FactSage thermochemical software and databases — recent developments

C.W. Bale [a,*], E. Bélisle [a], P. Chartrand [a], S.A. Decterov [a], G. Eriksson [b], K. Hack [b], I.-H. Jung [a], Y.-B. Kang [a], J. Melançon [a], A.D. Pelton [a], C. Robelin [a], S. Petersen [b]

[a] CRCT - Center for Research in Computational Thermochemistry, Department of Chemical Eng., École Polytechnique (Campus de Université de Montréal), Box 6079, Station Downtown, Montréal, Québec, Canada H3C 3A7 [1]

[b] GTT-Technologies, Kaiserstrasse 100, 52134 Herzogenrath, Germany [2]

ABSTRACT

FactSage® was introduced in 2001 as the fusion of the **F*A*C*T/FACT-Win** and **ChemSage** thermochemical packages. 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. This paper presents a summary of the recent developments in the **FactSage** thermochemical software and databases. In the article, emphasis is placed on the new databases and the calculation and manipulation of phase diagrams and complex phase equilibria.

© 2009 Published by Elsevier Ltd

0. Introduction

FactSage® was introduced in 2001 as the fusion of two well-known software packages in the field of computational thermochemistry: **F*A*C*T/FACT-Win** and **ChemSage**. It is used worldwide at approximately 400 installations in universities, governmental and non-governmental research laboratories and industry. The original F*A*C*T package [1] was designed to simulate the thermochemistry of pyrometallurgical processing. With the migration to the Windows-based **FACT-Win** and then to **FactSage** the applications have been expanded to include hydrometallurgy, electrometallurgy, corrosion, glass technology, combustion, ceramics, geology, environmental studies, etc.

While an understanding of chemical thermodynamics is useful in order to run the modules, it is not essential to be an expert in the field. With program usage 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.

An article on **FactSage Thermochemical Software and Databases** was published [2] in this journal. Since then extensive modifications and additions have been carried out to both the software and the databases. These developments are the subject of this current article with emphasis placed on the new databases and the calculation and manipulation of phase diagrams and complex phase equilibria. The reader who is unfamiliar with **FactSage** is encouraged to consult the original publication [2].

The **FactSage** package runs on a PC operating under Microsoft Windows®. The 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**.

1. Info

The **General** module provides slide shows (Microsoft Power Point® and Adobe PDF® presentations) of all the modules as well as database documentation, answers to frequently asked questions (FAQ) and a list of useful addresses and telephone numbers.

The module also includes information on the **FactSage Family of Products and Services**. Both GTT-Technologies and Thermfact/CRCT offer a suite of software products that can access the FactSage databases or enhance the FactSage environment. In addition, other software developers have programmed interfaces to access the FactSage data and software within their own packages. These products now include:

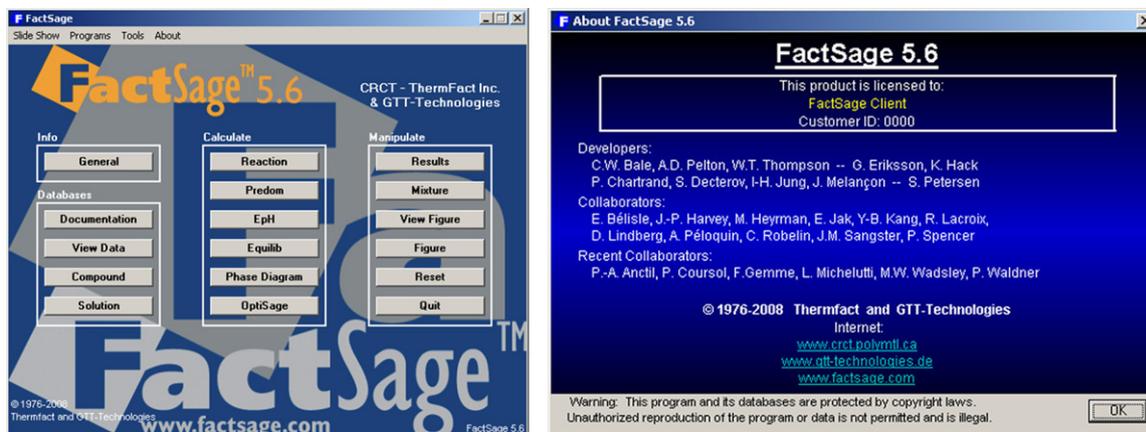**FactSage-Teach**—the thermochemical teaching package based on FactSage.

Fig. 1. FactSage Main Menu and *About Window*.

ChemApp—the thermochemistry library dynamically linked for software applications.

ChemSheet—the spreadsheet tool for process simulation.

SimuSage—the component library for rapid process modeling.

CSFAP—ChemSage File Administrator Program.

OLI Systems—FactSage Interface: the link to the OLI aqueous databanks.

METSIM—FactSage Link for the coupled chemical process simulation.

2. Databases

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 database files. These modules were presented in the previous **FactSage** article.

The **Documentation** module is new. A large amount of time has been devoted to developing new databases, introducing extensive documentation and displaying calculated phase diagrams.

In the **Documentation** module a new program, the **FactSage Browser**, has been developed that enables one to manipulate the database and documentation files in a 'phase diagram friendly' environment. For example, a 'click' on the Databases 'Documentation' button (Fig. 1) opens the **FactSage Browser** (Fig. 2) that displays database information, documentation and phase diagram previews. There is a 'search phase diagram' mode that scans the hundreds of phase diagrams stored in **FactSage**; Fig. 3 lists the phase diagrams and database source for systems containing SiO_2 or Al_2O_3.

FactSage accesses both solution databases and pure compound databases. The former contain the optimized parameters for solution phases. The latter contain the properties of stoichiometric compounds, either obtained from phase diagram optimizations or taken from standard compilations, for example [3–7]. The **FACT** and **SGTE** compound and solution databases were presented in the previous publication. During the past five years the diversity and number of databases have been expanded. The new databases are summarized in the following sections.

2.1. FACT databases — FToxid, FTsalt, FThall, FThelg, FTmisc, FTpulp

The **FACT** databases are the largest set of evaluated and optimized thermodynamic databases for inorganic systems in the world and have been under development for over 25 years. During the period 2001–2003, major additions and modifications were made as part of the "FACT Database Consortium Project" with funding from the Natural Sciences and Engineering Research

Council of Canada and 15 industries (Noranda, INCO, Teck Cominco, Rio Tinto, Alcoa, Shell, Corning, Dupont, Pechiney (now Alcan), St. Gobain Recherche, Schott Glass, Sintef, Norsk Hydro, Mintek, IIS Materials). The updated databases were publicly released in 2004 so the present databases are much expanded beyond what was available in the former **FACT** databases.

FToxid — oxide database for slags, glasses, minerals, ceramics, refractories, etc. contains data for stoichiometric oxides and oxide solutions of the following components: Al_2O_3, As_2O_3, B_2O_3, CaO, CoO, CrO, Cr_2O_3, Cu_2O, FeO, Fe_2O_3, GeO_2, K_2O, MgO, MnO, Na_2O, NiO, PbO, SiO_2, SnO, TiO_2, Ti_2O_3, ZnO, ZrO_2. Not all binary, ternary and higher-order subsystems have been evaluated and optimized, nor are all composition ranges covered. However, the system Al_2O_3–CaO–FeO–Fe_2O_3–MgO–SiO_2 has been fully optimized from 25 °C to above the liquidus temperatures at all compositions and oxygen partial pressures. Components CoO, CrO, Cr_2O_3, Cu_2O, MnO, NiO, PbO, SnO, TiO_2, Ti_2O_3, ZnO and ZrO_2 were added to this core six-component system and the relevant subsystems were optimized over the composition ranges important for applications in ferrous and non-ferrous metallurgy, production of ceramics, refractories and paint pigments. Currently we are working on the addition of B_2O_3, K_2O and Na_2O to the core six-component system for applications in the glass industry, combustion, coal gasification and waste management. Many subsystems with these three components are being re-evaluated and re-optimized using more advanced solution models that we have recently developed. The documentation module contains more detailed description of the systems that have been optimized.

The liquid/glass solution phase is called FToxid-Slag. As well as all the oxide components mentioned above, it includes dilute solutions of S, SO_4, PO_4, H_2O/OH, CO_3, F, Cl, I. We have also developed a new model for the viscosity of oxide melts [8]. It takes into account the information on the short-range ordering and formation of a silica network in liquid oxides obtained from the thermodynamic modeling of slags. The model uses many fewer adjustable parameters than the other viscosity models presently available and shows very good predictive ability. By critical evaluation of experimental viscosity data and optimization of the model parameters, a state-of-the-art viscosity database is being built which will soon become available to FactSage users.

There are many oxide solid solutions in the database. Some of the most extensive solutions include

Spinel: $(Al, Co^{2+}, Co^{3+}, Cr^{2+}, Cr^{3+}, Fe^{2+}, Fe^{3+}, Mg, Ni^{2+}, Zn)^T[Al, Co^{2+}, Co^{3+}, Cr^{3+}, Fe^{2+}, Fe^{3+}, Mg, Ni^{2+}, Zn]_2^O O_4$

Pyroxene: $(Ca, Fe^{2+}, Mg)^{M2}(Al, Fe^{2+}, Fe^{3+}, Mg)^{M1}(Al, Fe^{3+}, Si)^{T1} Si^{T2}O_6$

Melilite: $(Ca, Pb)_2^A[Al, Fe^{2+}, Fe^{3+}, Mg, Zn]^{T1}\{Al, Fe^{3+}, Si\}_2^{T2}O_7$

Fig. 2. **FactSage Browser** module — databases and preview window.

Olivine: $(Ca, Co, Fe^{2+}, Mg, Mn, Ni, Zn)^{M2}[Ca, Co, Fe^{2+}, Mg, Mn, Ni, Zn]^{M1}SiO_4$.

FTsalt — salt database contains data for pure salts and salt solutions formed among various combinations of the 20 cations Li, Na, K, Rb, Cs, Mg, Ca, Sr, Ba, Mn, Al, Fe(II), Fe(III), Co, Ni, Pb, La, Ce, Nd and 8 anions F, Cl, Br, I, NO_3, OH, CO_3, SO_4. The molten salt phase is called FTsalt-Salt and includes dilute solutions of O^{2-} and OH^-. **FTsalt** is by far the most extensive thermodynamic database available in the world on salt systems.

FThall — Hall aluminum database contains data for all pure substances and 17 solution phases formed among Al–Mg–Na–Li–Ca–F–O. The molten cryolite phase is called FThall-bath and the molten alloy phase is called FThall-liq. Calculations with NaF–AlF$_3$–CaF$_2$–Al$_2$O$_3$ electrolytes containing LiF, MgF$_2$ and dissolved metal can be made for liquidus calculations, emfs, partial pressures, etc. With this database, accurate liquidus temperatures of Na$_3$AlF$_6$, CaF$_2$, AlF$_3$, Na$_5$Al$_3$F$_{14}$, NaCaAlF$_6$ and NaF among others can be calculated. Alumina solubility in standard cryolite-based electrolyte can be computed from low eutectic temperatures ($>690\,^\circ$C) up to 1100 $^\circ$C. This is also valid for low concentrations of additives such as LiF, Li$_3$AlF$_6$ and MgF$_2$. Cubic-Na$_3$AlF$_6$ high temperature solid solution with excess AlF$_3$, CaF$_2$ and LiF has also been modeled. The gaseous species from the FACT53 database are consistent with phases found in FThall.

FThelg — aqueous (Helgeson) database contains infinite dilution properties for over 1400 aqueous solute species taken from the GEOPIG-SUPCRT Helgeson public database and include the Helgeson equation of state for temperatures up to 350 $^\circ$C and