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CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry

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Reprint of: 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.

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.

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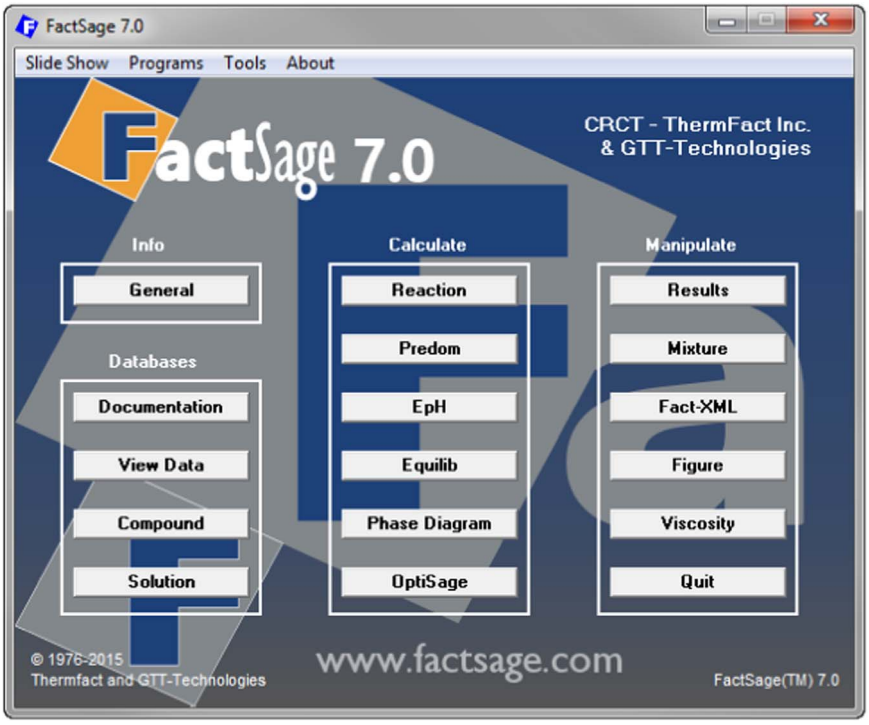

Fig. 1. FactSage 7.0 Main Menu Window.

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.

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 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,

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