbonitrides, concentrated aqueous solutions, ceramics, salts, mattes, slags, etc. The data are stored in the form of Gibbs energy functions for the phase constituents and temperature dependent model parameters for calculating the Gibbs energy of mixing among the phase constituents. **FactSage** supports 11 different solution models including simple polynomial models (Redlich-Kister and Legendre polynomials) combined with different higher order extrapolations (Muggianu, Kohler, Toop), the Unified Interation Parameter Model, Modified Quasichemical models for short-range ordering in pair and quadruplet approximations, the Pitzer model (for concentrated aqueous solutions) and sublattice models such as the Compound Energy Formalism. Additional solution models are planned.

The following databases are currently available in **FactSage**:

Compound Databases – note: a compound may contain several phases

- FACT - F*A*C*T 5.0 compound database (over 4,400 compounds)
- SGPS - SGTE pure substances database (over 3,400 compounds)
- SGSL - SGTE intermetallic compounds (for use with SGSL solutions)

Solution Databases

- FACT - F*A*C*T 5.0 solution database (120 non-ideal multicomponent phases)
- SGSL - SGTE alloy solutions database (63 non-ideal multicomponent alloy and carbonitride phases)

SGTE (Scientific Group Thermodata Europe) is a consortium of mainly European centers engaged in the development of thermodynamic databanks for inorganic and metallurgical systems and their application to practical problems. Both **GTT** and the **CRCT** are members of **SGTE**. The **FACT** and **SGTE** compound (pure substances) databases are quite similar in content. However the **FACT** solution database and the **SGTE** solution database are complementary. As they are combined in **FactSage** they permit unique application cases to be calculated, e.g. the corrosion of stainless steel alloys in sulfur- and oxygen-containing atmospheres.

The **FACT** solution database contains consistently assessed and critically evaluated thermodynamic data for $\text{SiO}_2\text{-CaO-Al}_2\text{O}_3\text{-Cu}_2\text{O-FeO-MgO-MnO-Na}_2\text{O-K}_2\text{O-TiO}_2\text{-Ti}_2\text{O}_3\text{-Fe}_2\text{O}_3\text{-ZrO}_2\text{-CrO-Cr}_2\text{O}_3\text{-NiO-B}_2\text{O}_3\text{-PbO-ZnO}$ melts/glasses with dilute solutes of $\text{S-SO}_4\text{-PO}_4\text{-CO}_3\text{-F-Cl-I-OH-H}_2\text{O}$. Many solid solutions (ceramics) of these components are also stored: monoxide, perovskite, spinels, pseudobrookite, melilite, olivine, wollastonite, etc. Most solid and molten salt solutions of the system Li, Na, K, Rb, Cs, Mg, Ca/F, Cl, Br, I, SO_4 , CO_3 , OH, NO_3 are also available as well as liquid sulfides (mattes) $\text{Fe-Ni-Co-Cr-Cu-Pb-Zn-As-S}$, several alloys, Pitzer parameters for concentrated aqueous solutions, etc. The **FACT** solution databases are being constantly extended and updated through a large internationally-funded research program.

The **SGTE** intermetallic compound and solution databases (**SGSL**) contain consistently assessed data on several hundred binary, ternary and quaternary alloy systems. These cover application fields such as noble metals, solders, semi-conductors or hard-metal systems. A special strength of the **SGTE** solution database is its application to Fe-based multi-component alloys, for example $\text{Fe-Cr-Co-Mo-W-Ni-C-N}$ with the formation of face- or body-centered cubic matrix phases and precipitates of intermetallic (rho, phi, Laves etc.), carbide (cementite, M_{23}C_6 , M_7C_3 , Cr_3C_2 , ksi etc.), nitride or carbonitride ($\text{Me}(\text{C,N})$, $\text{Me}_2(\text{C,N})$, Fe_4N) phases.

It is planned to make other databases available in **FactSage** including an extensive aqueous solution database from **Oli Systems** [02Oli], Inc., a light alloys database based on the European **COST507** project, **ThermoTech** Ni, Al, Fe and Ti alloy databases, **AEA** and **Thermodata** databases for nuclear applications, etc.

A user may also create and edit his own private databases using the **Compound** and **Solution** modules. With the **Optimize** module, thermodynamic assessments of experimental phase diagram and thermodynamic data can be performed in order to obtain the coefficients of G-functions of compounds or of the constituents of solid and liquid solution phases as well as the parameters of Gibbs energy models for the solutions.

Note that **FactSage** contains software permitting **ChemSage** and **ChemApp** users to automatically convert **ChemSage** datafiles into **FactSage** compatible databases and to permit the creation of **ChemApp** files from the **FactSage** databases.

With **View Data** one can display species and phases from the databases. For example Fig. 2 shows the input/output to list all compounds of the Fe-Si-O-S system that are stored in the **FACT** compound database. The mouse has been clicked on SiO_2 where it is noted that the compound has 8 solid allotropes (s1 to s8) and a liquid phase (L). Fig. 3 shows a summary of phases and a partial listing of the $\Delta\text{H}^\circ(\text{T})$, $\text{S}^\circ(\text{T})$ and $\text{Cp}(\text{T})$ compound data for SiO_2 . Fig. 4 is a partial listing summarizing the solution phases stored in the **FACT** database that contain the elements Fe-Si-O-S .

The **Compound** module is illustrated in Fig. 5. By using ‘drag and drop’, SiO_2 is copied from the read-only (r) **FACT** database (FACTBASE) into a private read/write (r/w) database USERBASE where the $\text{Cp}(\text{T})$ expressions for quartz, $\text{SiO}_2(\text{s}1)$ are being edited. Other properties such as magnetic (e.g. Fig. 6) (thermal expansivity, compressibility, etc.) can also be edited. It is also possible to add new phases or new compounds.

Figs. 7 and 8 show some of the features of the **Solution** module where one can list, edit, manipulate and store solution data. For example, Fig. 7 is a partial listing of the phases stored in the **SGTE** alloy solution

database, including general information on the liquid phase and its parameters. Fig. 8 displays the components of the MoNi_Delta phase together with a summary of functions and the contents of the GCRFCC function.

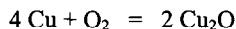
3. Calculate Modules

This group of modules is the heart of **FactSage**. One can interact with the software and databases in a variety of ways and calculate thermochemical equilibria in various forms.

Reaction Module

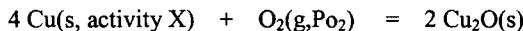
The **Reaction** module calculates changes in extensive thermochemical properties (H, G, V, S, Cp, A) for a single species, a mixture of species or for a chemical reaction. The species may be pure elements, stoichiometric compounds or ions (both plasma and aqueous ions). In the **Reaction Reactants Window** (Fig. 9) after a new reaction has been entered, data are automatically retrieved from the compound (pure substances) databases that are currently active. In the default mode the reaction is taken to be isothermal with all reactants and products in their most stable states. Alternatively, the temperature, pressure, state and activity of each species may be independently specified and the path by which the reactants become the chosen products may be specified as non-isothermal (adiabatic, isentropic, etc.). A tabular display in the form of an interactive spreadsheet is generated in the **Reaction Table Window** (Fig. 10).

Fig. 9 shows the entry of the isothermal standard state reaction for copper oxidation:



where the units selected are K, atm, J, mol. It is noted that the phases are not specified (i.e. *most stable*). In Fig. 10 the T(K) temperature range (300 to 2000 in steps of 300) is entered and **Reaction** determines the most stable phases at each temperature and lists common thermodynamic values including the transition temperatures. For example at 1200 K: the stable phases are Cu(s), O₂(g), Cu₂O(s); ΔH° = -332.62 kJ, ΔG° = -162.43 kJ, ΔS° = -141.83 J/mol-K, K_{eq} = 1.176 × 10⁶.

Fig. 11 shows entry of the non-standard state reaction:



In Fig. 12 the power of the interactive spreadsheet format of the *Table Window* is demonstrated. For example, in line 1 the activity of Cu(s) and the partial pressure of O₂ are given for standard conditions (a = X = 1, P = 1) and the changes in the standard enthalpy (ΔH° = -33.35 kJ), Gibbs energy (ΔG° = 191.16 kJ) etc. are calculated at 1000 K. In line 2 the activity of Cu(s) is still unity (X = 1.0), the Gibbs energy change is set to zero (i.e. equilibrium) and the equilibrium oxygen pressure is calculated to be P_{O₂} = 1.0359 × 10⁻¹⁰ atm. In line 3 the equilibrium activity of Cu(s) is calculated (3.1903 × 10⁻³) when P_{O₂} = 1.0 atm. In the last entry (line 4) O₂ with P_{O₂} = 10⁻¹² atm and Cu with a(Cu(s)) = 1 are at equilibrium (ΔG = 0) at the calculated temperature 897.01 K.

By appropriate entries one can perform heat balances, calculate adiabatic flame temperatures, solve simple equilibria, determine vapor pressures, calculate aqueous solubilities, etc. The results may also be automatically displayed as graphs and stored or exported (for example to Excel®) in the form of spreadsheets.

Predom and EpH Modules

With the **Predom** module one can calculate and plot isothermal predominance area diagrams for one-, two or three-metal systems using data retrieved from the compound databases. Fig. 13 shows the entry and resulting diagram for the one-metal Cu-P_{SO₂}-P_{O₂} system at 1000 K. After the components (Cu, S and O) have

been specified, the user clicks on "Next" and is presented with a list of possible axes, $\log_{10}X$ and $\log_{10}Y$ (X and Y are pressure or activity of S, S_2 , ... S_n , SO, SO_2 , SO_3 , O_2 etc.), and possible product species (gases, solids, liquids – these may be edited by clicking on the "List" button). A useful feature of the module is the option to include the calculated total pressure isobar on the predominance diagram (plotted as "+"s in Fig. 13). Along such an isobar the total pressure is the sum of the partial pressures of *all* the gas species (in Fig. 13 $P(\text{total}) = 1 \text{ atm} = P_S + P_{S_2} + \dots + P_{S_n} + P_{\text{SO}} + P_{\text{SO}_2} + P_{\text{SO}_3} + P_{O_2} + P_{\text{Cu}} \dots$ etc.). Such a line represents the reaction path whereby, for example, Cu_2S oxidizes to, say, Cu_2O .

With **Predom** one can also calculate more complex predominance area diagrams such as a two-metal diagram of $\log_{10}(P_{\text{SO}_2})$ versus $\log_{10}(P_{\text{CO}})$ for M_1 - M_2 -S-O-C system at constant P_{O_2} and $M_1/(M_1+M_2)$ metal ratio. All equilibrium partial pressures and activities at any point on the diagram can be calculated, as can the coordinates of all invariant points. Diagrams can be stored, edited, and exported.

The **EpH** module (not shown here) is similar to the **Predom** module and permits one to generate Eh vs pH (Pourbaix) diagrams for one-, two or three-metal systems using data retrieved from the compound databases that also include infinitely dilute aqueous data.

Equilib Module

The **Equilib** module is the Gibbs energy minimization workhorse of **FactSage**. It calculates the concentrations of chemical species when specified elements or compounds react or partially react to reach a state of chemical equilibrium. In most cases the user makes three entries as shown in the **Equilib Reactants Window** (Fig. 14) and **Menu Window** (Fig. 15):

1st entry: Define the reactants, then click on 'Next >>'.

2nd entry: Select the possible compound and solution products.

3rd entry: Set the final conditions - T and P, or other constraints, then click on 'Calculate >>'.

The **Reactants Window** (Fig. 14) shows the entry for a copper-based pyrometallurgical system (variable amounts $<A>$ of FeO and SiO_2 with CaO, Cu_2O , Fe_2O_3 , Pb, Zn, Cu and Cu_2S). In the **Menu Window** (Fig. 15) the possible products are identified (gas phase, pure solids and slag, spinel, matte, copper alloy solution phases) together with a range of composition ($<A> = 40, 41, 42, \dots 57$), the temperature (1250°C) and total pressure (1 atm.). Not shown here is how one can set various constraints, options, targets, etc. (in the example the equilibrium partial pressure of oxygen was fixed at $P(O_2) = 10^{-8}$ atm). One then clicks the "Calculate >>" button and the computation commences. When the calculation is finished one is automatically presented with the **Results Window** where **Equilib** provides the equilibrium products of the reaction and where the results may be displayed in **F*A*C*T** and **ChemSage** output formats. The equilibrium product amounts are positive, satisfy the mass balance constraints with respect to the system components and correspond to the lowest possible Gibbs energy for this particular selection of possible products. For example Fig. 16 displays the results in **F*A*C*T** format at $<A> = 40$; this equilibrium point corresponds to silica saturation, $a(\text{SiO}_2) = 1.0$. The equilibrium compositions of the slag, matte and blister copper are also listed. Fig. 17 shows a **ChemSage** format for $<A> = 57$ that now corresponds to spinel saturation. The calculated values may also be presented and manipulated via the **List Window**. For example Fig. 18 shows the distribution of the elements (Cu, Fe) among the phases when $<A> = 50$.

One may enter up to 48 reactants consisting of up to 32 different components (elements and electron phases). Reactants may include "streams" - these are equilibrated phases stored from the results of previous calculations (useful in process simulation). Phases from the compound and solution databases are retrieved and offered as possible products in the **Menu Window**. These may include pure substances (liquid, solid), ideal solutions (gas, liquid, solid, aqueous) and non-ideal solutions (real gases, slags, molten salts, mattes, ceramics, alloys, dilute solutions, aqueous solutions, etc.) from the databases described earlier.

Equilib employs the Gibbs energy minimization algorithm and thermochemical functions of **ChemSage** [90Eri] and offers great flexibility in the way the calculations may be performed. For example, the following are permitted: a choice of units (K, C, F, bar, atm, psi, J, cal, BTU, kwh, mol, wt.%, ...); dormant phases in equilibria; equilibria constrained with respect to T, P, V, H, S, G, U or A or changes thereof; user-specified product activities (the reactant amounts are then computed); user-specified compound and solution data; and much more. Phase targeting and one-dimensional phase mappings with automatic search for phase transitions are possible. For example, one can calculate all equilibrium (or Scheil-Gulliver non-equilibrium) phase transitions as a multicomponent mixture is cooled.

Equilib offers a post-processor whereby the results may be manipulated in a variety of ways: tabular output ordered with respect to amount, activity, fraction or elemental distribution; post-calculated activities; user-specified spreadsheets of $f(y)$ where $y = T, P, V, H, S, G, U, A, Cp$ or species mole, gram, activity, mass fraction and $f = y, \log(y), \ln(y), \exp(y)$ etc. for Lotus 1-2-3, Microsoft Word or Excel. For example Fig. 19 shows post-processing of the results and the generation of a $Cu\text{ wt.\% vs }Fe(\text{total})/SiO_2\text{ wt.\%}$ diagram for the complete set (18) of equilibrium calculations. Fig. 20 shows (top) a display of the thermodynamic partial properties functions, and (bottom) a partial listing of the calculated integral properties of a solution phase (FACT-MATT) for all 18 calculations.

Phase Diagram and Figure Modules

Phase Diagram is a generalized module that permits one to calculate, plot and edit unary, binary, ternary and multicomponent phase diagram sections where the axes can be various combinations of T, P, V, composition, activity, chemical potential, etc. The resulting phase diagram is automatically plotted by the **Figure** module. It is possible to calculate and plot: classical unary temperature versus pressure, binary temperature versus composition, and ternary isothermal isobaric Gibbs triangle phase diagrams; two-dimensional sections of a multi-component system where the axes are various combinations of T, P, V, composition, activity, chemical potential, etc.; predominance area diagrams (for example P_{SO_2} vs P_{O_2}) of a multicomponent system (e.g. Cu-Fe-Ni-S-O) where the phases are real solutions such as mattes, slags and alloys; reciprocal salt phase diagrams; etc.

The calculation of the binary temperature versus composition phase diagram for the CaO-SiO₂ system is shown in Figs. 21 and 22. In the **Phase Diagram** module the system components (CaO, SiO₂) are first entered in the *Reactants Window* (Fig. 21-top). Then the type of phase diagram is defined in the *Variables Window* (Fig. 21-bottom) where the user selects the type of diagram (Y vs X, or Gibbs triangle), the type of axes (composition, activity and chemical potential), the possible composition variables, and the limits and constants of the phase diagram. Data from the compound and solution databases are offered as possible product phases in the *Menu Window* (Fig. 22-top). In the case of CaO-SiO₂, the slag solution phase (FACT-SLAG) and all pure solids (including those outside the plane CaO-SiO₂) are selected as possible product phases. By clicking on the 'Calculate >>' button the phase diagram is automatically calculated and plotted in real time (Fig. 22-bottom). When the calculation is complete the **Figure** module uses the graph as a dynamic interface. By pointing to any domain, tie lines and stable phases are automatically labeled. Optionally the figure can be manipulated: tie lines can be inserted in the plot, the equilibrium compositions and phase amounts at a point on the diagram can be calculated and shown in a table, and the diagram can be edited (add experimental data points, text, change font and colors etc.). Examples of edited diagrams are shown later.

The versatility of the choice of axes in the *Variables Window* enables one to generate many different types of phase diagrams. Fig. 23 is a classical isothermal predominance area diagram for the Cu-SO₂-O₂ system. The system components are Cu, SO₂, O₂; the axis variables are $\log_{10}(P_{SO_2})$ and $\log_{10}(P_{O_2})$ and the temperature is set constant; the possible phases in the phase diagram are gas and stoichiometric solids taken from the FACT compound database. This diagram may be compared the one (Fig. 13) produced by the **Predom** module for the same system.

Unlike the **Predom** module, **Phase Diagram** can produce diagrams that also include real solution data. Fig 24 shows the $\log_{10}(P_{O_2})$ vs $Cr/(Cr+Fe)$ phase diagram at 1573 K where the system components are Fe, Cr and O₂. The possible phases are the gas and various real solutions taken from the **FACT** (oxides) and **SGTE** (alloys) databases. Fig. 25 is the input/output for an isopleth of T(C) vs TiO₂/(FeO+TiO₂) ratio at 50 mol % Fe in the FeO-TiO₂-Fe system again using both **FACT** and **SGTE** solution databases. An example of the interactive power of **Phase Diagram** is the equilibrium calculation shown in Fig. 26 where the user has first selected the *phase equilibrium mode* and then pointed and clicked at the coordinates 1450°C and TiO₂/(FeO+TiO₂) = 0.7. Note, these results would be identical to an **Equilib** calculation at 1450°C and 1 atm where the reactants are 0.35 TiO₂ + 0.15 FeO + 0.5 Fe.

Fig. 27 is the input/output for a Gibbs ternary section of the CaO-Al₂O₃-SiO₂ system at 1600°C using **FACT** data.

Examples of the combined use of the **Phase Diagram**, **Equilib** and **Figure** modules to generate phase diagrams are shown in Figs. 28 to 31.

How the Phase Diagram Module Works

The possible types of phase diagram sections that may be calculated are based on a *thermodynamically consistent theory of generalized phase diagram mapping* [01Pel]. Similar to the rules outlined by Hillert [97Hil] a set of simple rules has been derived that dictate what axes and constants constitute a true phase diagram. The Zero Phase Fraction (ZPF) line principle was introduced by Morral and co-workers [84Bra, 84Mor, 86Gup]. All true two-dimensional sections consist of a collection of ZPF lines, one for each phase. The phase appears on one side of its ZPF line and does not appear on the other, and the ZFF line either forms a closed loop inside the diagram or terminates at the edges of the diagram. In **FactSage** this has been combined with the phase diagram rules in order to derive a strategy for the mapping of a complete phase diagram without the need for user-defined starting points. This greatly simplifies the strategy for mapping the complete phase diagram since it is simply a question of tracing all ZPF lines.

Especially in higher-order systems the correct choice of axes and constants may not be obvious. For example, in the Fe-Cr-O system it may not be evident that for a true phase diagram at constant T (and total P) one may plot log P_{O₂} versus n_{Cr}/(n_{Cr} + n_{Fe}) but not versus n_{Cr}/(n_{Cr} + n_{Fe} + n_O). The reason for this is that in the latter case certain regions of the diagram may not represent unique equilibrium conditions. The **Phase Diagram** module has been conceived such that only inputs leading to true phase diagram sections are allowed. Future work includes calculating polythermal projections (e.g. the liquidus surfaces) of multicomponent phase diagrams, and the calculation of Pourbaix diagrams, Eh vs pH, of a multicomponent alloy where non-ideality of the aqueous and metallic phases is taken into account.

4. Manipulate Modules

FactSage offers a variety of modules that can post-process the tabular and graphical results or preprocess reactant inputs for complex equilibrium calculations in **Equilib**. The **Results** module enables one to generate graphical output from **Equilib** calculations and produce a variety of plots from a single set of equilibrium tables. **Mixture** is used to combine a *group* of reactant substances, e.g. 0.21 O₂(g) and 0.79 N₂(g), into a *single* stream, e.g. [air], that can then be imported as such as a reactant to **Equilib**. In this manner it is possible to store very complex mixtures and streams (e.g. slags, minerals, bunker oil). Also the results of an **Equilib** calculation may be automatically stored – for example the gas products of FeS oxidation could be stored as a stream and given a name such as “roaster_gas” that can be then edited by the **Mixture** program before being imported as a reactant to **Equilib** for a subsequent calculation.

Although mainly used for phase diagrams, **Figure** is a generalized plotting program that permits one to display, edit and manipulate the various graphs and plots produced by the **FactSage** modules. *.fig files may

be opened and edited by *Edition, Format, Frame & Axes Windows* and *Menu Bars*. For example Fig. 28 shows the use of the *View menu bar* to edit the calculated binary phase diagram for CaSiO₃-MgSiO₃. Figs. 29 to 31 illustrate sample edited figures. The diagrams may be exported as *.fig (ASCII for repeated use with **Figure**), *.bmp, *.emf and *.wmf files (bitmap, enhanced metafile and windows metafile) for subsequent use with other Windows® software.

Conclusions

This article has presented a summary of the modules offered in the **FactSage** thermochemical software and database package. Although emphasis has been placed on the calculation and manipulation of phase diagrams, the reputation of **FactSage** has been established mainly in the field of complex chemical equilibria and process simulation where the software has unique capabilities. For example with **FactSage** one is able to access both **FACT** (slag, matte, salt, ceramic, aqueous) and **SGTE** (alloy, carbonitride) solution databases; import and export streams and mixtures; import and export **ChemSage/ChemApp** files; perform open and closed system calculations; perform a predominant calculation involving thousands of possible product species (where the program does the species selection for the user); etc.

In addition to the continuous ongoing improvements to the modules and databases, our plans for the future include addition of aqueous databases for concentrated solutions, for example **OLI** [02Oli], and the development of a process simulation module (**SimuSage**). Through the use of exported **ChemSage** files it is already possible to combine kinetic and phase equilibrium calculations in the Excel add-in **ChemSheet**.

FactSage is a 32-bit application written with a blend of Visual-Basic (45%), Delphi (20%), C++(10%) and FORTRAN-90 (25%) - all the modules run in a Windows environment. It requires Microsoft Windows 95, 98, 2000, Millennium, NT (SP4, SP5 or SP6) or XP and a PC (recommend at least Pentium 200) with at least 32 MB RAM and 100 MB free disk space. Additional information is available through the Internet at www.factsage.com.

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- 97Hil M.Hillert, *J. Phase Equilibria*, **18** (1997) 249-263.
- 01Pel A.D. Pelton, *Thermodynamics and Phase Diagrams of Materials*, Chapter 1 in "Phase Transformations in Materials", ed. G. Kostorz, Wiley-VCH, Ny, 2001, p 1 – 80.
- 02Crc CRCT – Centre for Research in Computational Thermochemistry, École Polytechnique (Université de Montréal), Québec, Canada: www.crct.polymtl.ca
- 02Oli OLI Sytems, Inc., New Jersey, U.S.A.: www.olisystems.com

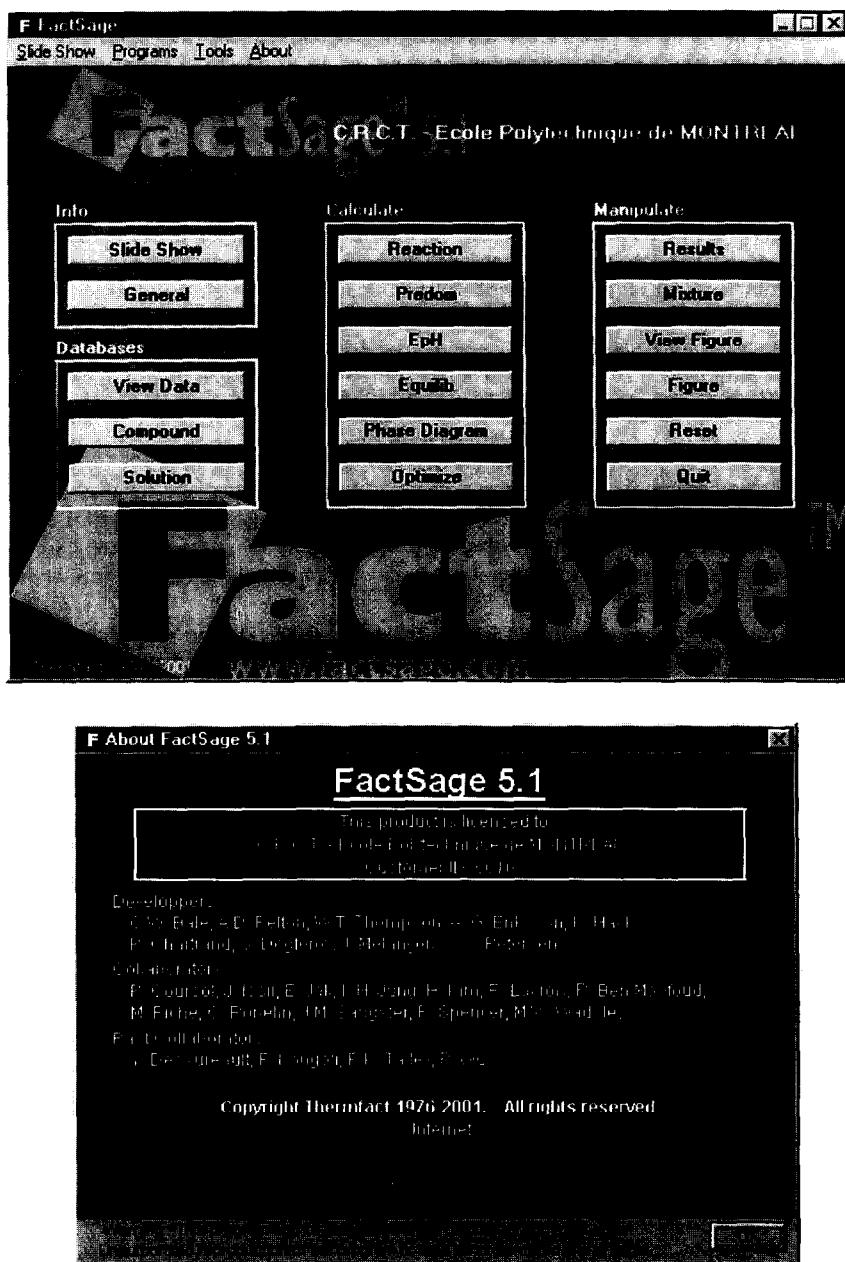


Figure 1 FactSage Main Menu and *About* Window.

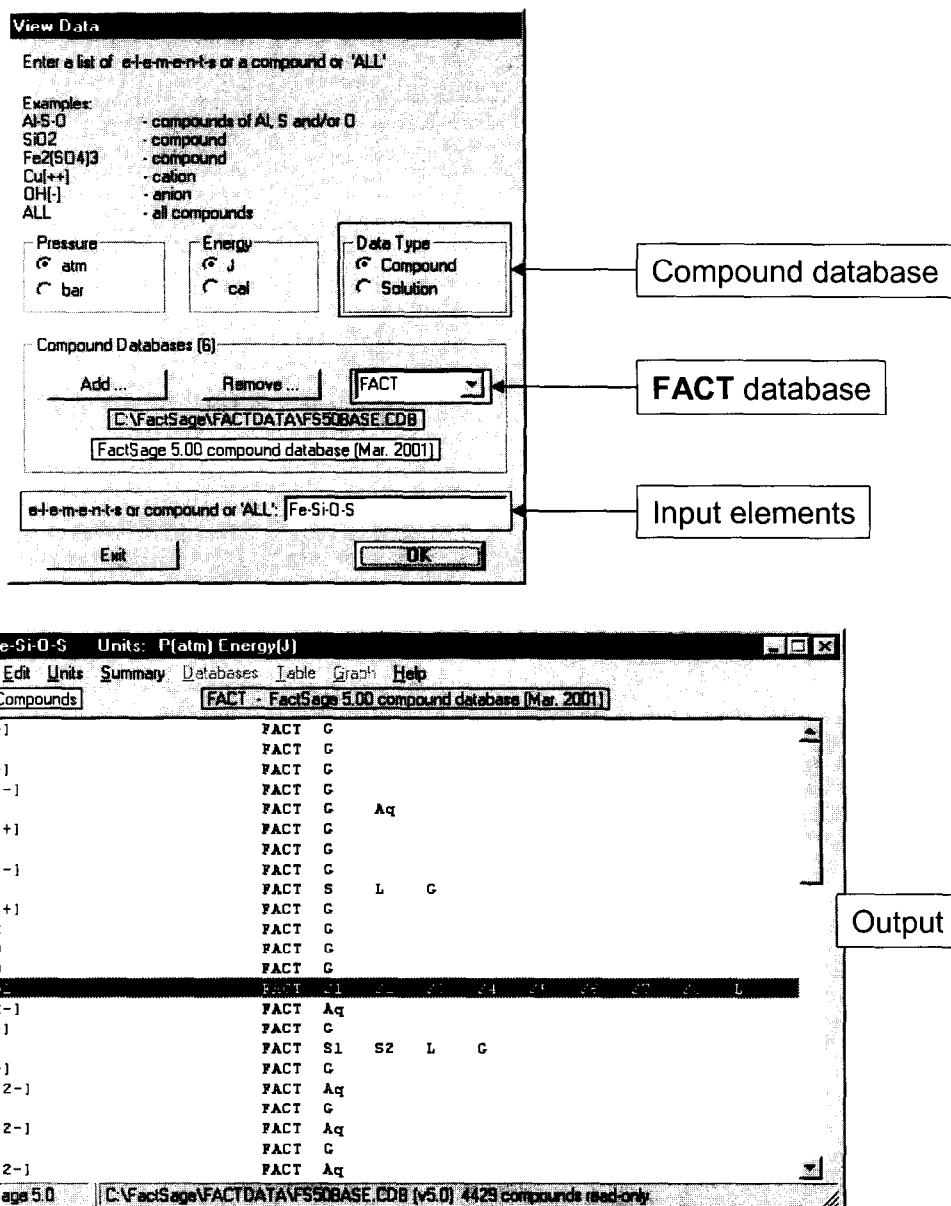


Figure 2 View Data Module – listing all Fe-Si-O-S species stored in the FACT compound database.

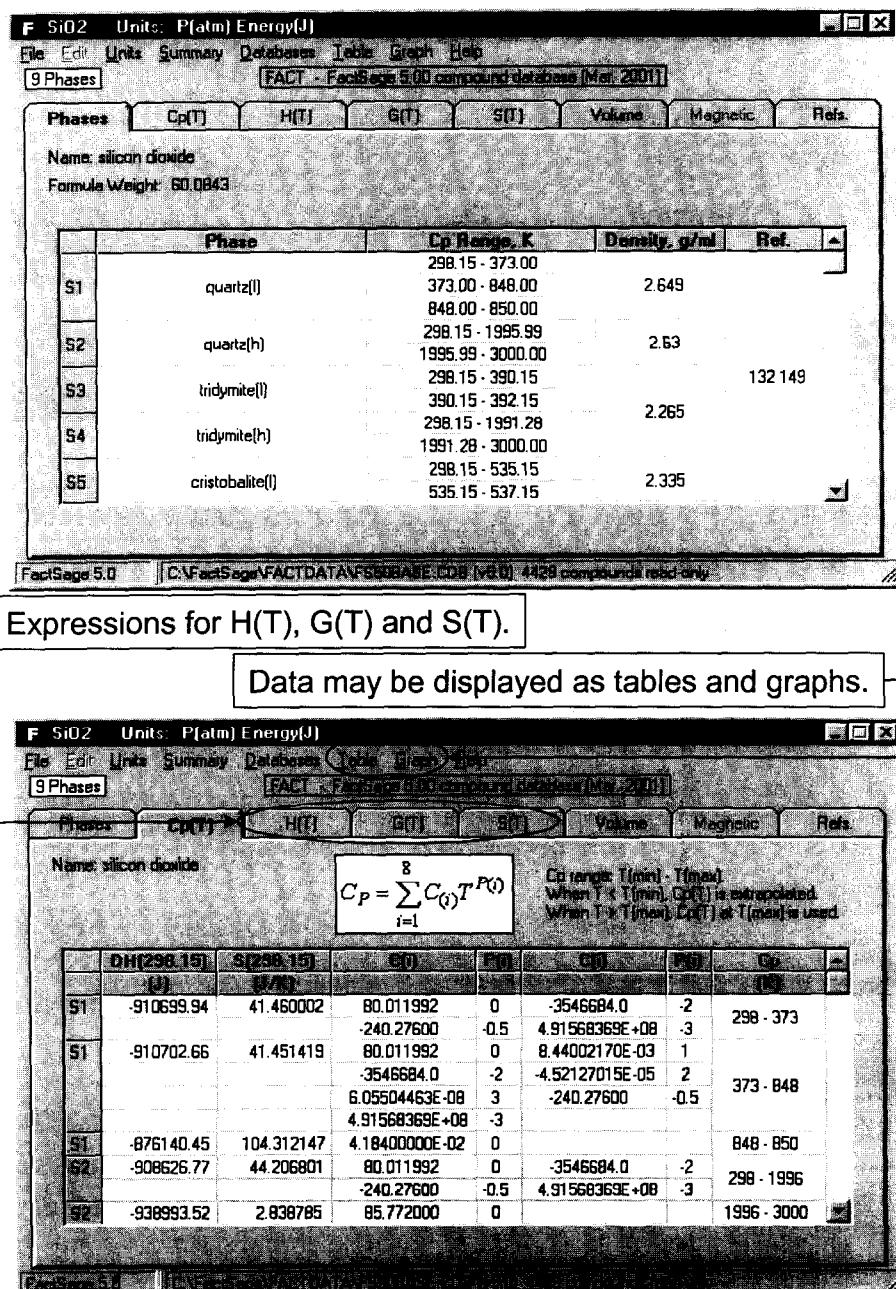


Figure 3 View Data Module – summary of phases (top) and compound data (bottom) for SiO₂.

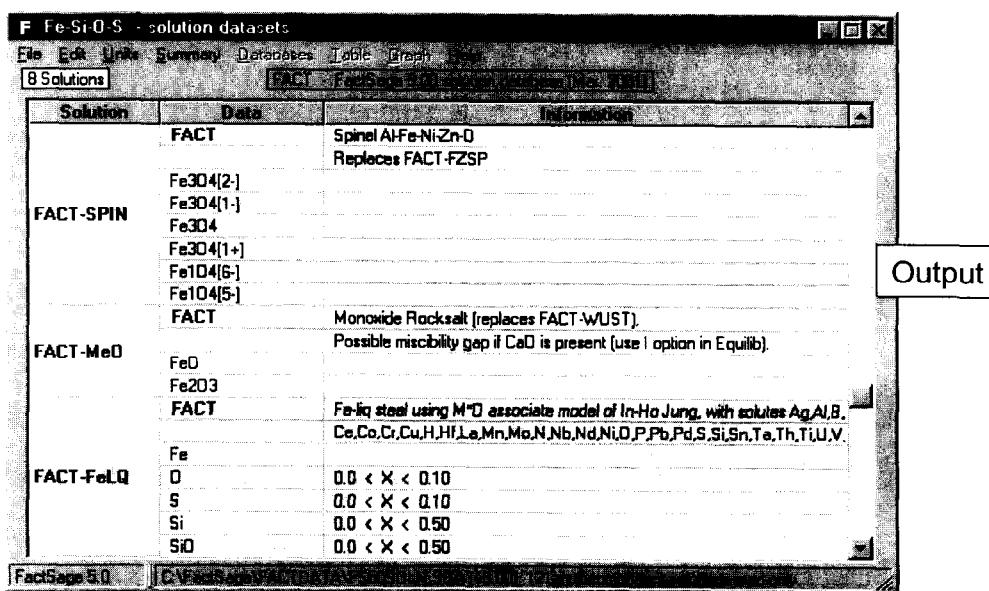
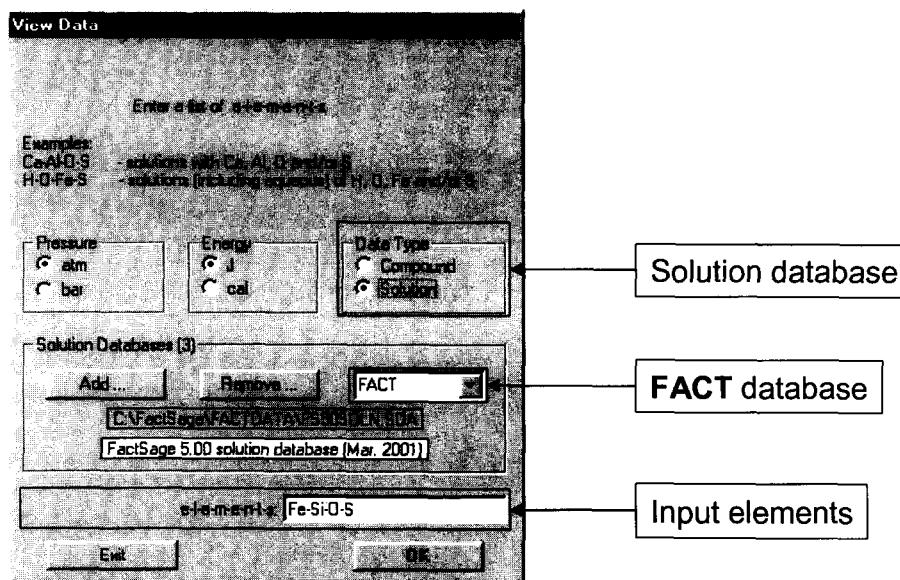


Figure 4 View Data Module – listing the Fe-Si-O-S phases stored in the FACT solution database.

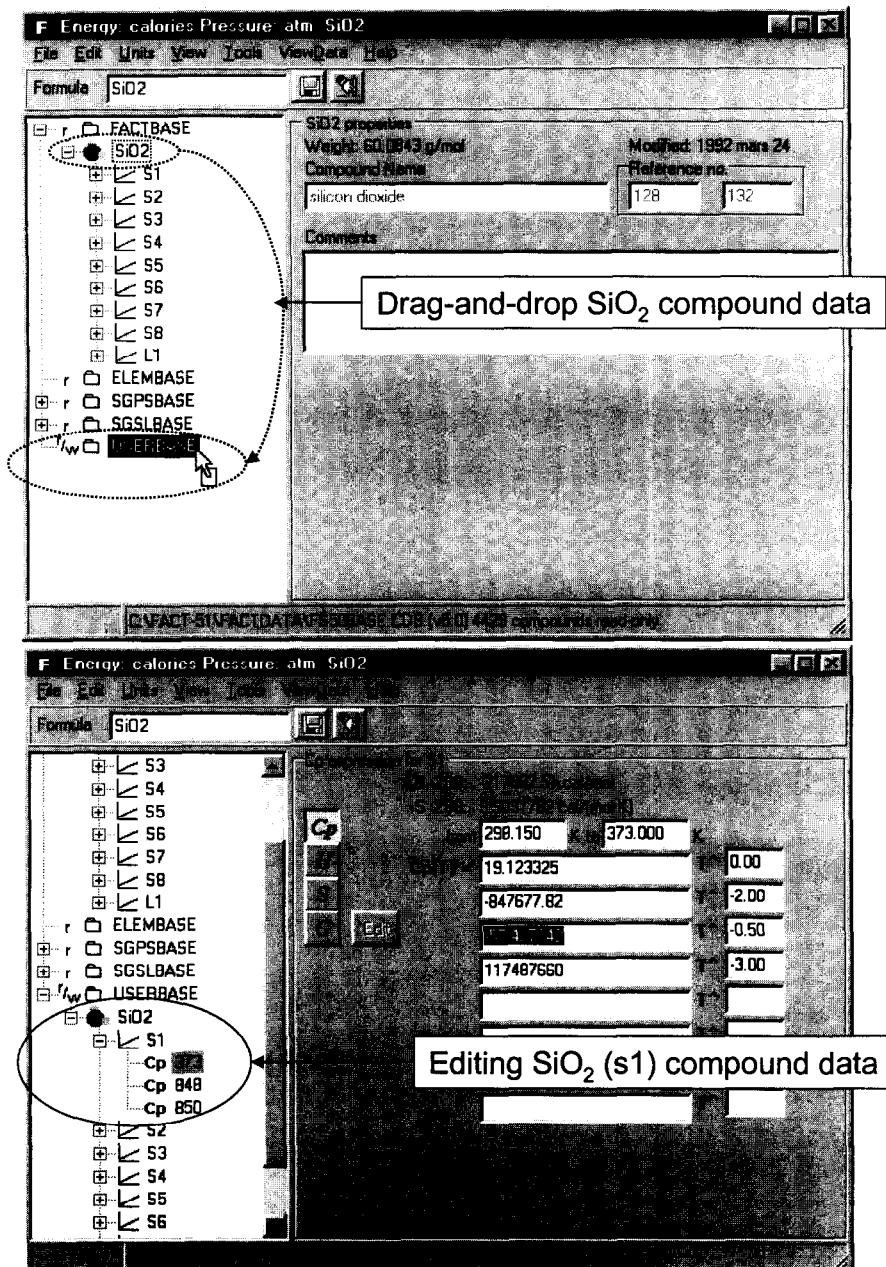


Figure 5 Compound Module – Top: drag-and-drop of SiO₂ data from the FACT to the private USER database. Bottom: manipulation of Cp(T) data in the USER database.

Magnetic contribution expression to the Gibbs free energy G_{mag} :

$$G_{mag} = RT \ln(\beta + 1) g(\tau) \quad \text{where} \quad \tau = \frac{T}{T_c}$$

$$g(\tau) = \frac{1}{D} \left\{ 1 - \left[\frac{79\tau^{-1}}{140p} + \frac{474}{497} (p^{-1} - 1) \left(\frac{\tau^3}{6} + \frac{\tau^9}{135} + \frac{\tau^{15}}{600} \right) \right] \right\} \quad \text{when } \tau \leq 1$$

$$g(\tau) = \frac{1}{D} \left[\frac{\tau^{-5}}{10} + \frac{\tau^{-15}}{315} + \frac{\tau^{-25}}{1500} \right] \quad \text{when } \tau > 1$$

$$\text{where } D = \frac{518}{1125} + \frac{11692}{15975} (p^{-1} - 1)$$

p is the P factor and **β** is the structure factor.

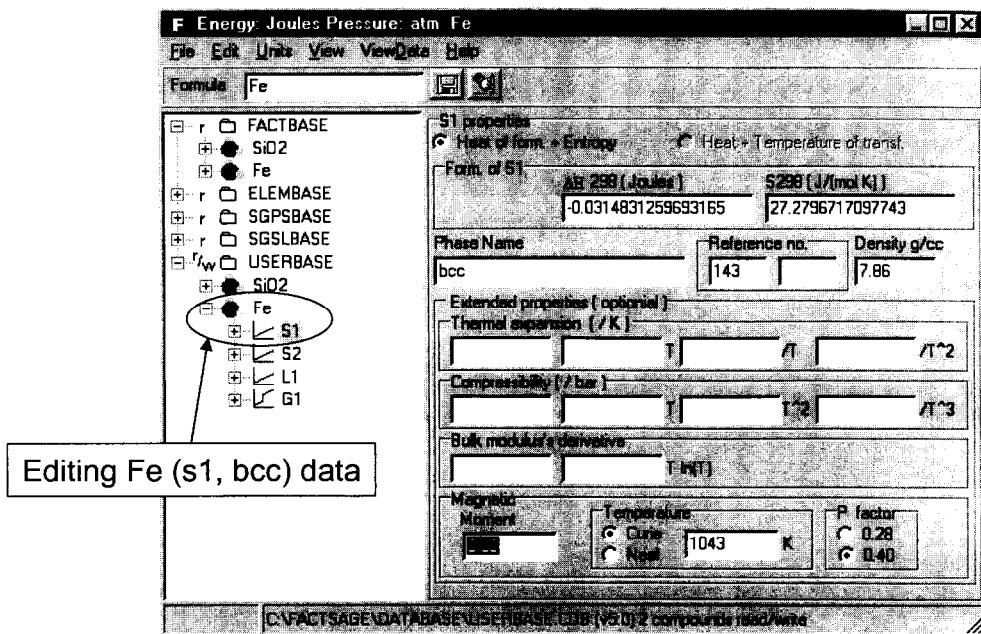


Figure 6 Compound Module – manipulating the magnetic data of Fe stored in the USER database.

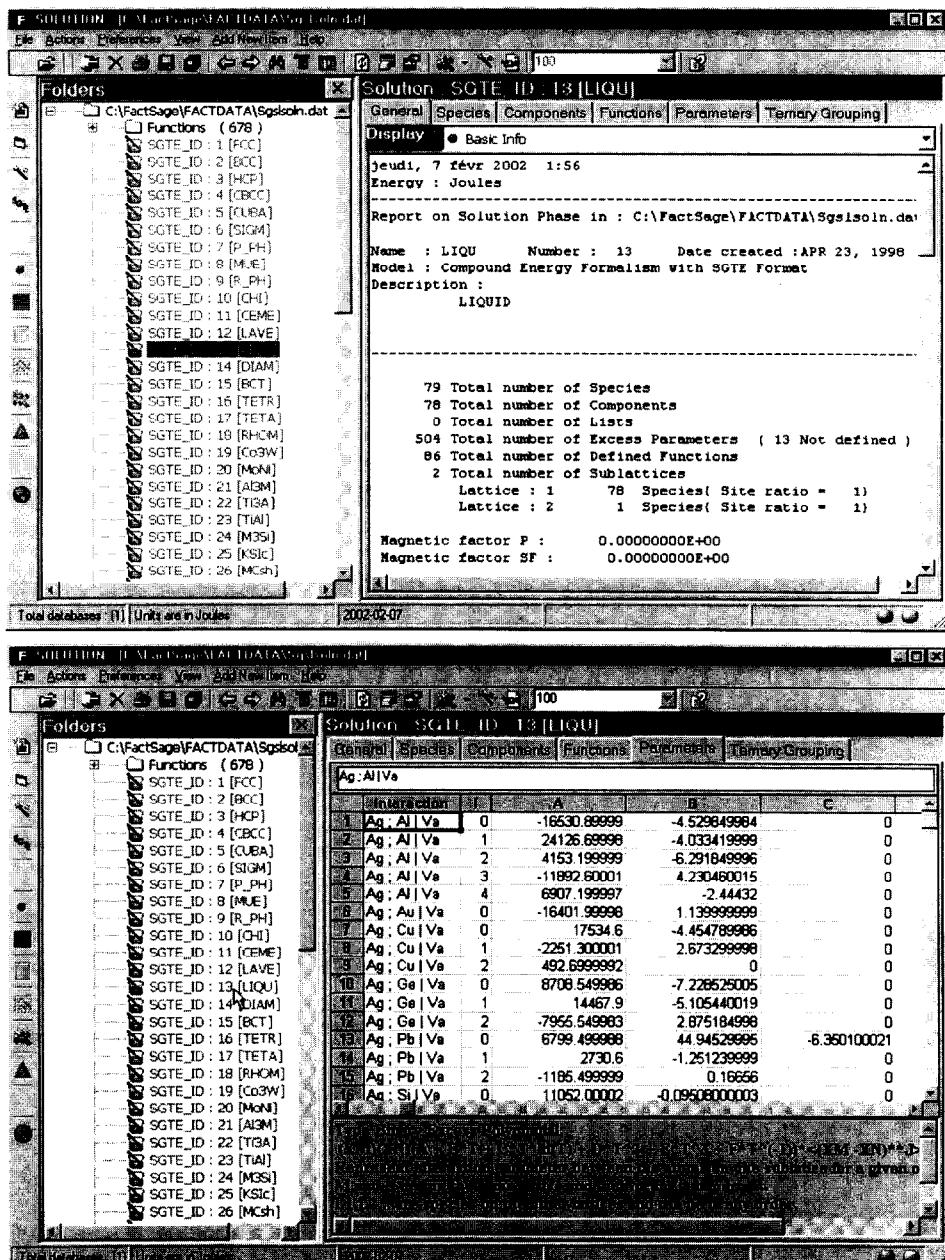


Figure 7 Solution Module – SGTE alloy database. Top: listing the solution phases.
Bottom: displaying the parameters of the liquid phase.

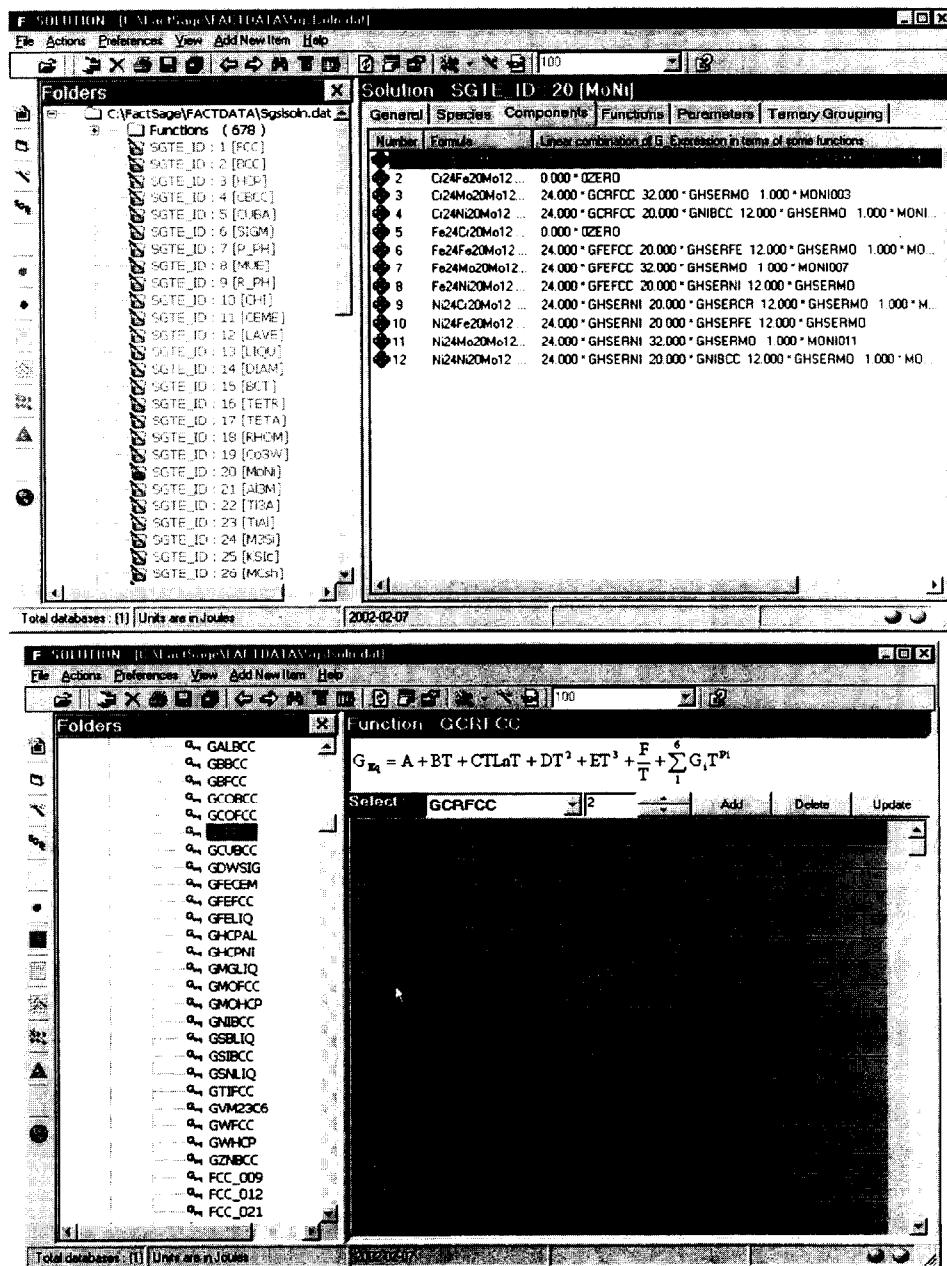


Figure 8 Solution Module – SGTE alloy database. Top: displaying the components of the MoNi_Delta phase. Bottom: displaying the contents of the GCRFCC function.

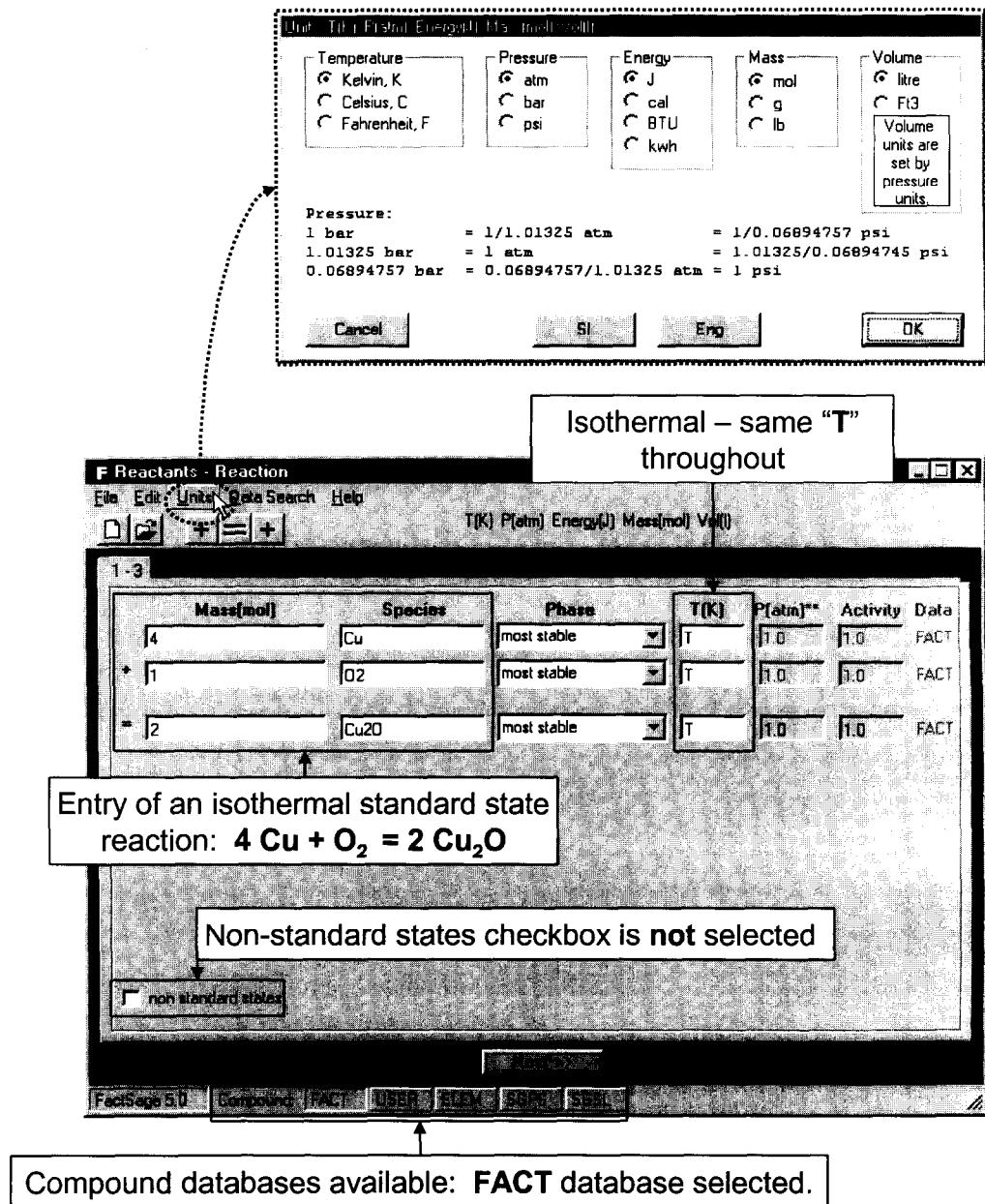


Figure 9 Reaction Module – *Reactants Window* Cu-O₂-Cu₂O system. Entry of the isothermal standard state reaction for copper oxidation.

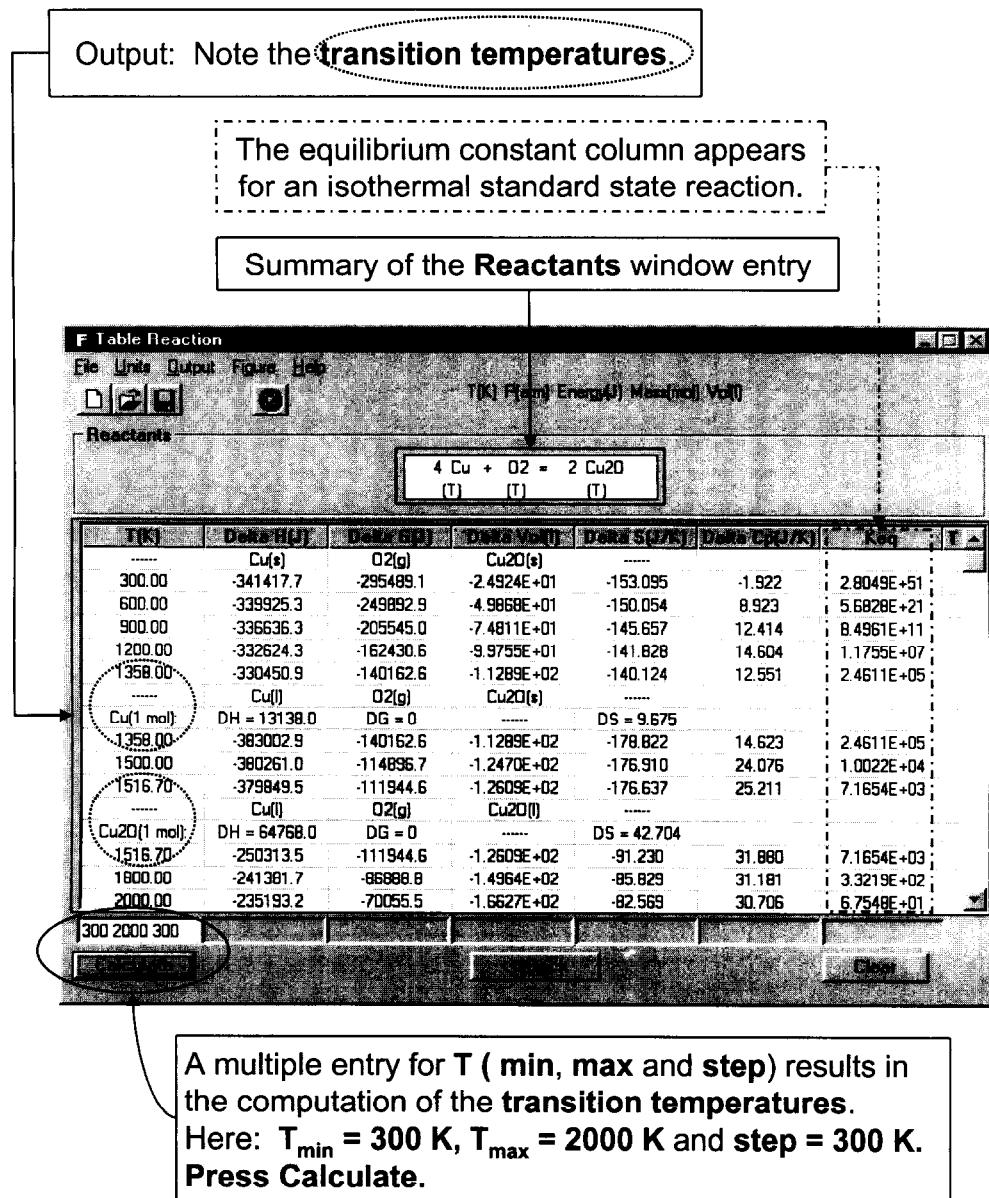


Figure 10 Reaction Module – Table Window Cu-O₂-Cu₂O system. Calculation of common thermodynamic values.

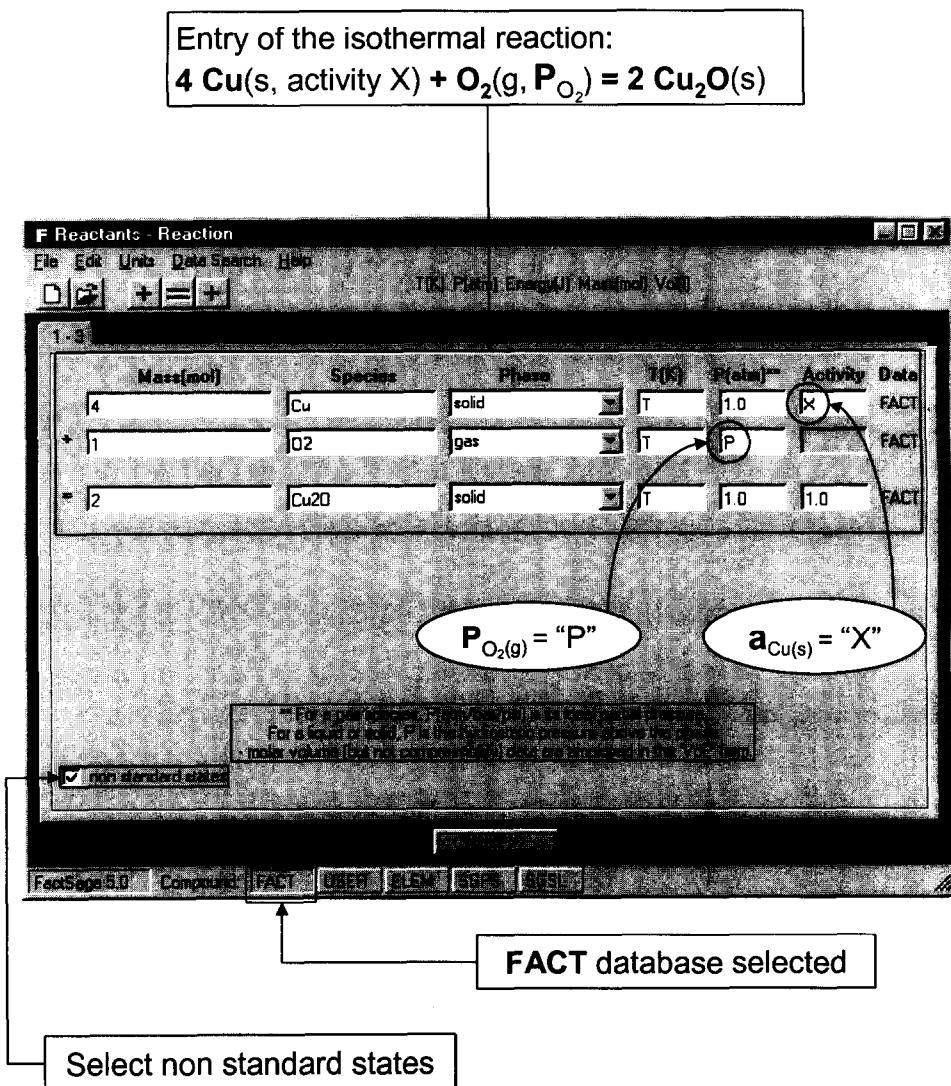


Figure 11 Reaction Module – Reactants Window Cu-O₂-Cu₂O system. Entry of the isothermal non-standard state reaction for copper oxidation.

Line 1:**Input:**

Standard state reaction at $T = 1000 \text{ K}$, $P_{\text{O}_2(\text{g})} = 1 \text{ atm}$ and $a_{\text{Cu(s)}} = 1$

Output: $\Delta H^\circ = -335.38 \text{ kJ}$, $\Delta G^\circ = -191.16 \text{ kJ}$, etc.

Line 2:

Input: Reaction at $T = 1000 \text{ K}$, $a_{\text{Cu(s)}} = 1$ and $\Delta G = 0 \text{ J}$

Output: $P_{\text{O}_2(\text{g})} = 1.3059 \times 10^{-10} \text{ atm}$, etc.

Line 3:

Input: Reaction at $T = 1000 \text{ K}$, $P_{\text{O}_2(\text{g})} = 1 \text{ atm}$ and $\Delta G = 0 \text{ J}$

Output: $a_{\text{Cu(s)}} = 3.1903 \times 10^{-3}$, etc.

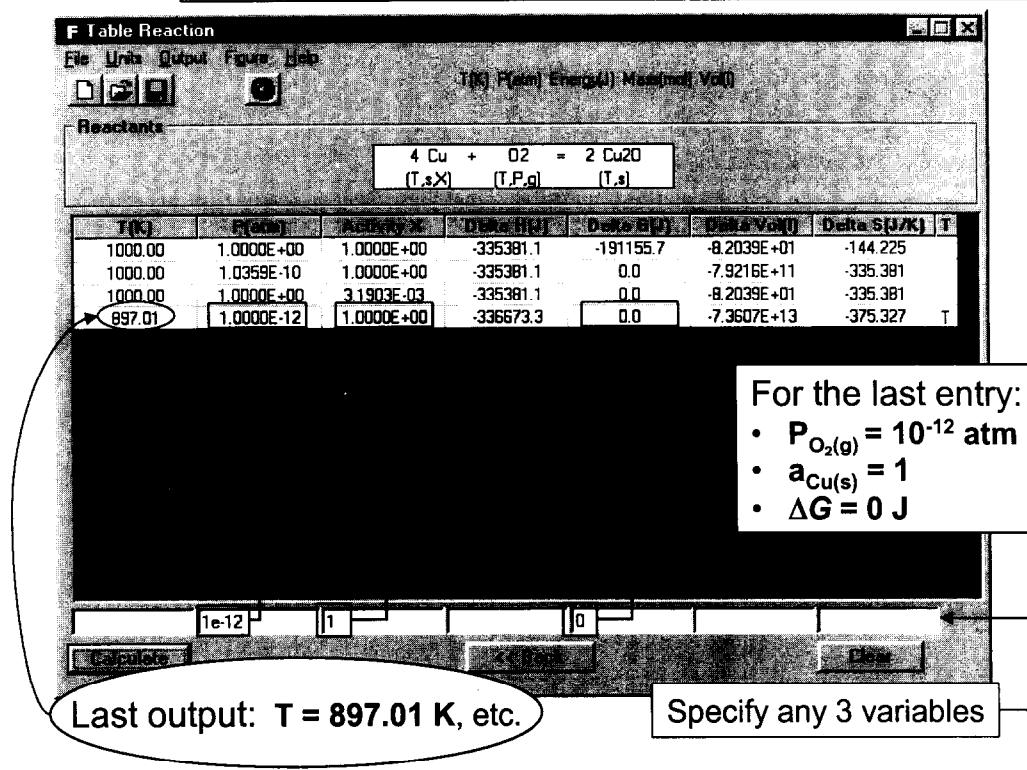


Figure 12 Reaction Module – Table Window Cu-O₂-Cu₂O system. Calculation of thermodynamic values by the interactive spreadsheet format.

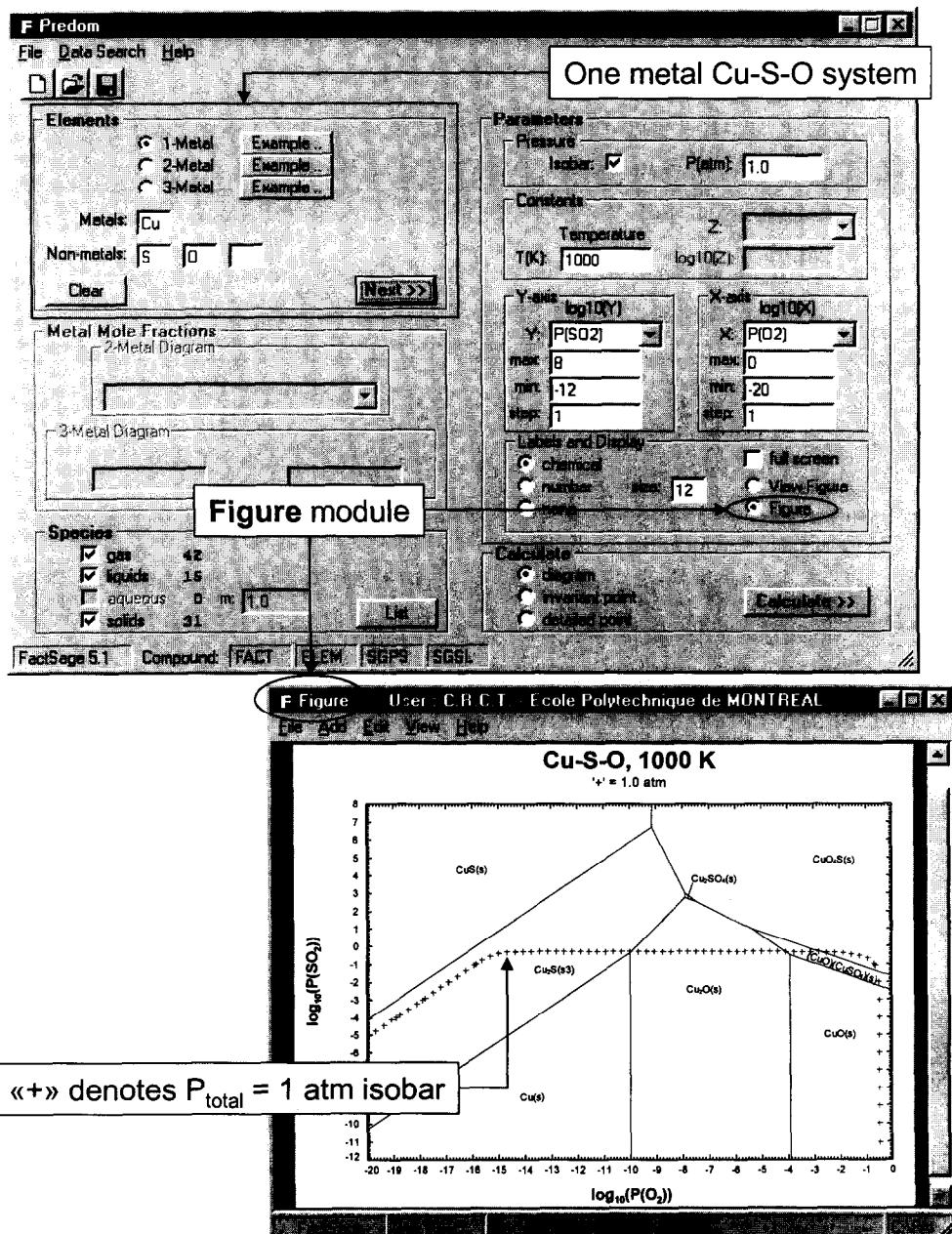


Figure 13 Predom Module – Top: entry of the one-metal Cu-p(SO₂)-p(O₂) system at 1000 K.
Bottom: resulting calculated predominance diagram.

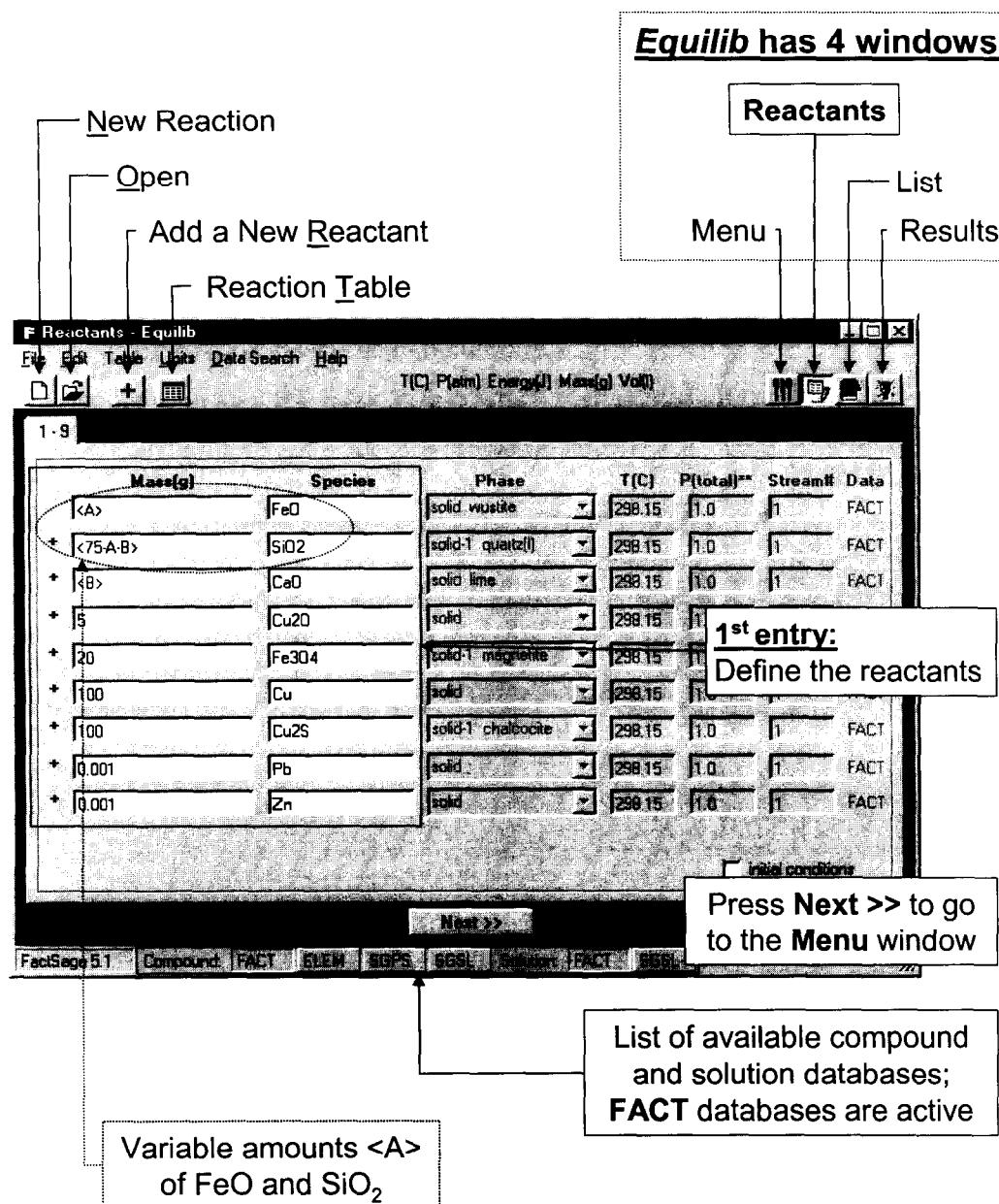


Figure 14 **Equilib Module – Reactants Window Cu-matte-slag system.** Entry of the reactants including a variable <A> amount of FeO and SiO₂.

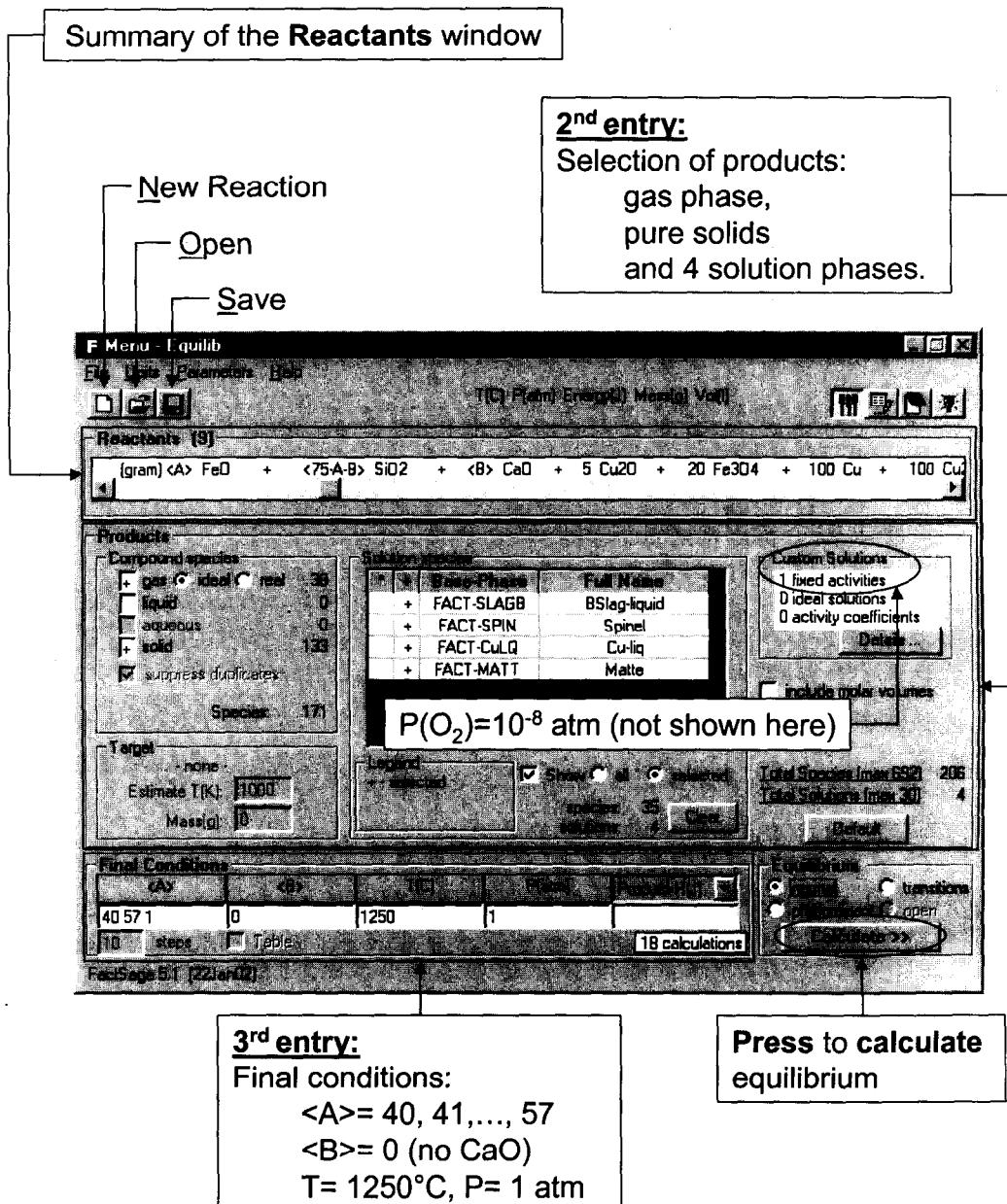


Figure 15 Equilib Module – Menu Window Cu-matte-slag system. Selection of possible product phases and definition of the final conditions.

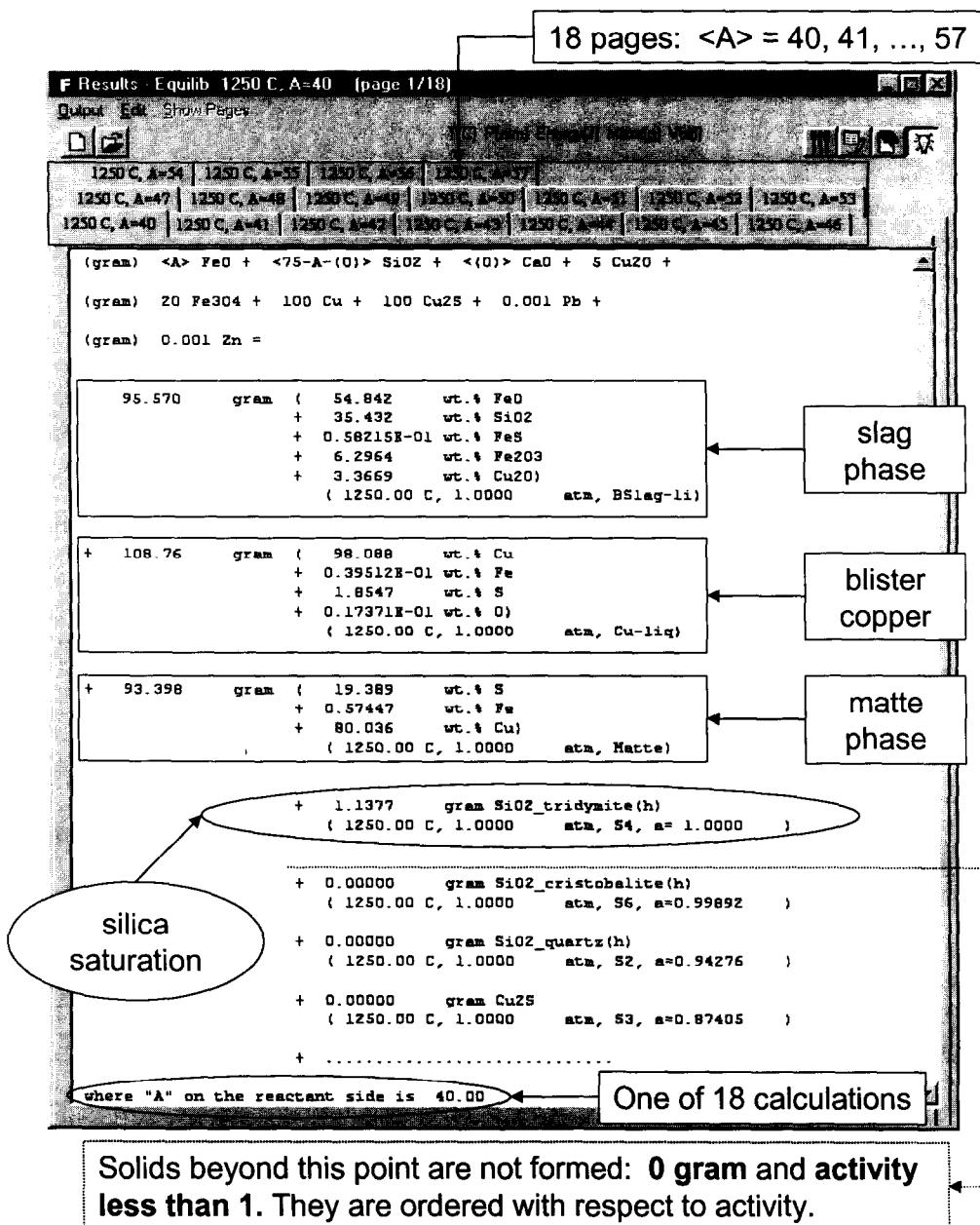


Figure 16 Equilib Module – Results Window Cu-matte-slag system. Display of the results in F^*A^*C*T Format for silica saturation ($\langle A \rangle = 40$).

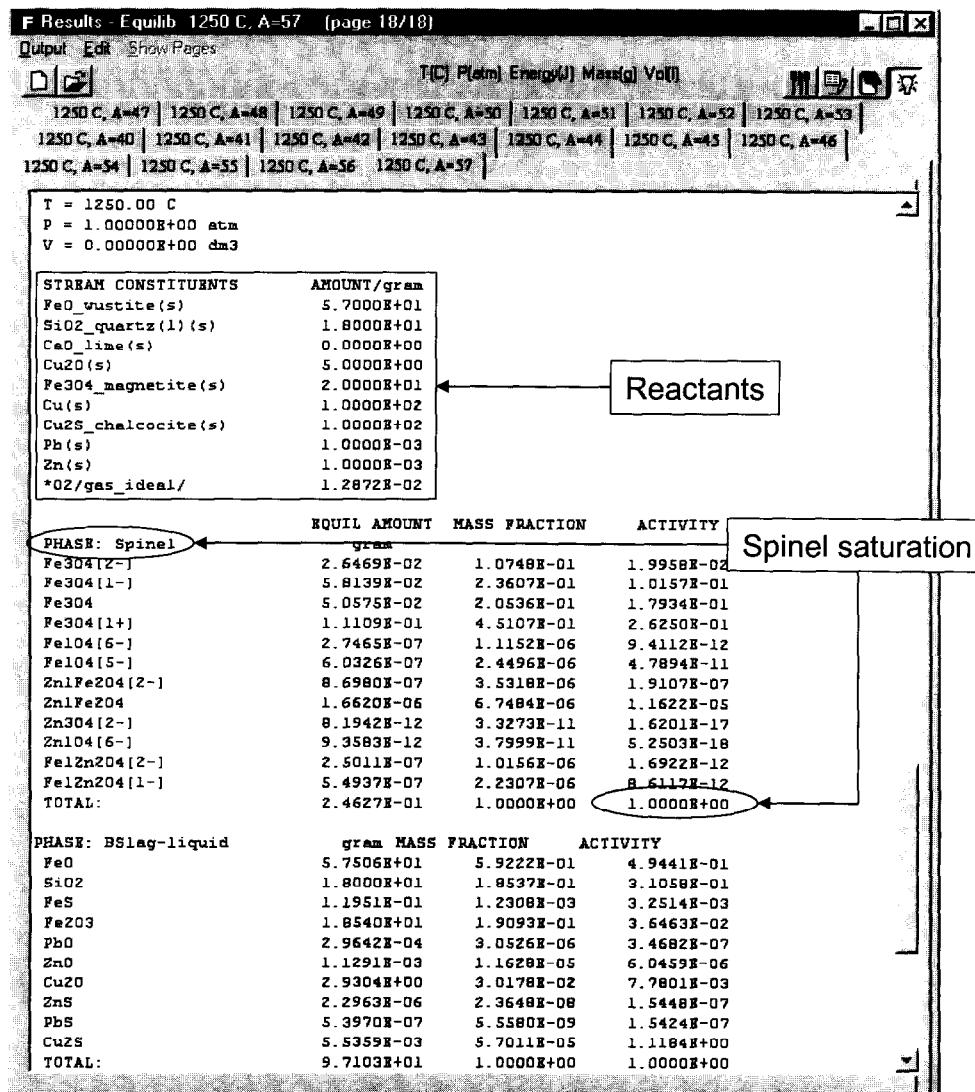
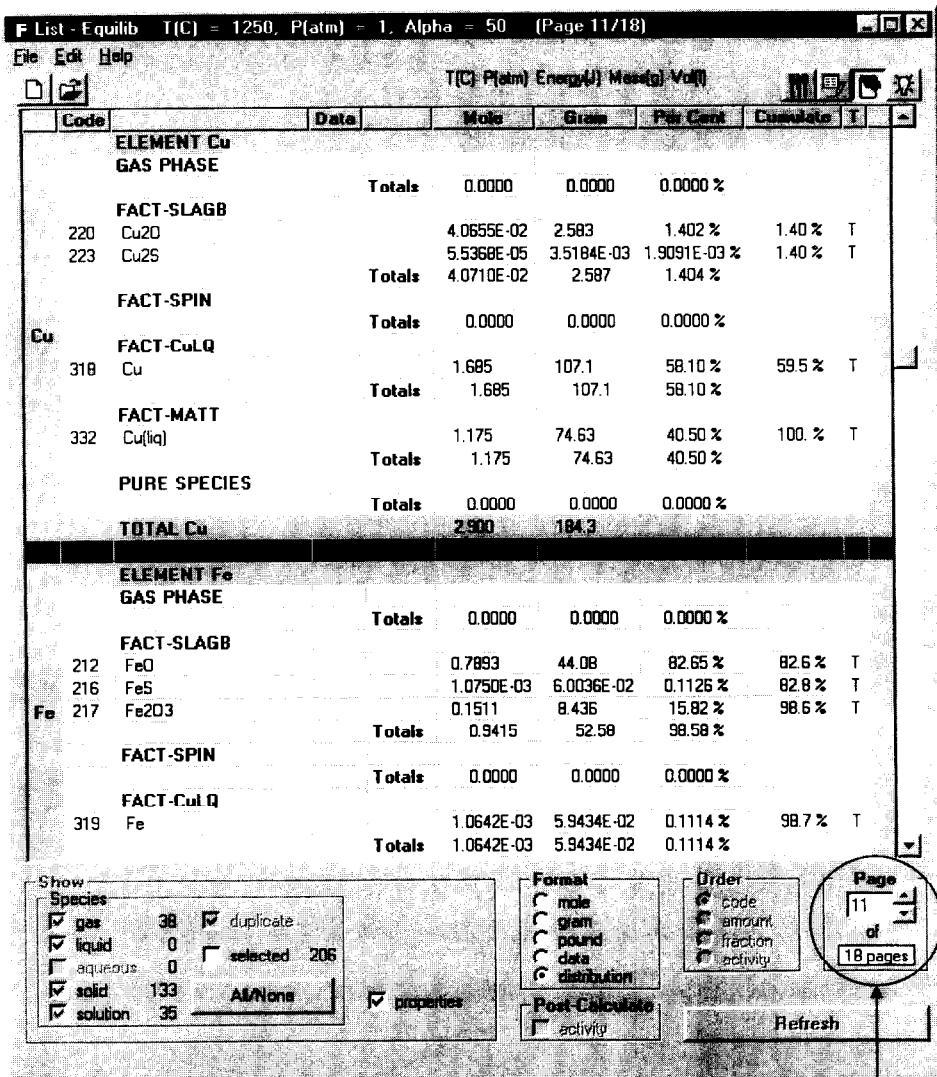


Figure 17 Equilib Module – Results Window Cu-mattc-slag system. Display of the results in ChemSage Format for spinel saturation (<A> = 57).



One of 18 calculations

Figure 18 Equilib Module – List Window Cu-matte-slag system. Distribution of the elements (Cu, Fe) among the phases when $\langle A \rangle = 50$.

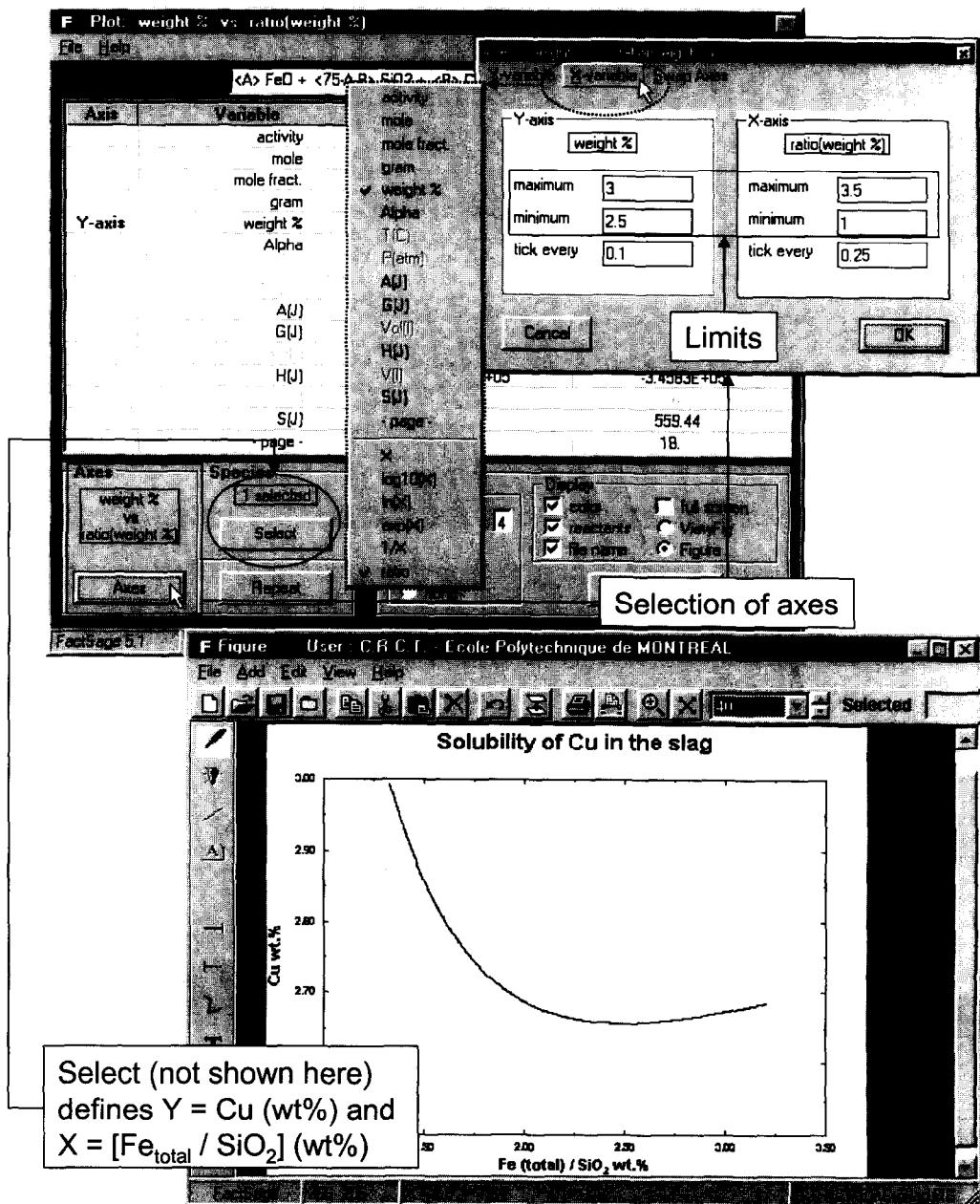


Figure 19 Equilib Module – Post-processor Window Cu-matte-slag system. Defining and plotting a Cu wt.% vs $Fe(\text{total})/SiO_2$ wt.% diagram for all results ($\langle A \rangle = 40$ to 57).

List of partial properties functions

F Molar Partial Properties FACT-MATT - Matte

Output Species Standard States

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

5/5 species 6 partial properties 16/16 properties

Property	Description
+ a(i)	activity of species i
+ gamma(i)	activity coefficient of species i = a(i)/a_ideal(i)
+ Delta_g(i)	= g(i) · go(i) = RT ln a(i)
+ Delta_h(i)	= h(i) · ho(i) = h(excess)(i)
+ Delta_s(i)	= s(i) · so(i)
+ g(i)	= h(i) - T · s(i)
+ h(i)	absolute h of species i with respect to elements at 25 C
+ s(i)	absolute s of species i
+ go(i)	g of species i in standard state
+ ho(i)	h of species i in standard state
+ so(i)	s of species i in standard state
+ a_ideal(i)	ideal activity of species i = mole fraction X(i)
+ Delta_g_ideal(i)	= RT ln a_ideal(i)
+ Delta_s_ideal(i)	= -R ln a_ideal(i)
+ g_excess(i)	= Delta_g(i) · Delta_g_ideal(i)
+ s_excess(i)	= Delta_s(i) · Delta_s_ideal(i)

Select All Close Close

F Molar Integral Properties FACT-MATT - Matte - Energy(J), Mass[mol]

File Edit

Page	Date	Delta_e	Delta_h	Delta_s	Energy	Delta_n_ideal	Delta_s_ideal
1	-43035.	-38667.	2.8676	-34668.	-2.6258	-8367.3	5.4934
2	-43038.	-38667.	2.8696	-34667.	-2.6259	-8370.3	5.4954
3	-43047.	-38666.	2.8767	-34666.	-2.6259	-8381.3	5.5026
4	-43057.	-38664.	2.8840	-34664.	-2.6258	-8392.3	5.5099
5	-43066.	-38662.	2.8913	-34663.	-2.6258	-8403.4	5.5171
6	-43076.	-38661.	2.8986	-34662.	-2.6257	-8414.3	5.5243
7	-43085.	-38659.	2.9057	-34660.	-2.6256	-8425.0	5.5313
8	-43094.	-38658.	2.9128	-34659.	-2.6254	-8435.5	5.5382
9	-43103.	-38656.	2.9195	-34657.	-2.6253	-8445.6	5.5448
10	-43111.	-38655.	2.9261	-34656.	-2.6251	-8455.3	5.5512
11	-43119.	-38653.	2.9323	-34655.	-2.6249	-8464.6	5.5573
12	-43127.	-38652.	2.9384	-34654.	-2.6247	-8473.3	5.5630
13	-43134.	-38650.	2.9440	-34653.	-2.6245	-8481.6	5.5685
14	-43141.	-38649.	2.9493	-34652.	-2.6242	-8489.4	5.5736
15	-43147.	-38647.	2.9544	-34651.	-2.6240	-8496.7	5.5784
16	-43153.	-38646.	2.9591	-34650.	-2.6237	-8503.5	5.5828
17	-43159.	-38645.	2.9635	-34649.	-2.6235	-8509.9	5.5870
18	-43164.	-38644.	2.9675	-34648.	-2.6233	-8515.6	5.5908

Figure 20 Equilib Module – Solution Properties Window Cu-matte-slag system. Top: list of the partial properties functions. Bottom: calculated integral properties of the matte phase.

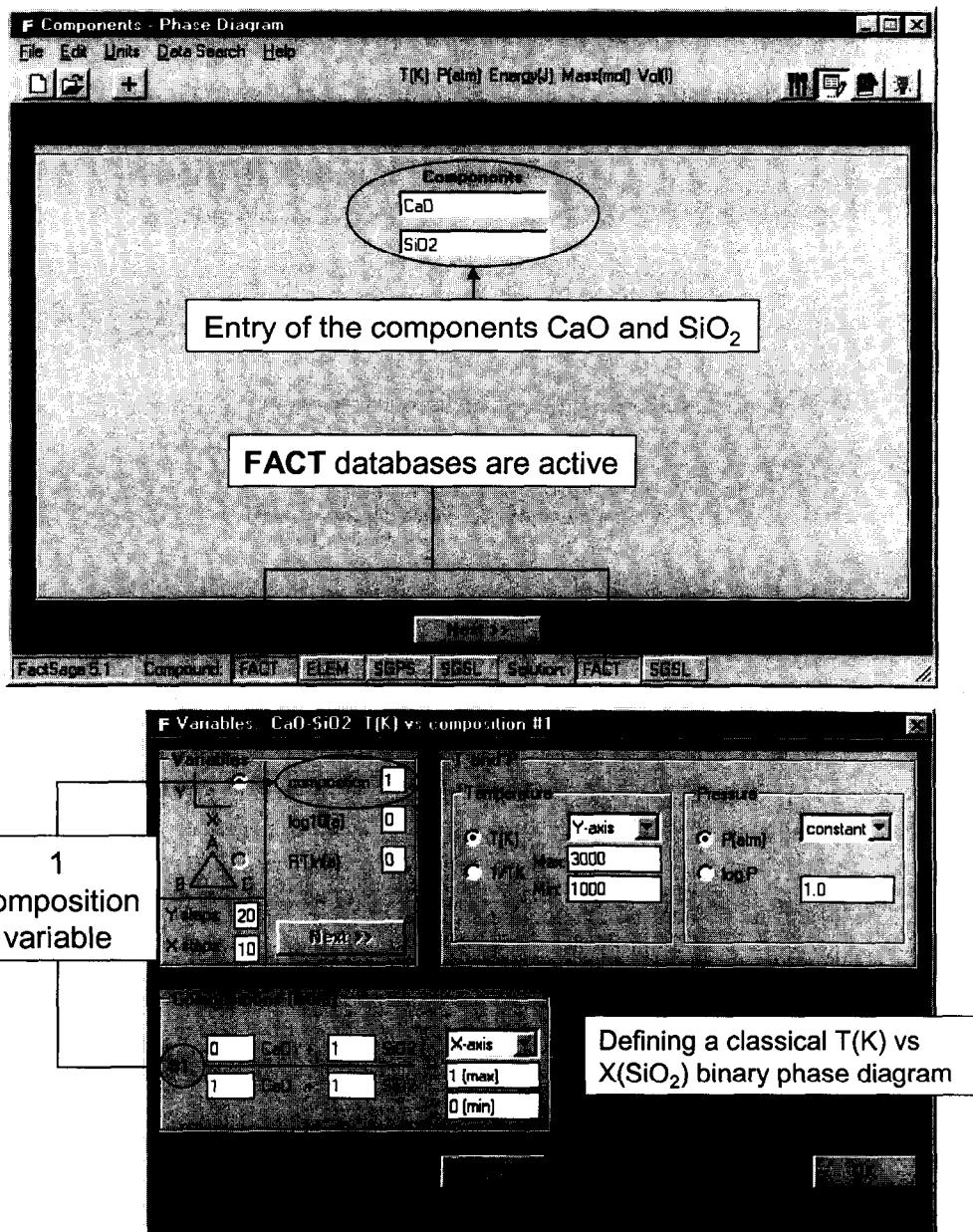


Figure 21 Phase Diagram Module – CaO-SiO₂ system. Top: Components Window – entry of CaO and SiO₂. Bottom: Variables Window – selection of T(K) and X(SiO₂) axes.

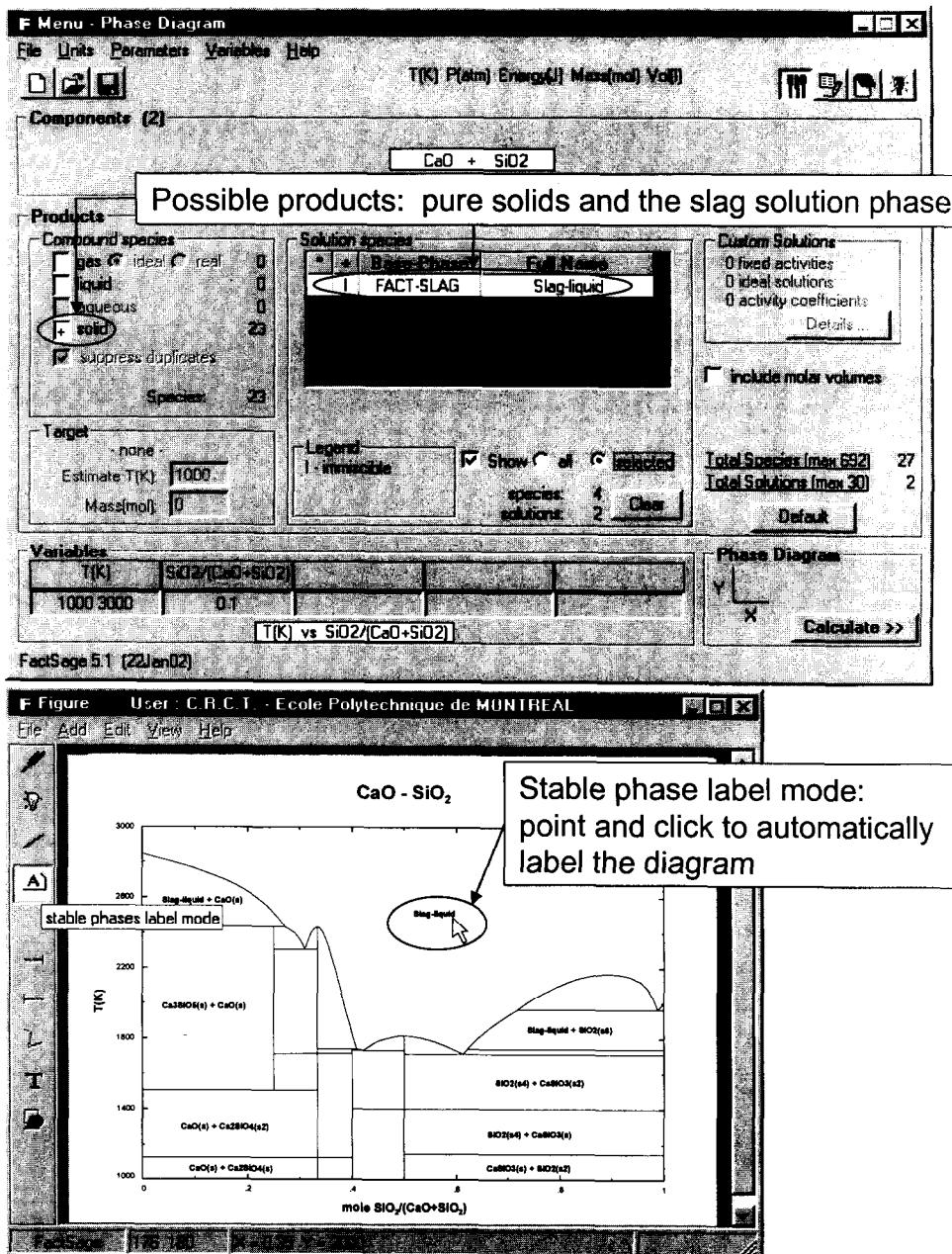


Figure 22 Phase Diagram Module – CaO-SiO₂ system. Top: *Menu Window* – selection of the possible products. Bottom: *Figure Window* - resulting binary CaO-SiO₂ phase diagram.

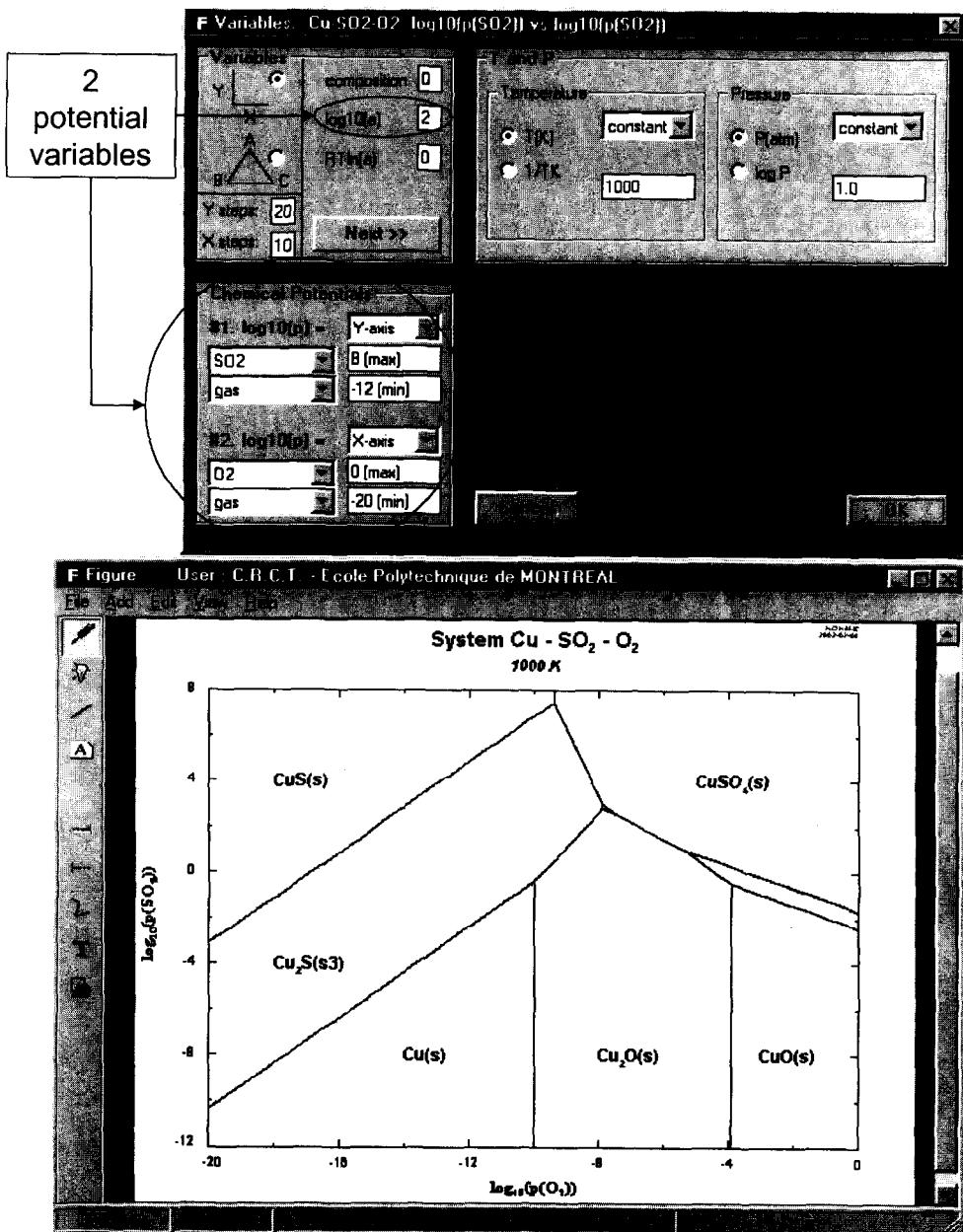


Figure 23 Phase Diagram Module – Cu-SO₂-O₂ system. Top: selection of the log₁₀(P_{SO₂}) and log₁₀(P_{O₂}) axes at 1000 K. Bottom: the resulting predominance area diagram.

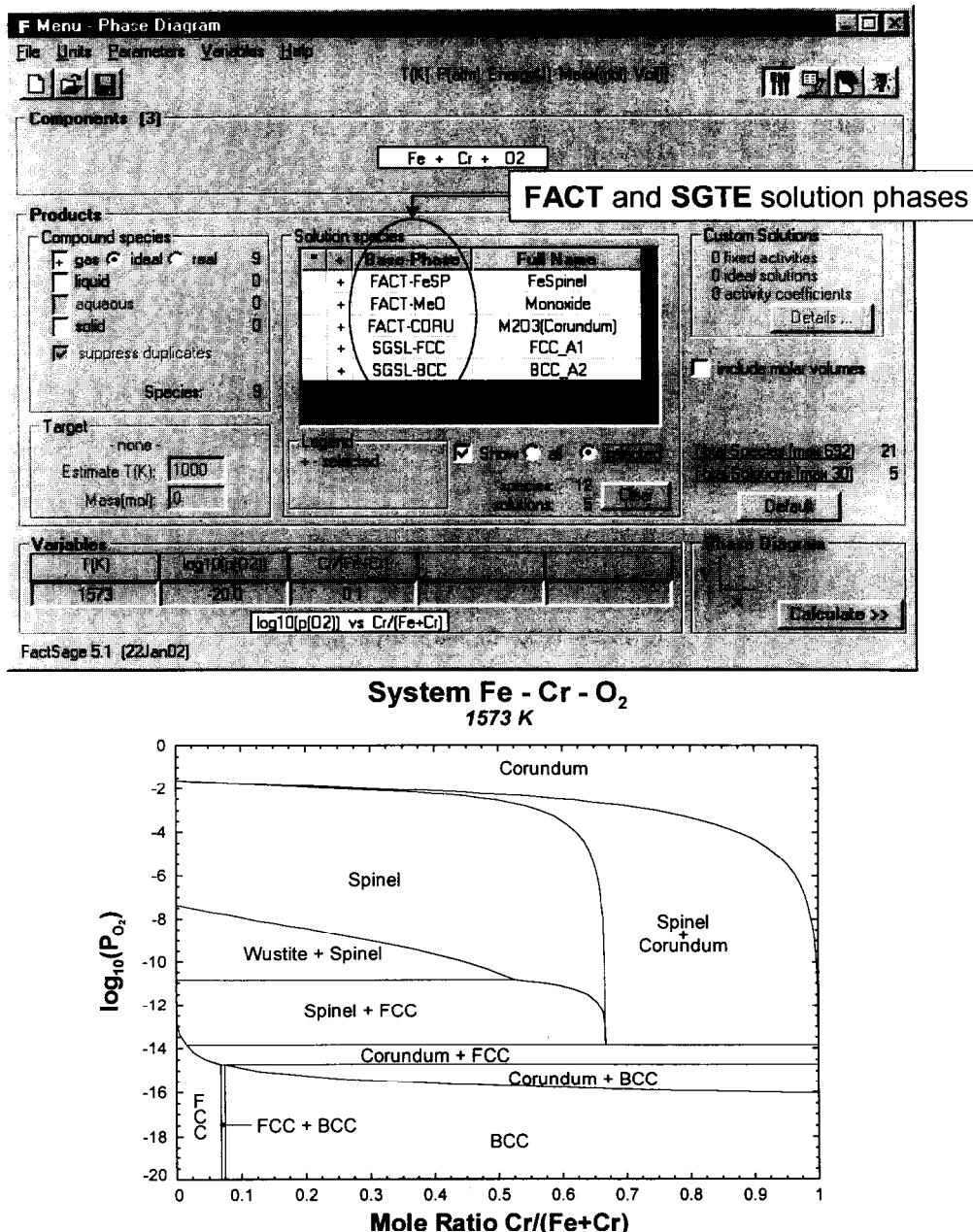


Figure 24 Phase Diagram Module – Fe-Cr-O₂ system. Top: selection of FACT (oxide) and SGTE (alloy) solution phases. Bottom: resulting log₁₀(P_{O₂}) vs Cr/(Cr+Fe) phase diagram at 1573 K.

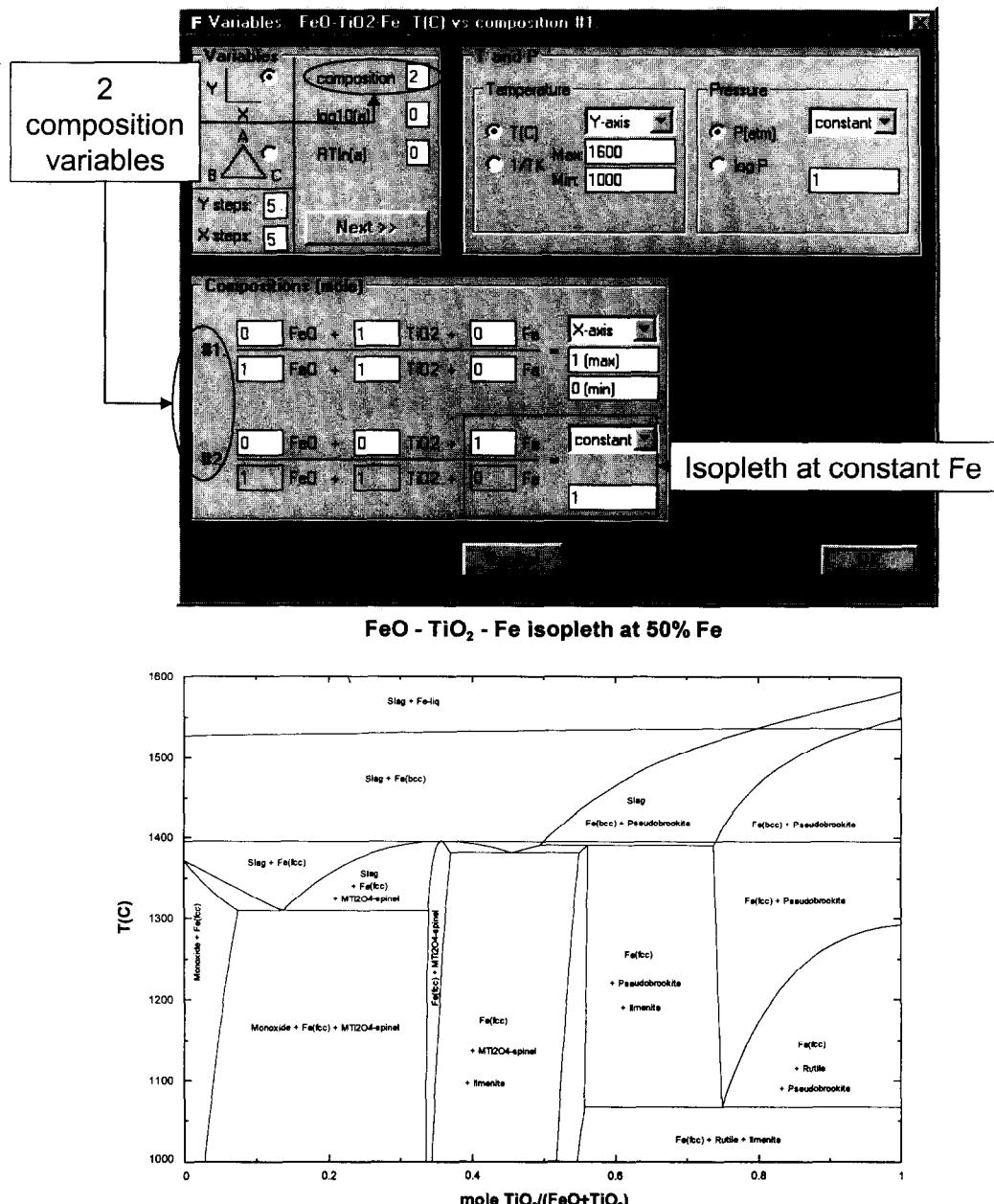


Figure 25 Phase Diagram Module – FeO-TiO₂-Fe system. Top: selection of the axes at constant Fe content. Bottom: resulting T(C) vs TiO₂/(FeO+TiO₂) isopleth at 50 mol % Fe.

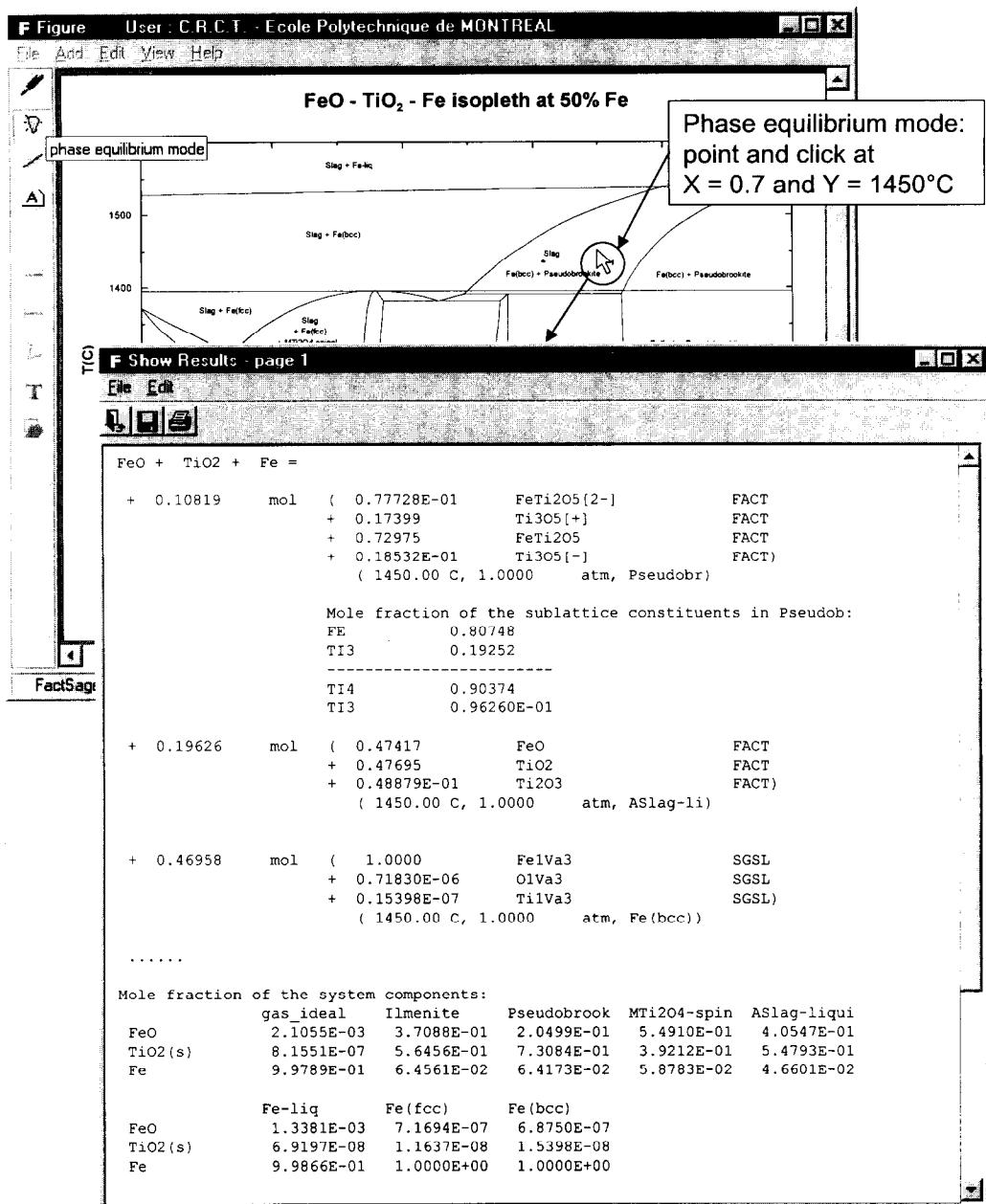


Figure 26 Phase Diagram Module – FeO-TiO₂-Fe system. Example of the *phase equilibrium mode* calculation at the coordinates 1450°C and TiO₂/(FeO+TiO₂) = 0.7.

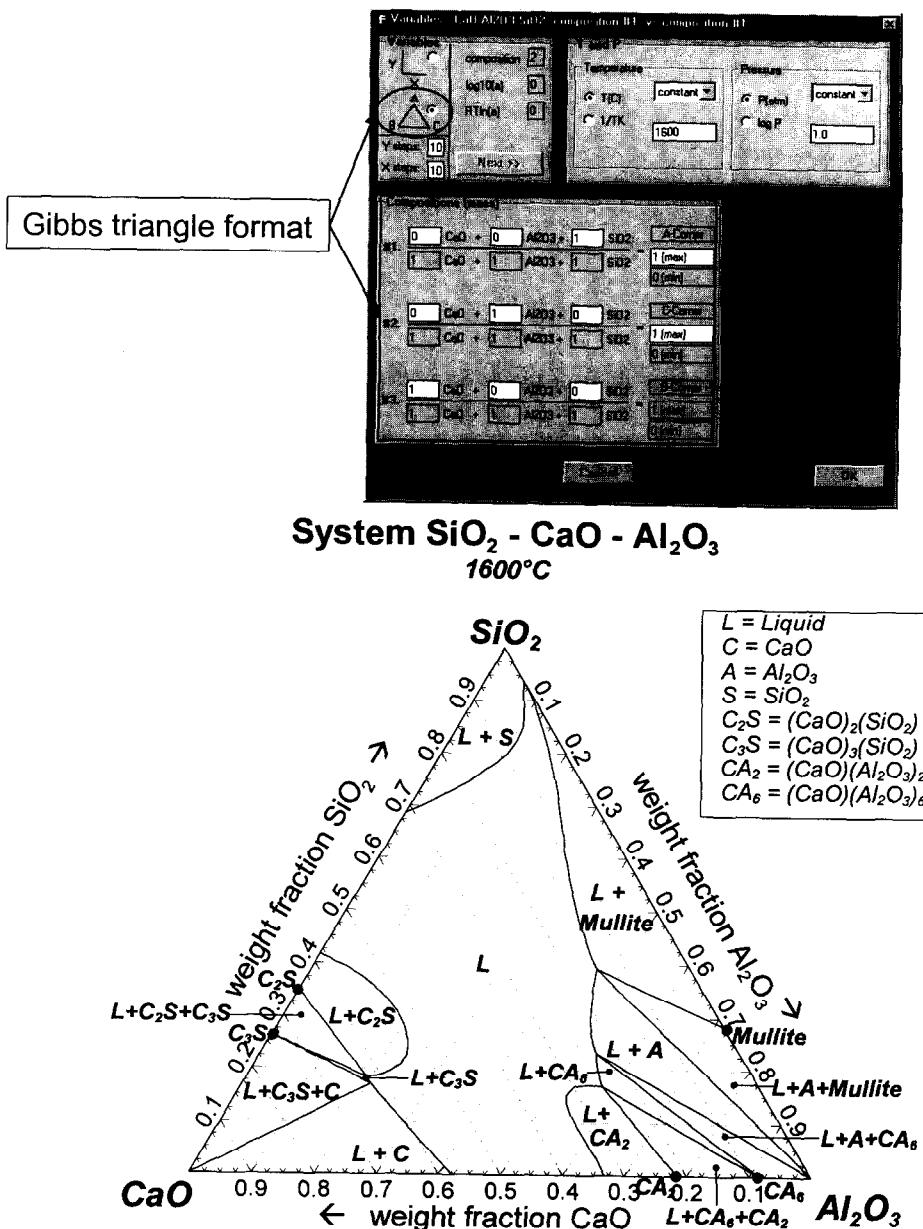


Figure 27 Phase Diagram Module – $\text{CaO}-\text{Al}_2\text{O}_3-\text{SiO}_2$ system. Top: selection of the Gibbs triangle format, axes and temperature. Bottom: resulting $\text{CaO}-\text{Al}_2\text{O}_3-\text{SiO}_2$ ternary phase diagram at 1600°C (the labels have been edited).

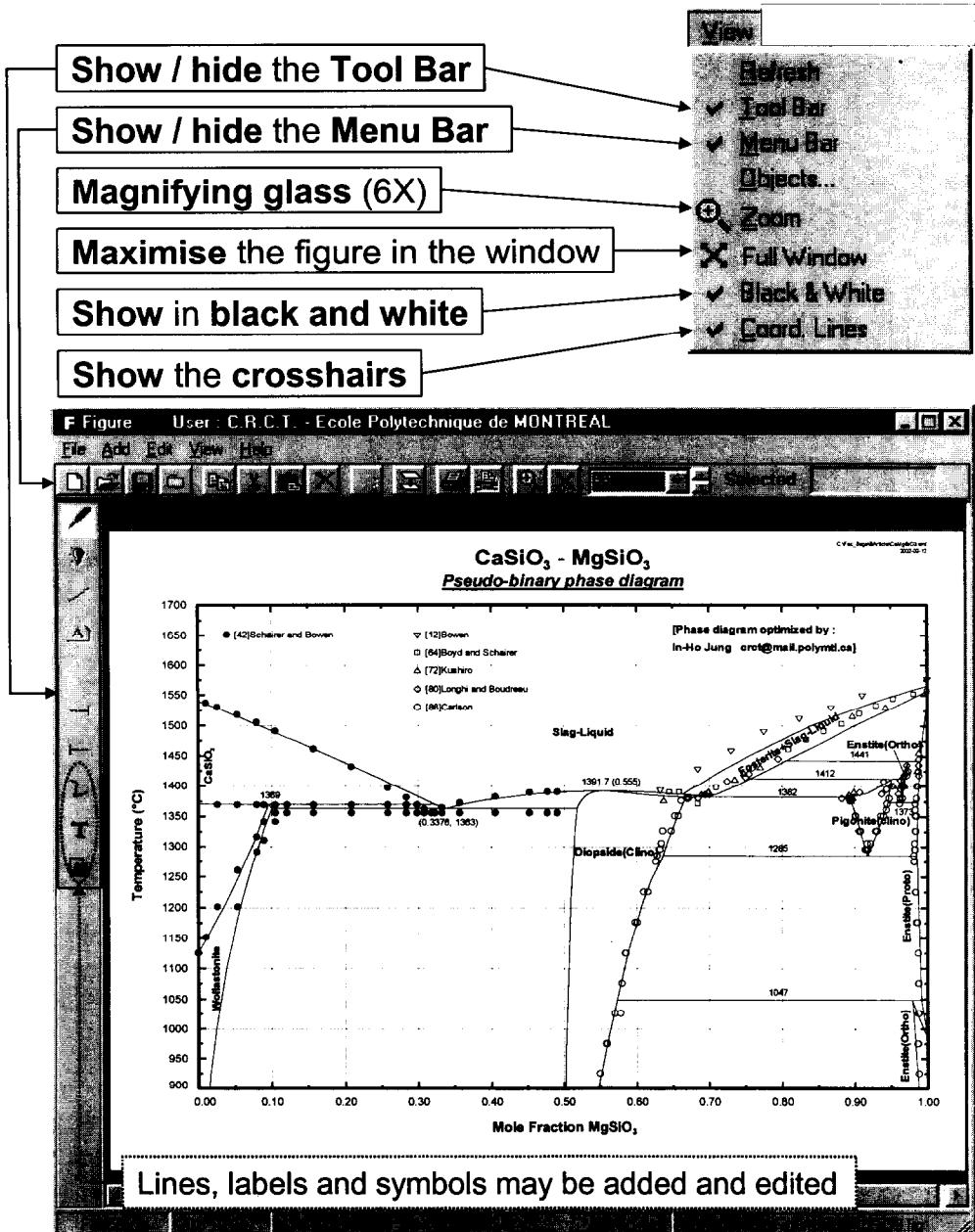


Figure 28 Figure Module – CaSiO₃-MgSiO₃ system. Example of the *View menu bar* used to edit calculated phase diagrams.

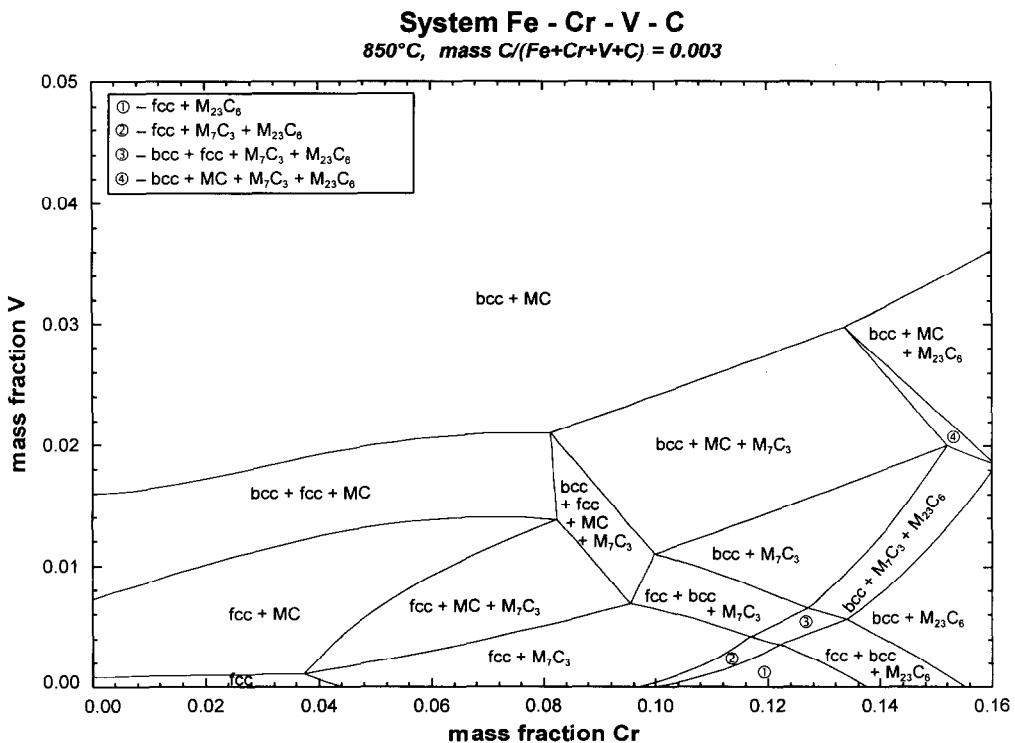


Figure 29 FactSage – Fe-Cr-V-C system. Mass fraction V versus mass fraction W isopleth at 0.3 wt.% C and 850°C calculated from SGTE data by Phase Diagram and editing the output in the Figure Module.

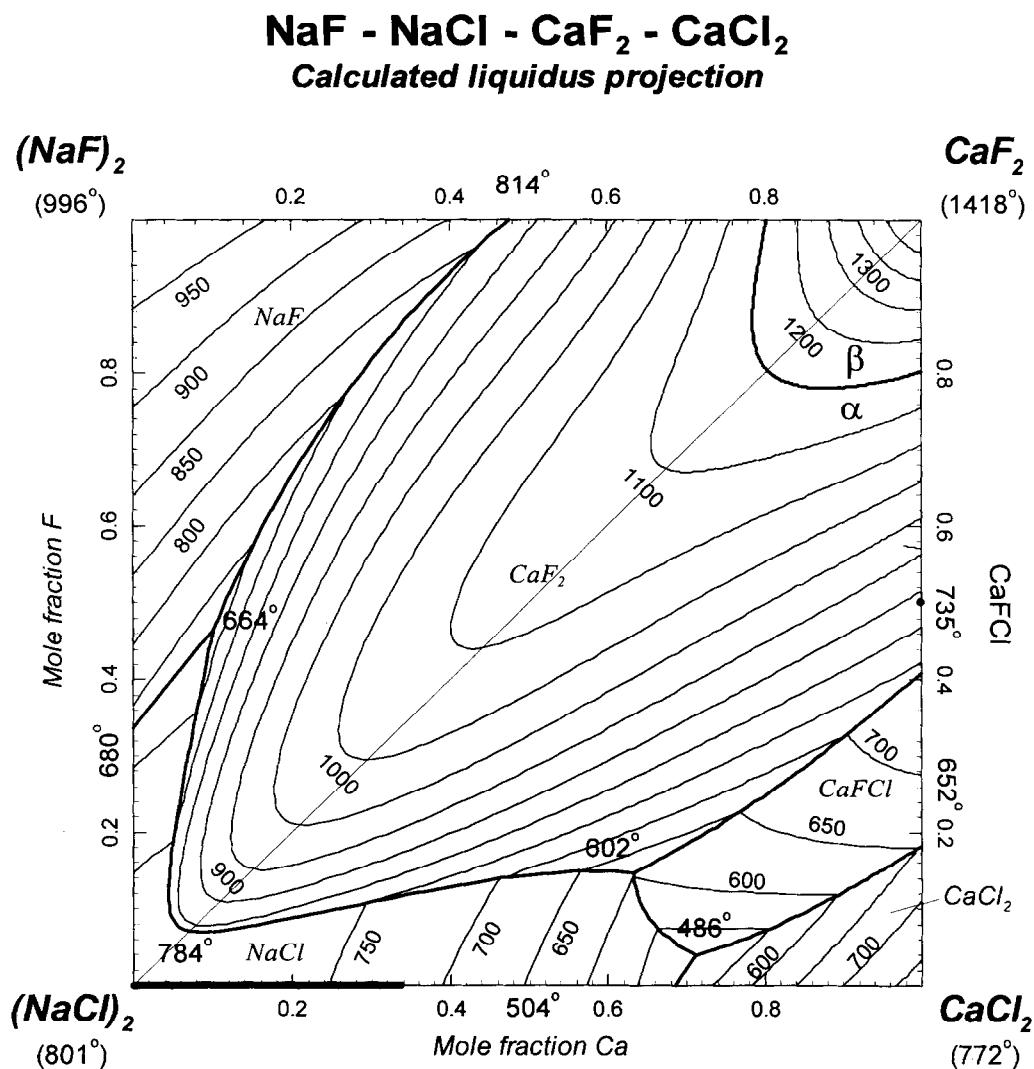


Figure 30 FactSage – NaF-NaCl-CaF₂-CaCl₂ reciprocal system. The liquidus projection was calculated from FACT data by editing the results and outputs from the Equilib, Phase Diagram and Figure modules.

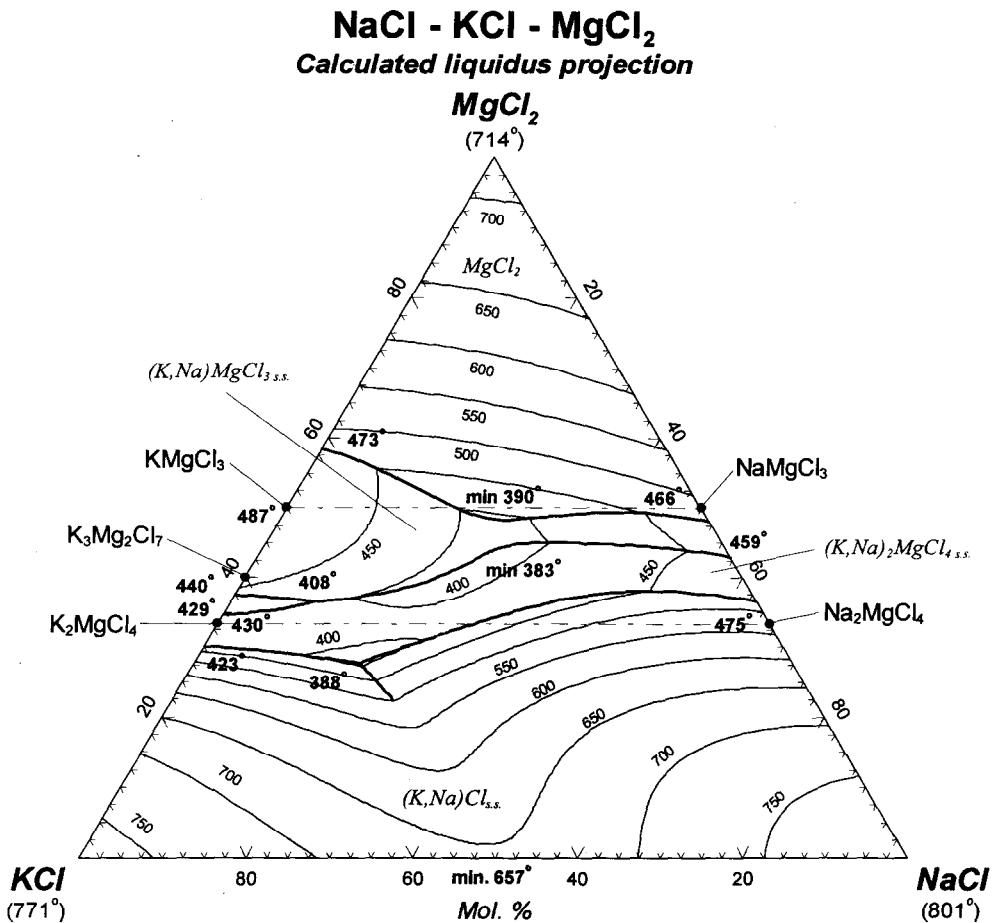


Figure 31 FactSage – NaCl-KCl-MgCl₂ ternary system. The liquidus projection was calculated from FACT data by editing the results and outputs and from the Equilib, Phase Diagram and Figure modules.