Technical product information

GTT-Technologies

FactSage

FactSage is an integrated thermodynamic databank system (ITDS) with thermochemical application modules for the calculation

- of thermodynamic properties of phases and their constituents,
- of isothermal and non-isothermal stoichiometric reactions,
- of complex equilibrium states under standard conditions and with special constraints, and
- of all types of classical phase diagrams, among these EpH diagrams for aqueous systems.

Results can be obtained in tables and plots, and can be exported in files for use in other software, e.g. in Microsoft Office, especially in EXCEL.

Furthermore, FactSage provides by way of the special module OptiSage the capability of assessing experimental thermochemical information (phase diagrams, activity or enthalpy measurements etc.) in the form of optimised Gibbs energy coefficients. These data can be stored in the user's own private databank(s).

FactSage comprises a standard and extended version of the Equilib module (the extended version covering systems with up to 1500 species and 40 non-ideal solution at the same time), and contains special software modules for the administration of thermodynamic databases. It comes with an element database, the SGTE Unary database for metallic components in a multitude of phase states and the SGTE binary alloy database included in the price. The use of all other general databases or customised mini-databases is subject to a charge. See DATABASES.

The licence fee includes two dongles and free Maintenance and Support as well as up-dates during the time of the lease.

The use of FactSage is subject to acceptance of the terms defined in a non-transferable and non-exclusive licence. Stand-alone and net-work licences are available. Terms for other licences are available upon request.

Stand-alone installations are protected by hardware security blocks (dongles) which can be supplied for use on parallel or USB ports. Please specify which on order.
Net-work installations are protected by a software key which is supplied when installing the software.

ChemApp

ChemApp is a highly versatile, programmable applications library incorporating the data-handling and phase equilibrium calculation modules of ChemSage. It can be used to design application-specific programs or be linked into third party programs. It is supplied in object code or as a DLL for a large number of platforms.

The use of ChemApp is subject to acceptance of the terms defined in a non-transferable and non-exclusive licence. Single-user and multi-user licences are available for PCs and workstations. Terms for other system licences are available upon request. The licence fee includes a Programmer's Handbook and hotline support.

The use of ChemApp is restricted; it is specifically prohibited to develop a competitive product to FactSage/ChemSage, or to develop programs that are released into the public domain, or distributed as free- or shareware. The use of ChemApp to develop a commercial product is subject to approval, issue of a licence, and payment of a royalty fee.

A special, restricted version of ChemApp (ChemApp "light"), made available for free for non-commercial purposes, can be used to evaluate whether ChemApp can be linked to a user's own or a third party program, and generally allows anybody interested in ChemApp to get to know it at no risk. To obtain ChemApp "light", please visit the ChemApp section on our web page.

ChemSheet

ChemSheet combines the flexibility and practicality of spreadsheet applications with rigorous, multi-phase thermodynamic calculations. Each application is defined as an independent worksheet in Excel, in which the entire simulation can be done. Please note that Microsoft Excel is not included in ChemSheet. In fact, its availability on the user's PC is a requirement for ChemSheet.

The input and output of the spreadsheet model are linked to the ChemApp thermodynamic programming library. Repetitive complex thermodynamic calculations for a diverse range of applications both in chemistry and metallurgy are thus enabled directly from the spreadsheet. It is even possible to integrate reaction kinetic related data into the calculations. Therefore, ChemSheet is a tool of interest to professionals and scientists in process engineering and metallurgy, as well as to those working with geochemistry and environmental sciences.

The use of ChemSheet is subject to a licence agreement.

SimuSage

SimuSage is a special tool for the field of thermochemistry based process modelling. It uses ChemApp inside, however the user sees and makes use of the interface of the DELPHI program development tool with special graphical components integrated into it that represent the toolbox SimuSage. The icons of SimuSage permit the generation of a themochemistry based process simulation by a simple drag-and-drop method on a graphics screen. Only in particular cases the user has to add explicit own code to the program. The major part of the programming is done by DELPHI interpreting the logical interlink of the graphical icons of SimuSage assembled by the user on the screen.

Each SimuSage application makes use of a special application oriented datafile that the user can either extract via FactSage from one of the many general databases, or which can be supplied to the user by GTT according to his special requirements.

The use of SimuSage is subject to a licence agreement.

ChemSage – FILE ADMINISTRATION PROGRAM (CSFAP)

CSFAP is a multi-purpose data handling software for users who work with own databases or who need to manipulate ChemSage.DAT files for use in kinetic applications. Furthermore CSFAP has the ability to translate datafiles from the Thermocalc ® world (*.TDB files) into the FactSage/ChemApp/ChemSheet/SimuSage world.

CSFAP can be used to manipulate all data entries in a ChemSage.DAT file. The names of phases or phase constituents can be modified just as easy as the actual thermochemical data in Gibbs energy expressions or the basic coefficients of the stoichiometry formula of a substance. Thus it provides the basis for a users work on own databases. This work is further support by the capability of merging two files, i.e. data from a literature source which have been tested in a small datafile can easily be incorporated into a large database. On the other hand CSFAP provides a means for extraction of an application specific datafile from a large database. Although the format of the database file is the same as that for a ChemSage.DAT file the size of such a file for use with CSFAP is NOT restricted.

In addition to the classical ChemSage.DAT format CSFAP support two other formats of database files. The first is the well known *.TDB file format that is used in the Thermocalc world. TDB files can thus easily be read into CSFAP and written out by CSFAP as ChemSage.DAT files. However, it is also possible to go the other way, i.e. from ChemSage.DAT to *.TDB. In this direction it is of course necessary to make sure that no Gibbs energy models are used which are not compatible with Thermocalc. Not all Gibbs energy models which can be used in FactSage/ChemApp/ChemSheet/SimuSage are available in Thermocalc.

The second format is a CSFAP inherent own format. It combines the flexibility of TDB files with respect to the use of functions with the multitude of Gibbs energy models available in FactSage/ChemApp/ ChemSheet/SimuSage. Furthermore, this new format is based on the concept of XML files. Thus it is easy to change data even in an editor or to exchange data with other CSFAP users on a general level.

NOTE: If a database used with CSFAP becomes larger than a standard ChemSage.DAT file GTT has an additional tool which permits the translation of such large file for use in FactSage. Please let us know if you are in need of such a tool.

THERMOCHEMICAL DATABASES

The FACT and SGTE Pure Substance databases cover both approximately 4.200 entries for gases as well as stoichiometric condensed substances, both in the solid and in the liquid state. A special group of entries only available in the FACT database pertains to aqueous species.

The FACT Solution database is now split into several more application oriented sub-sections which all have special names:
FToxid contains oxide systems based on the Ca-Mg-Al-Si-Fe(2+/3+)-O system with many additions for metallurgical slags as well as glasses
FTsalt is a general salt database with non-ideal solid and liquid solutions
FThall is a special salt database based on NaF-AlF3-Al2O3 for the thermochemistry of the Hall-Herroult process
FTmisc is a collection of miscellaneous liquid and solid solutions pertaining mainly to metallurgical systems
FThelg is a special database for aqueous solution using the Helgeson approach.

The SGTE Solution database is a general database for alloy systems now covering 78 elementary metallic components. From among these elements, there are some 300 completely assessed binary alloy systems together with about 120 ternary and higher-order systems for which assessed parameters are available for phases of practical relevance. The systems now incorporate 177 different solution phases and 588 stoichiometric intermetallic compound phases.

The Steel database (FSstel) contains 28 elementary components in Fe. It comprises approximately 120 completely assessed binary alloy systems, together with 85 ternary and 17 quaternary systems for which assessed parameters are available for phases of practical relevance. As such, the database is intended to provide a sound basis for calculations covering a wide range of steelmaking processes, but also solid-liquid interactions during solidification and the solid-solid phase equilibria related to heat treatments. It is the first complete alloy database that is also compatible with the liquid slag phase data of the Ftoxid database mentioned above.

The Light Metal database (FSlite) covers 24 elementary components which permit the calculation of alloy equilibria in Al-, Mg-, and Ti-based systems. From among these elements, there are 117 completely assessed binary alloy systems together with 30 ternary and 3 quaternary systems for which assessed parameters are available for phases of practical relevance. A large number of new published assessments (44 binary, 9 ternary, 3 quaternary), some amendments and some updates are incorporated in this light alloy database. As such, the database is intended to provide a sound basis for calculations relating to the production and heat treatment of Al-, Mg-, and Ti-based alloys. The SGTE Noble Metal database (FSnobl) contains evaluated thermodynamic parameters for alloys of Ag, Au, Ir, Os, Pd, Pt, Rh, Ru alloyed amongst themselves and also in alloys with the metals Al, As, Bi, C, Co, Cr, Cu, Fe, Ge, In, Mg, Ni, Pb, Sb, Si, Sn, Ta, Te, Ti, Tl, Zn, Zr. The evaluated parameters in the Noble Metal Alloys Database are based on data collected from publications and internal project reports or have been assessed as part of the development of the database.

The Copper database (FSCopp) covers mainly the liquid state of Cu-based binary and higher-order systems. It is based on relevant sub-systems from the old SGTE Solution Database, but now incorporating updates of those systems as well as many new published assessments. Data compiled by Coursol (Report from CRCT, Ecole Polytechnique de Montreal, August 2001) for the Cu-rich liquid phase have also been incorporated. Altogether 43 components (39 metals: Ag, Al, As, Au, Ba, Be, Bi, C, Ca, Cd, Ce, Co, Cr, Fe, Ga, Ge, In, Li, Mg, Mn, Nb, Nd, Ni, Pb, Pd, Pt, Pr, Sb, Se, Si, Sm, Sn, Sr, Te, Ti, Tl, V, Y, Zn, Zr) including C, O, S and P have been compiled or assessed together with Cu. While the optimized thermodynamic parameters contained in FScopp are intended primarily to provide a sound basis for calculations relating to copper production and refining, copper-rich *solid phases* are also included in the database. This makes possible the calculation of liquidus temperatures and solidification characteristics relevant to the casting of certain copper-rich alloys, although, because of the more limited amount of assessed data for solid ternary and higher-order phases available, the results should be treated with caution.

The Lead database (FSLead) covers mainly the liquid state of Pb-based binary and higher-order order systems. It is based on relevant sub-systems from the old SGTE Solution Database, but now incorporating updates of those systems as well as many new published assessments. In particular, the assessed information contained in Dessureault 's thesis [Ph.D.Thesis, Ecole Polytech., Univ.Montreal, Nov.1993] for the liquid phase of Pb-rich ternary systems has also been incorporated and a few new assessments have been carried out as part of the present work. Altogether 28 components (25 metals: Ag, Al, As, Au, Bi, Ca, Cd, Cu, Fe, Ga, Ge, Hg, In, Mn, Ni, Pd, Sb, Se, Si, Sn, Sr, Te, Tl, Zn, Zr) including C, O and S have been compiled or assessed together with Pb. While the optimized thermodynamic parameters contained in FSlead are intended primarily to provide a sound basis for calculations relating to lead production and refining, lead-rich *solid phases* are also included in the database. This makes possible the calculation of liquidus temperatures and solidification characteristics relevant to the casting of certain lead-rich alloys, although, because of the more limited amount of assessed data for solid ternary and higher-order phases available, the results should be treated with caution. With the exception of Pb-Fe, Pb-Mn, Pb-S, Pb-Se, and Pb-Sr, the lead-containing binary systems are described over all ranges of composition and temperature, i.e. the assessed data provide a good description of the complete phase diagram and thermodynamic properties for the binary alloy system concerned.

The Ultra-pure Silicon database (FSUpSi) covers mainly the liquid state of Pb-based binary and higher-order order systems, with the particular aim of enabling calculation of impurity concentration levels in ultra-pure silicon. In addition, a number of elements are included in a Si-rich *solid solution phase (diamond structure)*, although assessed data for solid Si-rich alloys are fewer and less reliable. Solid phases which may precipitate at low concentration levels of B, C, N and O are also included in the database. Altogether 24 elements (18 metals: Al, Au, Ca, Co, Cr, Cu, Fe, Ge, In, Mg, Mn, Ni, Pb, Sb, Sn, Te, Ti, V, Zn) including B, C, N, O and P have been incorporated in the Si-rich melt. The elements included in the Si-rich solid solution are: B, C, Ge, N, Sn, Ti, Zn All other elements are treated as insoluble in solid Si. The major source of data has been the assessments contained in the SGTE2004 Solution Database, together with more recent published assessments. One or two original assessments have been carried out as part of the development work on this database.

The SGTE nuclear database (SGNucl) has been generated by Thermodata, Grenoble, as part of a much bigger database effort to cover many thermochemical aspects related to the field of nuclear reactors. The SGnucl database is specially made for the investigation of in-vessel chemical reactions. It is an SGTE approved database and has been converted for use with FactSage by GTT Technologies. The elements included in the database are: O, U, Zr, Fe, Cr, Ni, Ar, H. Also included are systems formed among the 6 oxides UO_2 - ZrO_2 - FeO - Fe_2O_3 - Cr_2O_3 - NiO. The database covers the entire composition range from pure metal to oxide regions and contains critically evaluated thermodynamic parameters for all relevant multicomponent condensed or gaseous substances and solution phases.

The full Thermodata nuclear database (TDNucl) covers the 18+2 component system O-U-Zr-Fe-Cr-Ni-Ag-In-B-Ba-C-La-Ru-Sr-Al-Ca-Mg-Si plus Ar and H in the gas phase. It contains data for the 15 component oxide sub-systemUO2-ZrO2-In2O3-B2O3-FeO-Fe2O3-Cr2O3-NiO-BaO-La2O3-SrO-Al2O3-CaO-MgO-SiO2. Altogether 153 metal-metal or metal-oxgen binary systems and 105 pseudo-binary oxide-oxide systems have been consistently assessed. 20 ternary metal-metal-metal, metal-metal-O, C or B systems and 12 pseudo-ternary metal oxide systems are contained in the database. These systems comprise 46 different condensed non-ideal solution phases and 512 stoichiometric solid compound phases, furthermore there are 202 gas species. The databases is suited for applications in severe nuclear accident investigations, both in the in-vessel and the ex-vessel range. It can be implemented in thermohydraulic or other simulation codes using the programmers library ChemApp. The Thermodata nuclear database is under constant developments. Up-dates will be announced as they become available.

FREE SGTE *Binary alloys* and *Unary element* data.
The SGTE free binary alloy database comprises some 115 of the BINARY systems contained in the SGTE alloy databases. The database contains model parameters for binary systems only. No model parameters for ternary or higher-order systems are included. The selection of systems has been made so as to provide users with assessed data for a cross-section of system types, the stored data for which provide information on the systems concerned as well as allowing practice in the use of different software for phase diagram and thermodynamic property calculations.
In conjunction with the restricted set of recommended assessed binary systems above SGTE also provides data for the so-called lattice stabilities of the elements. It is SGTEs general policy to make the data for the elements freely available to the scientific community. Please make appropriate use of them. In case you want to set up a new database for an alloy system you can extract the necessary phase component data from the unary database while you assemble the basic solution phases such as Liquid, FCC_A1, BCC_A2 etc.

For information on the contents and range of applicability of the OLI Aqueous databases please see the web page of OLI Systems at: www.olisystems.com.

THERMODYNAMIC DATA-FILES/Mini-Databases

Off-the-shelf 'Standard' and specially prepared 'Customised' data-files are offered for direct and easy use with FactSage, but especially with ChemApp, ChemSheet and/or SimuSage. For more details on the 'Standard' datafiles please visit the GTT-Web Page (DataGuide). Prices for thermodynamic data-files are quoted separately, upon request.

FactSage - TEACH

FactSage-TEACH is a thermochemical teaching package based on the FactSage ITDS. It comprises a series of application oriented small databases and a comprehensive workbook. The workbook illustrates the practical use of computational thermochemistry for solving everyday problems in industry, research and environmental science. Through gaining a knowledge of the practical use of thermochemistry, a student is more inclined to learn the theory behind a rather dry subject matter. The workbooks contains an extensive introduction into the theoretical background of computational thermochemistry, thereafter the assignments are given with questions and answers. The workbook also provides a quick reference guide to the FactSage software. Since the program is interactive it provides an easy means to the student to check out "What happens if?" by changing input parameters and detecting the effects in the result tables or graphical output.

SPECIAL THERMOCHEMICAL SERVICES

GTT provides consulting, calculation, data-file compilation and teaching courses. Calculation services are used by many customers to supplement their research efforts and customer support activities. We also see ourselves in the role of "matchmakers" for those customers who seek special experimental support. Our colleagues at RWTH Aachen and Forschungszentrum Jülich are there to help with calorimetry, mass-spectrometry, thermal analysis and other methods.

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