

FactSage Practical

MSE302

Practical 1. Info and Databases

Acknowledgements

The teaching team of MSE302 is grateful to:

Professor Mansoor Barati (UofT)

Professor Elmira Moosavi (ETS)

Professor Arthur Pelton (CRCT)

Professors In-Ho Jung and M. -A. Van Ende (Seoul National University)

Dr. Sina Mostaghel (SNC-Lavalin)

Professor Kinnor Chattopadhyay (UofT)

Drs. Daigen Fukayama, Takahiro Sasaki (RCCM)

Drs. Moritz to Baden and Guixuan Wu (GTT Technologies)

Outline

1. [FactSage Overview](#)
2. [Information Module](#)
3. [Directory Settings](#)
4. [Documentation Module](#)

FactSage Overview: Thermodynamic Packages

Several thermochemical software/database packages with applications in materials science have been developed over the last 40+ years.

These packages all contain large **critically evaluated** databases of **thermochemical properties** for thousands of compounds and hundreds of solution phases, as well as user interfaces of varying degrees of user-friendliness.

- ✓ HSC Chemistry
- ✓ Thermo-Calc
- ✓ HSC Chemistry
- ✓ Pandat
- ✓ **FactSage**

(The history of FactSage: Interview Part [1](#) and [2](#), highly recommended!!!)

FactSage Overview: Who is FactSage?

FactSage stands for Fact + Sage (2001)

F*A*C*T: Facility for the Analysis of Chemical Thermodynamics – started in 1976 as a joint research project between two universities, the École Polytechnique (Professors Christopher W. Bale & Arthur D. Pelton) and McGill University (Professor William T. Thompson), for treating thermodynamic properties and calculations in chemical metallurgy. In 1984, CRCT was founded. F*A*C*T is also the name of the thermodynamic database developed at CRCT. The Windows® version FACT-Win (1999) offered a fully integrated thermochemical database system that coupled proven software with self-consistent critically assessed thermodynamic data.

Sage: SOLGASMIX-based advanced Gibbs energy minimizer (SOLGAMIX is a historic program published in 1975 by a German company that calculates the equilibria of **SOL**ids, **GAS**es, and **MIX**tures). Since Sage was used in other software, it was released under the name ChemSage (1987).

FactSage Overview: Who is FactSage?

What does FactSage stand for? Fact + Sage (2001)

FactSage™ is a thermochemical software and database package developed jointly between [Thermfact/CRCT](#) (Montreal, Canada) and [GTT-Technologies](#) (Aachen, Germany), and is the result of over 30 years of collaborative efforts. The FactSage web site is www.factsage.com.

FactSage Overview: What is FactSage?

FactSage contains a number of high-quality, critically assessed thermodynamic compound and solution databases, and uses a **Gibbs energy minimizer** when performing thermodynamic calculations.

Thermochemical databases contain parameters giving the **Gibbs energy**, G , of all compounds as functions of T (and P) and of all solutions as functions of T , (and P) and composition. This dependence gives a complete database because **all** the other thermodynamic properties (H , C_p , μ , etc.) can be calculated by taking the appropriate derivatives of the G functions.

Gibbs energy minimizer is used when calculating the system's equilibrium state under **a given set of constraints** (such as temperature, total pressure, total mass of each element). Mathematically, this is equivalent to solving all the equilibrium equations simultaneously. Thermodynamic data are automatically extracted as required from the databases.

FactSage Overview: What can FactSage do?

Coupled with the **Gibbs energy minimizer** of FactSage, we can use the critically assessed thermodynamic databases to do the following.

- ✓ Make predictions within a short period of time. New technological ideas can thus be generated by calculating the composition and temperature (Metal, Waste Treatment).
- ✓ Increase the process productivity (Chemistry).
- ✓ Guide the selection of refractory materials in a high-temperature furnace, and thus improve the service life of refractory material (Chemistry).
- ✓ Assist in root cause analysis and countermeasures (Heavy Industry, Iron- and Steel-making)
- ✓ Find if a process is thermodynamically feasible (Iron- and steel-making)
- ✓ Predict the behavior of systems that are difficult to experiment with (Nuclear materials)

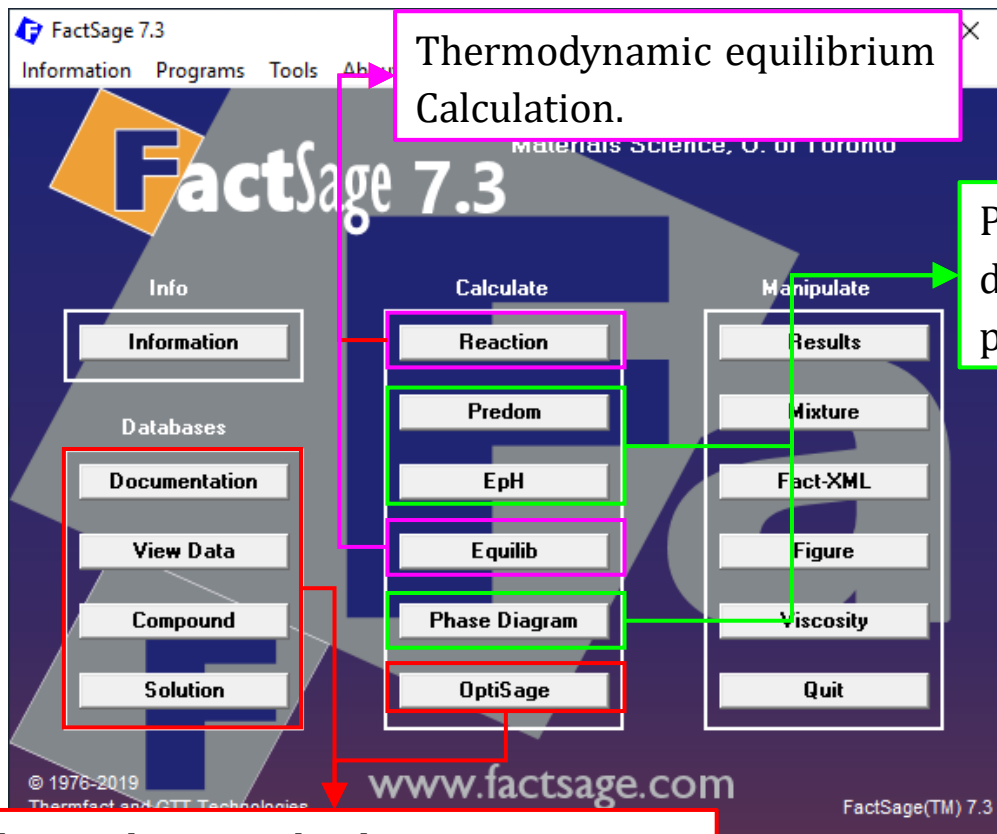
FactSage Overview: What can FactSage do?

Coupled with the **Gibbs energy minimizer** of FactSage, we can use the critically assessed thermodynamic databases do the following.

- ✓ Calculate any phase diagram sections (Isothermal, Isoplethal, etc.)
- ✓ Study the cooling paths of alloys (Equilibrium, Scheil-Gulliver, etc.)
- ✓ Determine the amounts of each phase (→ Estimation of amounts and composition of microstructural constituents.)
- ✓ Calculate the heat evolution during cooling, etc. (the thermodynamic database permits calculation of the driving force for diffusion, precipitation kinetics, etc. and can be coupled to software for phase field and kinetic modeling.)

FactSage Overview: What can FactSage do?

FactSage: Thermodynamic Databases Plus Gibbs Energy Minimizer (which Calculates Thermodynamic Phase Equilibria)



Thermodynamic equilibrium Calculation.

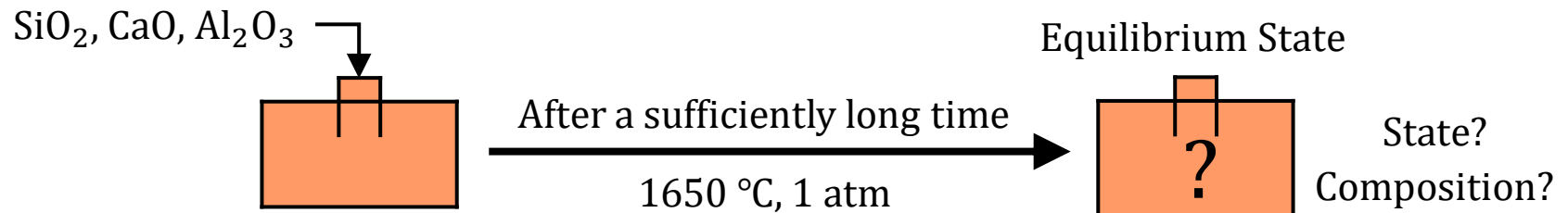
Phase Diagram Calculation (Phase diagram is graphical representation of phase equilibria).

Thermodynamic database management and editing.

FactSage Overview: Equilibrium Calculation

What is thermodynamic equilibrium calculation?

Say we place a number of substances in a container. Under given **external** conditions (e.g., temperature and pressure), if we put a lid or piston on top of the container and then leave the system for a sufficiently long time, the system's **macroscopic** properties such as temperature, pressure, volume, composition, etc. will remain unchanged with time. This indicates a **state of thermodynamic equilibrium** is reached.



In a thermodynamic equilibrium calculation, **the state of thermodynamic equilibrium** of a system is predicted by calculation based on thermodynamic laws (i.e., Gibbs energy minimization). This requires a fast and efficient algorithm and critically assessed thermodynamic database(s).

FactSage Overview: Thermodynamic Properties

What thermodynamic properties/diagrams can be calculated in FactSage?

With critically assessed thermodynamic databases...	
Reliable Estimation	Good Estimation
<ul style="list-style-type: none">✓ Equilibrium composition, partial pressure, activity✓ Equilibrium phase diagram (stable/metastable phases)✓ Melting and boiling point, phase transition temperatures<ul style="list-style-type: none">✓ Adiabatic combustion temperature✓ Gibbs energy, Enthalpy, Entropy, heat capacity	<ul style="list-style-type: none">✓ Viscosity of molten slag/glass✓ Viscosity of molten alloy✓ Thermal conductivity✓ Density and volume
Properties that can not be calculated	N/A
<ul style="list-style-type: none">× Mechanical properties (strength, hardness, etc.)<ul style="list-style-type: none">× Electrical conductivity× Permittivity× Crystallographic parameters× Magnetic susceptibility...	<ul style="list-style-type: none">× First principle calculation× Diffusion analysis× Fluid dynamic analysis

Information Module

The Information Module compiled all the teaching materials and examples files.

The screenshot displays the FactSage 7.3 Information Module interface. The main window shows a list of documents on the right and a sidebar on the left. Red boxes and arrows highlight specific features:

- FactSage 7.3** (top left)
- Information** (top left)
- Programs** (top left)
- Tools** (top left)
- About** (top left)
- Info** (left sidebar)
- Calculate** (left sidebar)
- Slide Shows** (left sidebar)
- Database Documentation ...** (left sidebar)
- FactSage Documentation ...** (left sidebar)
- Macro Processing** (left sidebar)
- FactSage-Teach** (left sidebar, highlighted with a red box)
- FactSage 7.3 -News- from www.FactSage.com ...** (left sidebar)
- What's New in FactSage 7.3 ...** (left sidebar)
- FAQ - Frequently Asked Questions ...** (left sidebar)
- Information, addresses, e-mails, phone numbers ...** (left sidebar)
- List of references ...** (left sidebar)
- FactSage Family of Products and Services ...** (left sidebar)
- © 1976-2019 Thermfact and GTT-Technologies** (bottom left)
- www.factsage.com** (bottom left)
- FactSage Overview - a quick look at FactSage Modules and Databases (pdf)** (right sidebar)
- FactSage Browser - a navigation tool for database documentation ...** (right sidebar)
- The theoretical background of FactSage ...** (right sidebar, highlighted with a red box)
- FactSage Applications Processing: Combustion and Heat (pdf)** (right sidebar)
- FactSage Applications Processing: Oxides and Pyrometallurgy (pdf)** (right sidebar)
- FactSage Applications Processing: Hall-Heroult Process (pdf)** (right sidebar)
- FactSage Ferrous Processing: Review of Thermodynamics (2015) (pdf)** (right sidebar)
- FactSage Ferrous Processing: Database Selection (2015) (pdf)** (right sidebar)
- FactSage Ferrous Processing: Applications I (2015) (pdf)** (right sidebar)
- FactSage Ferrous Processing: Applications II (2015) (pdf)** (right sidebar)
- FactSage Ferrous Processing: Process Simulation (2015) (pdf)** (right sidebar)
- FactSage Alloy Design: Basic and Advanced (2015) (pdf)** (right sidebar, highlighted with a red box)
- FactSage Alloy Design: Metal Treatment (pdf)** (right sidebar)
- FactSage Alloy Design: Solidification and Thermo. (pdf)** (right sidebar)
- FactSage Alloy Design: Solidification Microstructure (2017) (pdf)** (right sidebar)
- View Data ...** (right sidebar)
- Compound ...** (right sidebar)
- Solution - Introduction ...** (right sidebar)
- Solution - models and examples ...** (right sidebar)
- Reaction ...** (right sidebar)
- Predom ...** (right sidebar)
- Eph ...** (right sidebar)
- Equilib - Regular features ...** (right sidebar)
- Equilib - Advanced features ...** (right sidebar)
- Equilib - FactXML output ...** (right sidebar)
- Equilib - FactOptimal ...** (right sidebar)
- Equilib - Fact-Function-Builder ...** (right sidebar)
- Phase Diagram ...** (right sidebar)
- Phase Diagrams with Various X- and Y- ...** (right sidebar)
- Phase Diagram - Article - Scheil-Gulliver constituent diagrams (pdf)** (right sidebar)
- OptiSage ...** (right sidebar)
- Results ...** (right sidebar)

Advanced application examples using FactSage.

Some theoretical basis of FactSage. Ask your instructor if the relevant files can not be accessed.

Directory Settings

Before we carry out any thermodynamic calculations (in the Reaction, Predom, EpH, Equilib, Phase Diagram Module), we need to create a Directory. That can be on any hard drive or a movable USB.

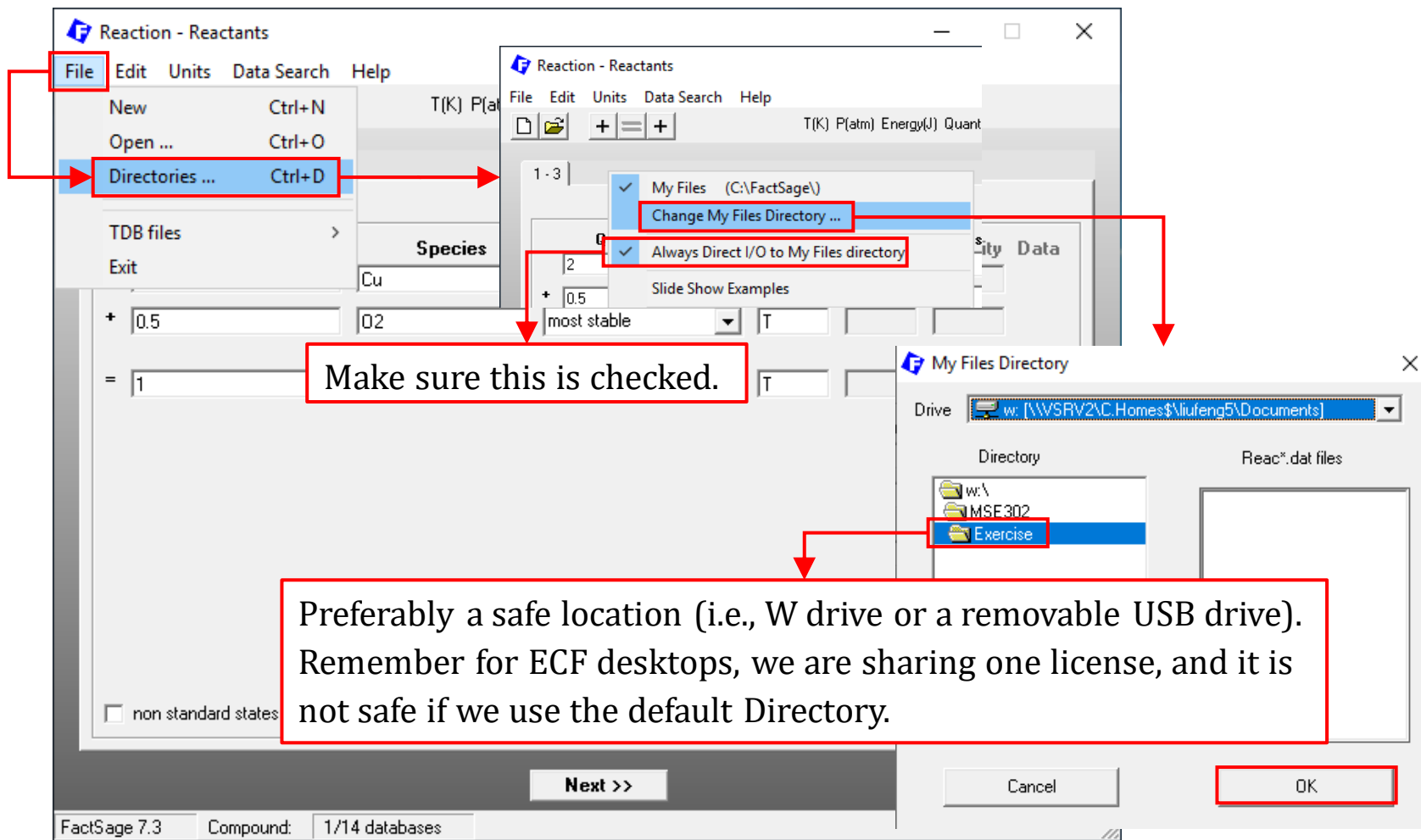
Note: the default Directory (C:\FactSage\) can be changed using any of the above-mentioned module.

Directory Settings



Run the "Reaction" Module

Directory Settings



File/Directories/Change My Files Directory

Directory Settings

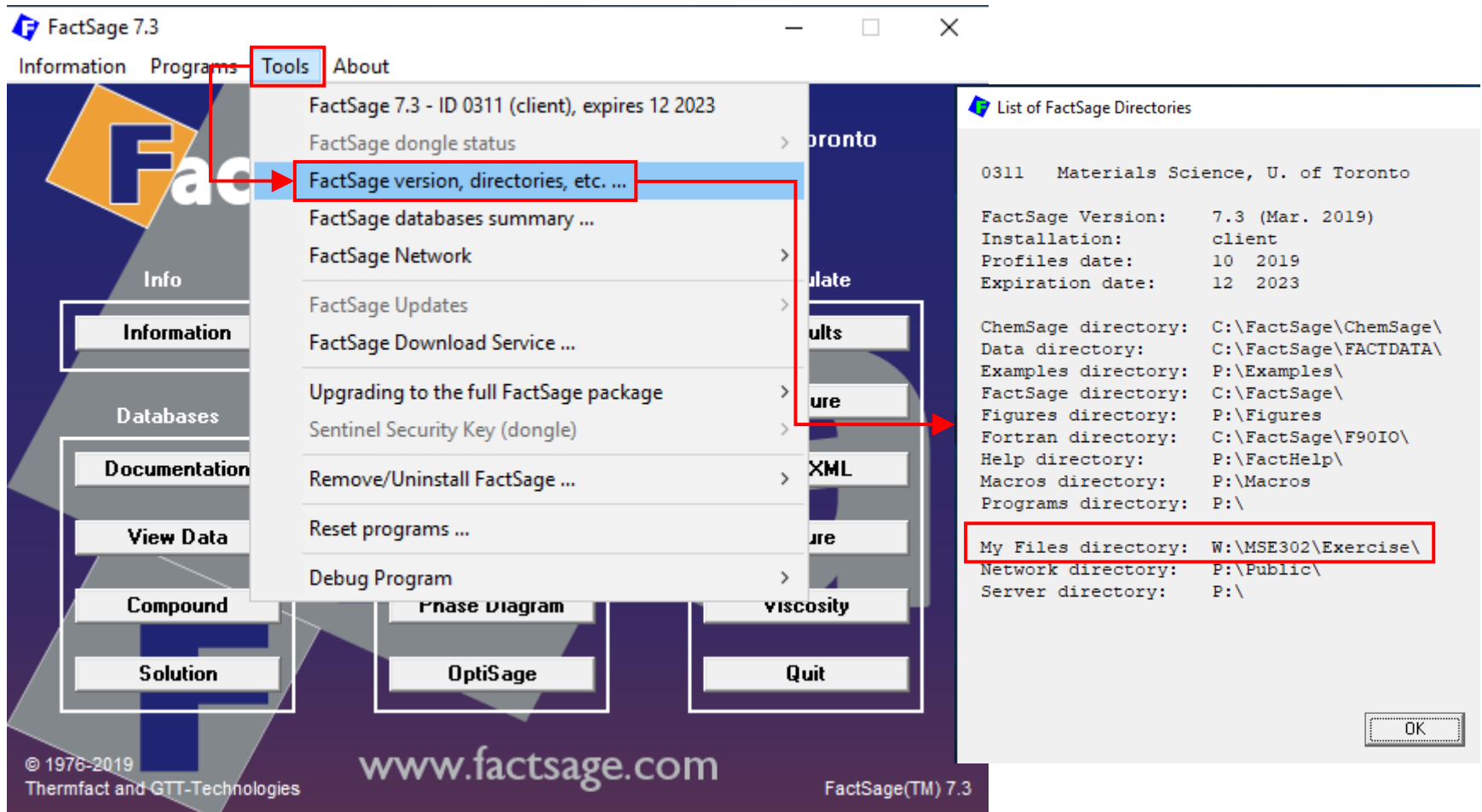
Now, if you run other modules, you should find that the Directory for these modules has also been changed.

Although it is not mandatory to change the default Directory, a carefully chosen Directory keeps your calculation files safe and well-organized.

Note: for the FactSage installed on the ECF desktop, all the FactSage settings will be restored to default every time you log out your ECF account. Therefore, it is recommended to check the directory settings before you perform a thermodynamic calculation.

Directory Settings

One can always check the Directory from the Main Screen

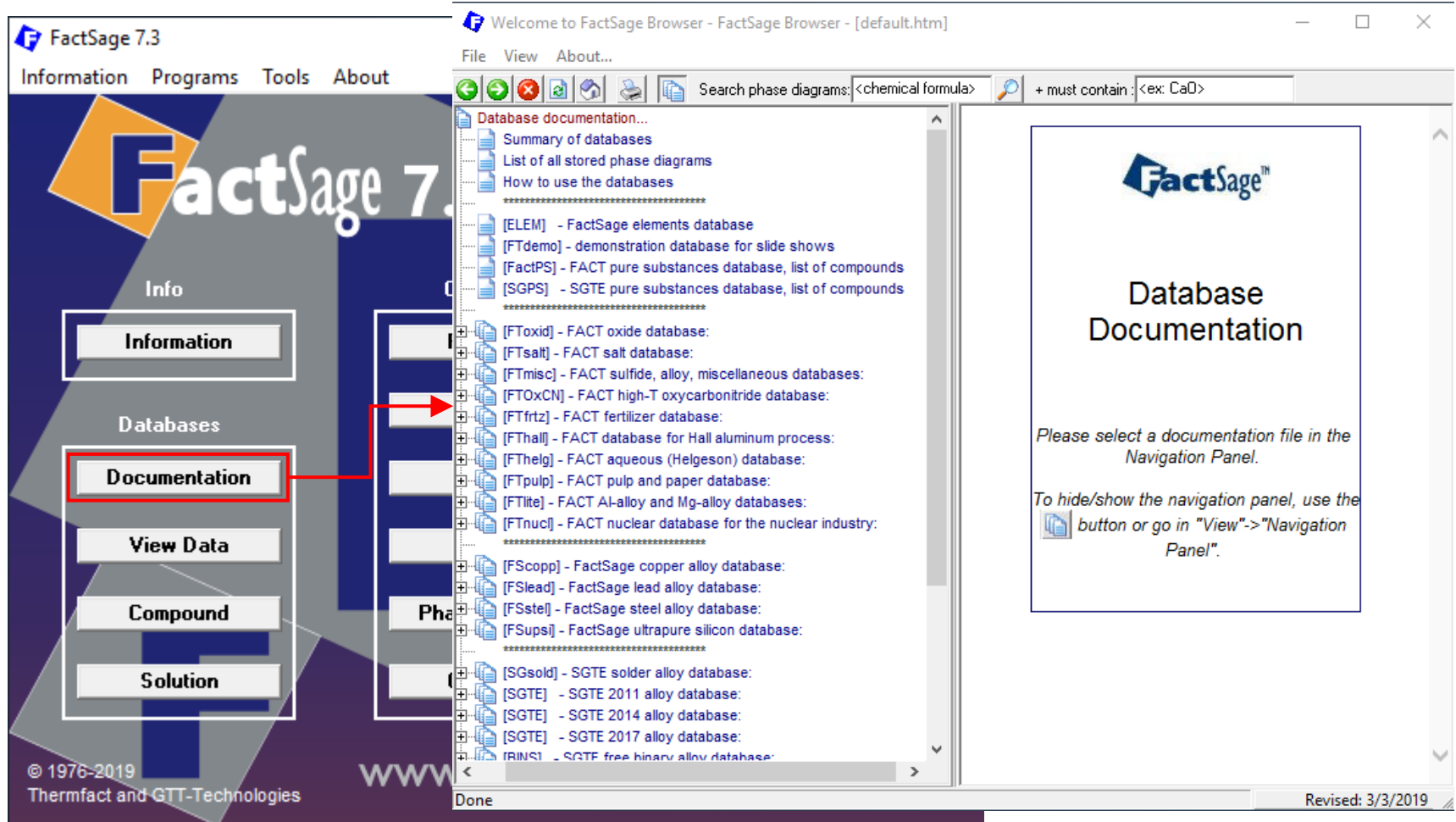


Documentation Module

The Documentation module is your **reference point** when using FactSage. Prior to performing a thermodynamic calculation, we need to “consult” the Documentation module to do the following.

- ✓ Choose the right database(s).
- ✓ Know the reliability of thermodynamic data.
- ✓ Determine if the thermodynamic calculations can be carried out within the effective composition range and effective temperature range.

Documentation Module



Run the "Documentation" Module

Documentation Module

Summary of Databases

The screenshot shows the FactSage 7.3 Summary of Databases window. The left sidebar lists various databases under 'Database documentation...'. The main panel displays a summary of these databases, categorized into 'Overview of databases', 'Compound Databases', 'Coupled Compound & Solution Databases', and 'Fact Package'. Red boxes and arrows highlight specific information:

- Advanced users of FactSage must be familiar with this content.** (Points to the top of the main panel)
- Only Stoi. Compounds.** (Points to the 'Overview of databases' section)
- Both Stoi. Compounds and Solutions.** (Points to the 'Coupled Compound & Solution Databases' section)
- By CRCT.** (Points to the 'Fact Package' section)
- By SGTE.** (Points to the 'SGTE' databases in the 'Coupled Compound & Solution Databases' section)

FactSage 7.3 - Summary of Databases

Overview of databases

- Compound Databases :**
 - FactPS** - FACT pure substances database
 - SGPS** - SGTE pure substances database
 - FTDemo** - FACT slide show demonstration database
 - SGun** - SGTE unary database

Coupled Compound & Solution Databases :

- Fact Package:**
 - FToxid** - oxide database for slags, glasses, ceramics, refractories
 - FTsalt** - salt database
 - FTHall** - Hall-Héroult aluminum database
 - FTHeig** - aqueous (Helge)
 - FTmisc** - miscellaneous database for sulfides, alloys, etc.
 - FTpulp** - pulp and paper database (also for corrosion and combustion)
 - FTftrtz** - fertilizer database (also for explosives)
 - FTOxCN** - oxycarbonitride high temperature database

Revised: 3/3/2019

Documentation Module

Summary of Databases

FactSage Summary of Databases - FactSage Browser - [FSDData.htm]

File View About...

Search phase diagrams: <chemical formula> + must contain: <ex: CaO>

Database documentation...

- Summary of databases
- List of all stored phase diagrams
- How to use the databases
- *****
- [ELEM] - FactSage elements database
- [FTdemo] - demonstration database for slide shows
- [FactPS] - FACT pure substances database, list of compounds
- [SGPS] - SGTE pure substances database, list of compounds
- *****
- [FToxid] - FACT oxide database:
- [FTsalt] - FACT salt database:
- [FTmisc] - FACT sulfide, alloy, miscellaneous databases:
- [FTOxCN] - FACT high-T oxycarbonitride database:
- [FTfrtz] - FACT fertilizer database:
- [FThall] - FACT database for Hall aluminum process:
- [FThelg] - FACT aqueous (Helgeson) database:
- [FTpulp] - FACT pulp and paper database:
- [FTlite] - FACT Al-alloy and Mg-alloy databases:
- [FTnucl] - FACT nuclear database for the nuclear industry:
- *****
- [FScopp] - FactSage copper alloy database:
- [FSlead] - FactSage lead alloy database:
- [FSstel] - FactSage steel alloy database:
- [FSup] - FactSage ultrapure silicon database:
- *****
- [SGsc] - SGTE 2011 alloy database:
- [SGTE] - SGTE 2014 alloy database:
- [SGTE] - SGTE 2017 alloy database:
- [BINS] - SGTE free binary alloy database:

By FactSage's collaborators.

Other databases:

- FTlite - Al-alloy and Mg-alloy databases
- FTnucl - FACT nuclear database.

By CRCT.

FactSage™ Databases:

- FScopp - copper alloy database
- FSlead - lead alloy database
- FSstel - steel database
- FSupsi - ultrapure silicon database

By CRCT and GTT.

SGTE Databases:

- SGTE - alloy database
- SGsold - solders database
- BINS - free alloy database

By SGTE.

Free but not complete.

Other Databases:

- SpMCBN - database for carbide, boride, nitride and silicide systems
- SGnobl - noble metal database
- TDnucl and TDmeph - Thermodata nuclear databases

General FactSage Database Documentation

Revised: 3/3/2019

Documentation Module

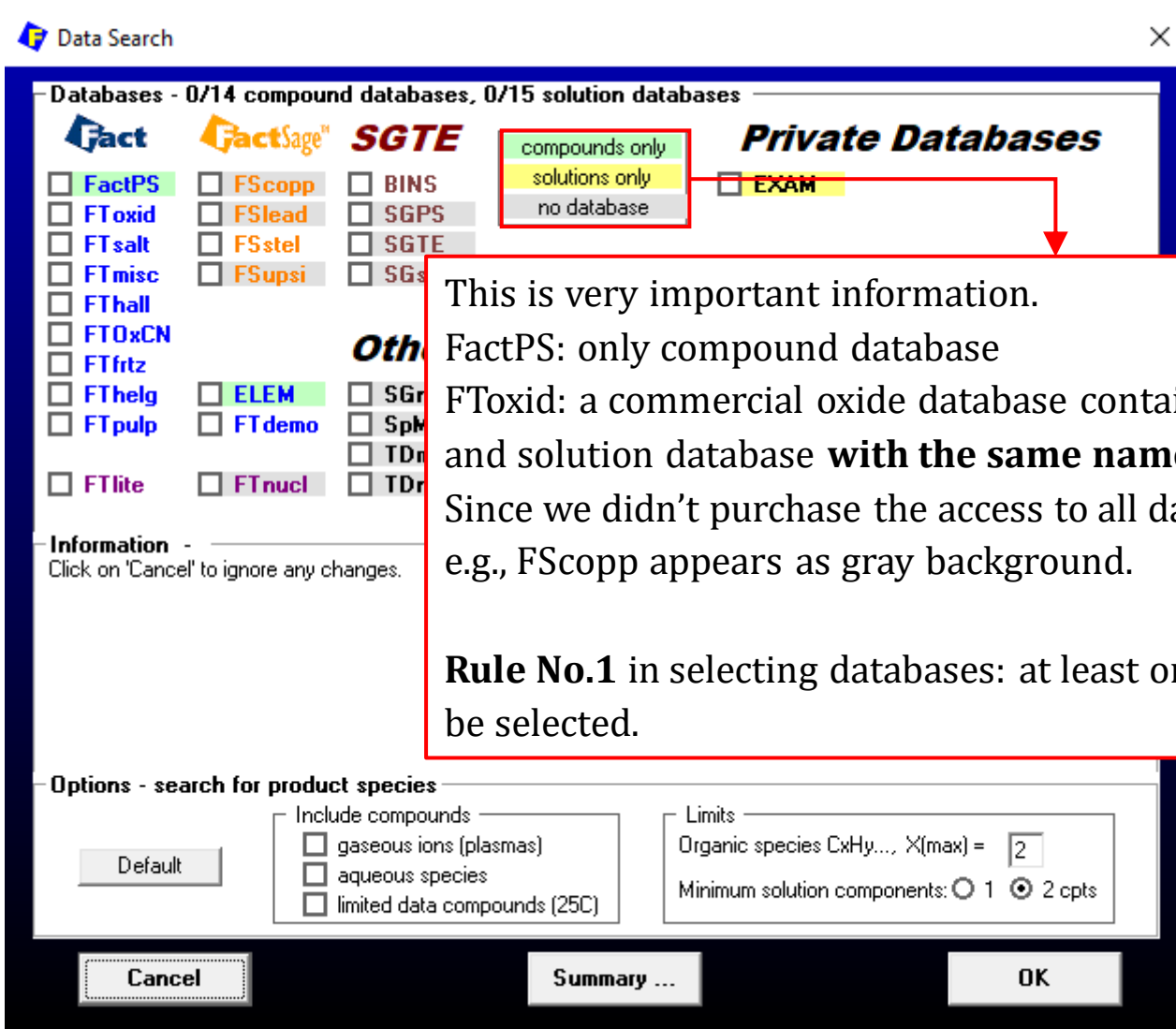
Compound Database	
FactPS	FACT compound database
SGPS	SGTE compound database

Compound Database & Solution Database (FACT)	
FToxid	Oxide (slag, glass, ceramics, refractory)
FTsalt	Salt
FThall	Hall-Hérault method (aluminum smelting)
FThelg	Dilute solution
FTmisc	Molten steel (main components are Fe, Cu, Ti, Pb, etc.), sulfur/sulfide compounds, solutions.
FTpulp	Black liquor discharged during the pulp manufacturing process
FTfrtz	Chemical fertilizer
FTOxCN	High temperature acid/charcoal/nitride (ceramics, etc.)
Ftlite	Aluminum alloy/Magnesium alloy
FTnucl	FACT nuclear fuel
FTdemo	Demonstration database. Used in help examples

Compound Database & Solution Database (Collaborators)	
FScopp	Copper alloy
FSlead	Lead alloy
FSstel	Iron alloy
FSupsi	Ultra-high purity silicon
SGTE	Alloys of various systems
SGsold	Solder system
BINS	Binary alloy
SpMCBN	Refractory (Metal C-B-N series)
SGnobl	Noble metals
Tdnucl	IRSN nuclear related systems
Tdmeph	IRSN nuclear fuel

FactSage Database { Compound Database
Solution Database

Documentation Module



Documentation Module

For the solution databases in FactSage...

- ✓ Not all databases contain a solution database; some databases only contain compound database.
- ✓ The thermodynamic data of solution phases such as molten slag, oxide solid solutions, liquid iron, molten steel, alloys, etc. are stored in the solution databases.
- ✓ While the gas mixture is classified as a solution phase, in FactSage, the thermodynamic data of gaseous species are stored in the compound database (FactPS). This is because the gas mixture is normally treated as ideal solution and the Gibbs energy of the gas mixture is determined by the Gibbs energy of the individual gas components.
- ✓ When using the solution databases, one should always consult the Documentation Module to ensure appropriate selection of solution databases and the solution phases.

Documentation Module

General tips when using the solution database

- ✓ The user should consult carefully the general description of the database in the Documentation Module for the systems that have been fully/partially assessed. Searching the relevant phase diagram is very helpful.
- ✓ Each solution database has its own unique feature, and thus the method/rule of phase selection might be different.
- ✓ Some databases by default set the immiscibility as [I]- or [J]-option for a solution phase; but these settings might not be necessary.
- ✓ There are phases that are exclusive to each other and should not be selected at the same time. This is especially true if multiple solution databases are selected. Typical examples: molten slag and liquid metal.
- ✓ For high-order systems (No. Components ≥ 4), one should be aware that it is impossible to know the optimal phase selection before calculation. Multiple trial-and-error calculations are usually needed.

Documentation Module

List of All Stored Phase Diagrams

The Documentation module provides a larger number of phase diagrams calculated using the commercial databases of FactSage (unfortunately, our school didn't purchase the full package and some commercial databases are inaccessible.) or SGTE alloy databases.

Documentation Module

List of All Stored Phase Diagrams

FactSage 7.3 - List of Stored Phase Diagrams (6845)

FACT Databases

FToxid FACT oxide data (454)	FTsalt salt data (338)	FTmisc sulfide, alloy, miscellaneous data (39)
FThall data for Hall aluminum process (14)	FTPulp pulp and paper data (22)	FThelg aqueous (Helgeson) data (0)
FTlite Al-alloy and Mg-alloy light metal data (854)	FTOxCN high-temperature oxycarbonitrides (55)	FTfrtz fertilizer (210)

FactSage Databases

FScopp copper alloy data (422)	FSlead lead alloy data (161)	FSstel steel alloy data (187)
FSupsi ultrapure silicon data (0)		

SGTE Databases

SGTE2011 2011 alloy data (535)	SGTE2014 2014 alloy data (970)	SGTE2017 2017 alloy data (1176)
SGsold solder alloy data (55)	BINARY free binary SGTE alloy data (108)	

Revised: 3/3/2019

Documentation Module

List of All Stored Phase Diagrams

FTlite - FACT Al-alloy and Mg-alloy Phase Diagrams (854) - FactSage Browser - [FTlite_Figs.htm]

File View About...

Search phase diagrams: <chemical formula> + must contain: <ex: CaO>

Database documentation...

- Summary of databases
- List of all stored phase diagrams
- How to use the databases

- [ELEM] - FactSage elements database
- [FTdemo] - demonstration database for slide shows
- [FactPS] - FACT pure substances database, list of compounds
- [SGPS] - SGTE pure substances database, list of compounds

- [FToxid] - FACT oxide database:
- [FTsalt] - FACT salt database:
- [FTmisc] - FACT sulfide, alloy, miscellaneous databases:
- [FTOxCN] - FACT high-T oxycarbonitride database:
- [FTfrtz] - FACT fertilizer database:
- [FTHall] - FACT database for Hall aluminum process:
- [FTHelg] - FACT aqueous (Helgeson) database:
- [FTpulp] - FACT pulp and paper database:
- [-] FTlite - FACT Al-alloy and Mg-alloy databases:
 - (pdf) general description and list of optimized systems
 - list of compounds and solutions
 - phase diagrams
- [FTnuc] - FACT nuclear database for the nuclear industry:

FTlite - FACT Al-alloy and Mg-alloy Phase Diagrams (854)

Click on a system to display the phase diagram.

Ag-Al

Ag-Bi

Ag-Cu

Ag-In

Ag-Na

Ag-Sb

Ag-Ta

Ag-Zr

Al-Be

Al-Bi

Al-Co

Al-Eu

Al-H

Al-La

Al-Na

Al-Pb

Al-Sm

Al-Ti

Al-Yb

Al-Zn

Al-Zr

Al-V

Al-W

As-Au

As-In

Preview

Ag - Al

Data from FTlite - FACT light alloy databases

FactSage

T/C

Al/(Ag+Al) (mol/mol)

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You can find the phase diagram for the system of interest under each database section.

Documentation Module

List of All Stored Phase Diagrams

Search Results - FactSage Browser - [search_results.htm]

File View About...

Search phase diagrams: Ag Al

You can ALSO search the phase diagram by typing the elements for the system of interest.

Database documentation...

- Summary of databases
- List of all stored phase diagrams
- How to use the databases

- [ELEM] - FactSage elements database
- [FTdemo] - demonstration database for slide shows
- [FactPS] - FACT pure substances database, list of compounds
- [SGPS] - SGTE pure substances database, list of compounds

- [FToxid] - FACT oxide database:
- [FTsalt] - FACT salt database:
- [FTmisc] - FACT sulfide, alloy, miscellaneous databases:
- [FToxCN] - FACT high-T oxycarbonitride database:
- [FTfrtz] - FACT fertilizer database:
- [FThall] - FACT database for Hall aluminum process:

- [SGsold] - SGTE solder alloy database:
- [SGTE] - SGTE 2011 alloy database:

List of Phase Diagrams:

- Ag - Al : | FScopp | **FTlite** | SGnobl | SGTE2011 | SGTE2014 | SGTE2017 | TDnucl |
- Al - Zn - Ag : | SGnobl |
- Al - Ti - Ag : | SGnobl |
- Al - Sn - Ag : | SGnobl |
- Al - Sn - Ag : | SGnobl |
- Al - Si - Ag : | SGnobl |
- Al - Si - Ag : | SGnobl |
- Al - Pb - Ag : | SGnobl |

Search results for: **Ag Al**

Preview

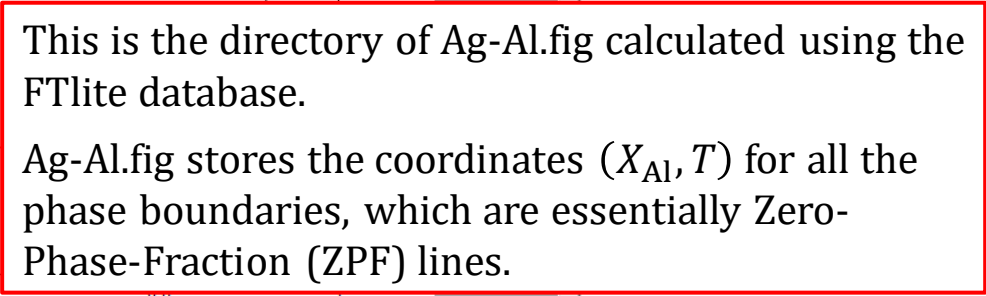
Ag - Al
Data from FTlite - FACT light alloy databases

FactSage

Revised: 3/3/2019

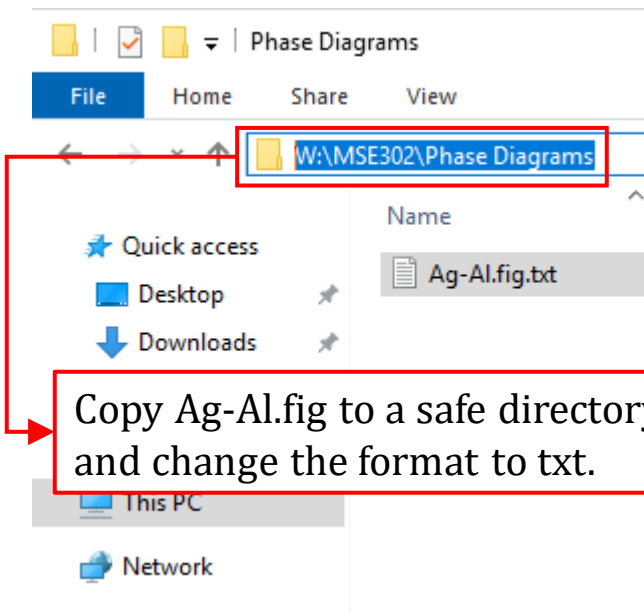
You might notice that the phase diagram of the Ag-Al system can be calculated by various databases. Although these diagrams look pretty similar, some details (phase boundaries) might differ depending on the corresponding assessment work.

List of All Stored Phase Diagrams



Documentation Module

List of All Stored Phase Diagrams



Ag-Al.fig.txt - Notepad

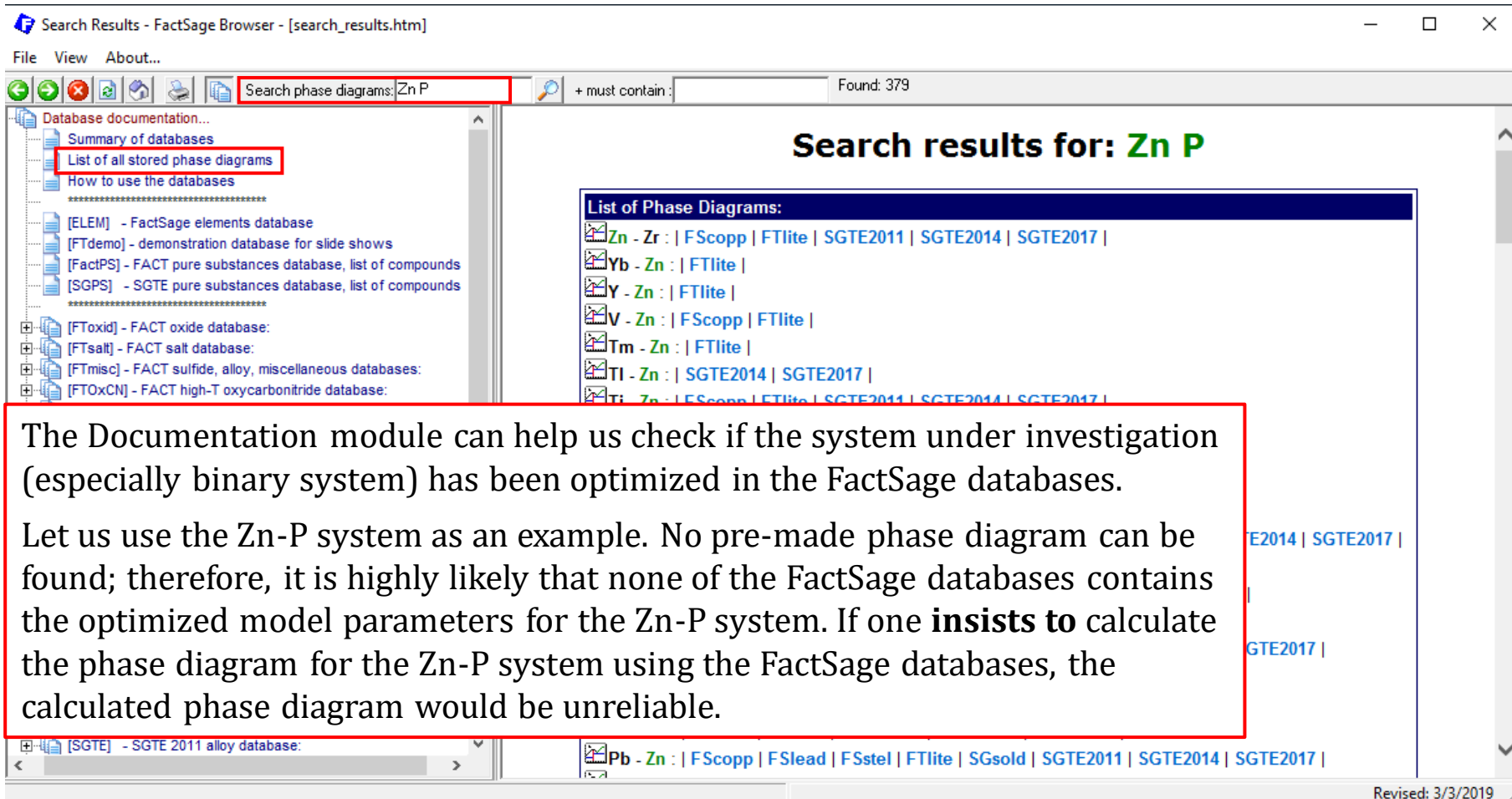
	File	Edit	Format	View	Help
210PEN	4	0	3.00000000000000E-0001	(mode style width)	
210PEN	4	0	2.00000002980232E-0001	(mode style width)	
701LIN	0	1	255 255 255 0 1	ZPF: Liquid#1	
120EXP	0	1	1.00000000000000E-0005	9.61779077000000E+0002	
120EXP	-1	1	1.00593838000000E-0003	9.61680277000000E+0002	
120EXP	-1	1	1.32368036000000E-0002	9.58843652000000E+0002	
120EXP	-1	2	4.65439390000000E-0002	9.53247320000000E+0002	
120EXP	-1	4	4.73869420000000E-0002	9.36872285000000E+0002	
120EXP	-1	6	2.31895700000000E-0002	9.17320671000000E+0002	
120EXP	-1	7	8.60559720000000E-0002	8.96457329000000E+0002	
120EXP	-1	9	4.24261220000000E-0002	8.75001013000000E+0002	
120EXP	-1	1	0.09594671000000E-0001	8.53297122000000E+0002	
120EXP	-1	1	2.48943070000000E-0001	8.31548484000000E+0002	
120EXP	-1	1	4.03067250000000E-0001	8.09896419000000E+0002	

Use Notepad to open the Ag-Al.fig.txt, you should be able to find the coordinates of various ZPF's for different phases. The third and fourth columns correspond to X_{Al} and T , respectively.

120EXP	-1	2	7.27010110000000E-0001	7.34430140000000E+0002	
120EXP	-1	2	7.69196900000000E-0001	7.31346699000000E+0002	
120EXP	-1	3	0.19191900000000E-0001	7.31346699000000E+0002	
120EXP	-1	3	2.53910180000000E-0001	7.31346699000000E+0002	

Documentation Module

List of All Stored Phase Diagrams



The screenshot shows the FactSage Browser interface. The search bar at the top contains 'Zn P' and 'Found: 379'. The left sidebar shows a tree view with 'List of all stored phase diagrams' highlighted. The main panel displays 'Search results for: Zn P' and a 'List of Phase Diagrams' table. The table lists various phase diagrams for Zn-P, Zn-Zr, Zn-Yb, Zn-Y, Zn-V, Zn-Tm, Zn-Tl, and Zn-Ti, each with associated database sources like FScopp, FTlite, SGTE2011, SGTE2014, and SGTE2017. A red box highlights the text below the table, explaining the documentation module's role in checking for optimized models and the unreliability of calculated diagrams for the Zn-P system.

The Documentation module can help us check if the system under investigation (especially binary system) has been optimized in the FactSage databases.

Let us use the Zn-P system as an example. No pre-made phase diagram can be found; therefore, it is highly likely that none of the FactSage databases contains the optimized model parameters for the Zn-P system. If one **insists to** calculate the phase diagram for the Zn-P system using the FactSage databases, the calculated phase diagram would be unreliable.

Documentation Module

How to use the databases?

The screenshot shows the FactSage Database Documentation browser window. The title bar reads 'FactSage Database Documentation - FactSage Browser - [Database_Documentation.htm]'. The menu bar includes 'File', 'View', and 'About...'. The toolbar contains icons for navigation and search. The search bar is labeled 'Search phase diagrams:' and the status bar shows 'Found: 899'. The left sidebar lists the following items: 'Database documentation...', 'Summary of databases', 'List of all stored phase diagrams', 'How to use the databases' (highlighted with a red box), '[ELEM] - FactSage elements database', and '[FTdemo] - demonstration database for slide shows'. The main content area displays the title 'HOW TO USE THE DATABASES' in red, followed by a 'Table of Contents' section. The table of contents lists the following sections and subsections: 1.0 INTRODUCTION (1.1 Overview, 1.2 References), 2.0 GENERAL COMPOUND DATABASES (2.1 The FactPS (FS53Base.cdb) general compound database, 2.2 SGPS (SGPSBase.cdb) - the SGTE pure substances database, 2.3 The former FACT pure compound (FS50Base.cdb) and solution (FS50soln.sda) databases), 3.0 CORRESPONDING SOLUTION AND COMPOUND DATABASES (3.1 Corresponding solution and compound databases: 3.1.1 Recommended procedure for species selection, 3.1.2 Database naming convention), 4.0 THE FACTSAGE ELEM COMPOUND DATABASE, and 5.0 DOCUMENTATION FOR ASSISTANCE WITH SPECIES AND PHASE SELECTION (5.1 General Description of a database, 5.2 List of optimized systems and calculated binary phase diagrams, 5.3 Phase Diagrams, 5.4 List of compounds and solutions). A red box highlights the text: 'This section provides a general guidance to the use of FactSage databases. **You are expected to** read this section thoroughly so that you feel confident when choosing the right database(s) and the right species from the database when carrying out a thermodynamic calculation.' The bottom right corner of the window shows 'Revised: 3/3/2019'.

FactSage Database Documentation - FactSage Browser - [Database_Documentation.htm]

File View About...

Search phase diagrams: + must contain: Found: 899

Database documentation...
Summary of databases
List of all stored phase diagrams
How to use the databases
[ELEM] - FactSage elements database
[FTdemo] - demonstration database for slide shows

HOW TO USE THE DATABASES

Table of Contents

1.0 INTRODUCTION
1.1 Overview
1.2 References

2.0 GENERAL COMPOUND DATABASES
2.1 The FactPS (FS53Base.cdb) general compound database
2.2 SGPS (SGPSBase.cdb) - the SGTE pure substances database.
2.3 The former FACT pure compound (FS50Base.cdb) and solution (FS50soln.sda) databases:

3.0 CORRESPONDING SOLUTION AND COMPOUND DATABASES
3.1 Corresponding solution and compound databases:
3.1.1 Recommended procedure for species selection
3.1.2 Database naming convention

4.0 THE FACTSAGE ELEM COMPOUND DATABASE

5.0 DOCUMENTATION FOR ASSISTANCE WITH SPECIES AND PHASE SELECTION
5.1 General Description of a database
5.2 List of optimized systems and calculated binary phase diagrams
5.3 Phase Diagrams
5.4 List of compounds and solutions

Revised: 3/3/2019

This section provides a general guidance to the use of FactSage databases. **You are expected to** read this section thoroughly so that you feel confident when choosing the right database(s) and the right species from the database when carrying out a thermodynamic calculation.

[SGsold] - SGTE solder alloy database:
[SGTE] - SGTE 2011 alloy database:
[SGTE] - SGTE 2014 alloy database:
[SGTE] - SGTE 2017 alloy database:
[IRINS] - SGTE free binary alloy database:

Documentation Module

[ELEM] – FactSage elements database

ELEM Compound Database - FactSage Browser - [ELEM_Documentation.htm]

File View About...

Search phase diagrams: + must contain: Found: 899

Database documentation...

- Summary of databases
- List of all stored phase diagrams
- How to use the databases
- *****
- [ELEM] - FactSage elements database**
- [FTdemo] - demonstration database for slide shows
- [FactPS] - FACT pure substances database, list of compounds
- [SGPS] - SGTE pure substances database, list of compounds
- *****
- [FToxid] - FACT oxide database:
- [FTsalt] - FACT salt database:
- [FTmisc] - FACT sulfide, alloy, miscellaneous databases:
- [FTOxCN] - FACT high-T oxycarbonitride database:
- [FTfritz] - FACT fertilizer database:
- [FThall] - FACT database for Hall aluminum process:
- [FThelg] - FACT aqueous (Helgeson) database:
- [FTpulp] - FACT pulp and paper database:
- [FTlite] - FACT Al-alloy and Mg-alloy databases:
- [FTnuc] - FACT nuclear database for the nuclear industry:
- *****
- [FScopp] - FactSage copper alloy database:
- [FSlead] - FactSage lead alloy database:
- [FSstel] - FactSage steel alloy database:
- [FSupsi] - FactSage ultrapure silicon database:
- *****
- [SGsold] - SGTE solder alloy database:
- [SGTE] - SGTE 2011 alloy database:
- [SGTE] - SGTE 2014 alloy database:
- [SGTE] - SGTE 2017 alloy database:
- [IRINS] - SGTE free binary alloy database:

The FactSage ELEM Compound Database

The **ELEM** compound database contains standard state data for all the elements taken from the **FactPS** compound database.

There is no need to select the **ELEM** database in your data search. If elemental data are required by a program it will automatically retrieve the data from the **FactPS** database.

Recall from MSE302, “absolute” Enthalpy and Gibbs energy require the selection of a reference state. The most common reference state is Standard Element Reference (SER) State, and FactSage databases use this SER State.

Done Revised: 3/3/2019

Documentation Module

[FTdemo] – demonstration database for slide shows

FTdemo Databases - FactSage Browser - [FS50_SlideShows.htm]

File View About...

Search phase diagrams: + must contain: Found: 899

Database documentation...

- Summary of databases
- List of all stored phase diagrams
- How to use the databases
- *****
- [ELEM] - FactSage elements database
- [FTdemo] - demonstration database for slide shows**
- [FactPS] - FACT pure substances database, list of compounds
- [SGPS] - SGTE pure substances database, list of compounds
- *****
- [FToxid] - FACT oxide database:
- [FTsalt] - FACT salt database:
- [FTmisc] - FACT sulfide, alloy, miscellaneous databases:
- [FTOxCN] - FACT high-T oxycarbonitride database:
- [FTfritz] - FACT fertilizer database:
- [FThall] - FACT database for Hall aluminum process:
- [FThelg] - FACT aqueous (Helgeson) database:
- [FTpulp] - FACT pulp and paper database:
- [FTlite] - FACT Al-alloy and Mg-alloy databases:
- [FTnucl] - FACT nuclear database for the nuclear industry:
- *****
- [FS Copp] - FactSage copper alloy database:
- [FSlead] - FactSage lead alloy database:
- [FSstel] - FactSage steel alloy database:
- [FSupsi] - FactSage ultrapure silicon database:
- *****
- [SGsold] - SGTE solder alloy database:
- [SGTE] - SGTE 2011 alloy database:
- [SGTE] - SGTE 2014 alloy database:
- [SGTE] - SGTE 2017 alloy database:
- [IRINS] - SGTE free binary alloy database:

FTdemo Demonstration Slide Show Databases

The **worked examples** ("slide show examples") which are included with the **Reaction, Predom, Equilib** and **Phase Diagram** modules generally use the **FTdemo** demonstration databases (these are the old **FACT** databases from **FactSage 5.0**). In this manner the species, phase selection and thermodynamic data presented in the **Slide Show** documentation will not change when **FTdemo** data are employed since these databases are not being updated.

The **FTdemo** databases should only be used for slide shows and teaching. Since the results can be imprecise and even totally wrong you must never publish results that employ **FTdemo** data.

Fact	FactSage	SGTE
<input type="checkbox"/> FactPS	<input type="checkbox"/> FS Copp	<input type="checkbox"/> BINS
<input type="checkbox"/> FToxid	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGTE
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSupsi	<input type="checkbox"/> SGsold
<input type="checkbox"/> FThall		
<input type="checkbox"/> FTOxCN		
<input type="checkbox"/> FTfritz		
<input type="checkbox"/> FThelg	<input type="checkbox"/> ELEM	Other
<input type="checkbox"/> FTpulp	<input type="checkbox"/> FTdemo	<input type="checkbox"/> SGnobl
<input type="checkbox"/> FTlite	<input type="checkbox"/> FTnucl	<input type="checkbox"/> SpMCBN
		<input type="checkbox"/> TDmeph
		<input type="checkbox"/> TDnucl

For research and publications use data from any protected public database except **FTdemo**.

Done

Revised: 3/3/2019

Documentation Module

[FTdemo] – demonstration database for slide shows

The screenshot displays the FactSage Browser window titled "FACT oxide database - documentation - FactSage Browser - [FToxid_Documentation.htm]". The left sidebar shows a tree view of databases, with "[FTdemo] - demonstration database for slide shows" selected and highlighted with a red box. The main content area displays the documentation for "THE FACT FToxid OXIDE DATABASES".

THE FACT FToxid OXIDE DATABASES

The FToxid solution database contains oxide solutions evaluated/optimized by the FACT group. The FToxid compound database contains all stoichiometric solid and liquid oxide compounds evaluated/optimized by the FACT group to be thermodynamically consistent with the FToxid solution database.

Systems and Components

The FToxid databases contain data for pure oxides and oxide solutions of 20 elements (as well as for dilute solutions of S, SO₄, PO₄, H₂O/OH, CO₃, F, Cl and I in the molten (slag) phase.) ~~Not all binary and ternary sub-systems have been evaluated and optimized, nor are all composition ranges covered. Sub-systems which have not been evaluated and optimized have been assumed ideal or have been approximated. The sub-systems and composition ranges which have been evaluated and optimized are described in the following. The most accurate calculations will be obtained in or near these sub-systems and composition ranges.~~

(1) Major oxide components: Al₂O₃, CaO, FeO, Fe₂O₃, MgO, SiO₂

All major oxide components have been fully optimized and evaluated together at all compositions. All available data for binary, ternary and quaternary sub-systems have been fully optimized [2004, 2020, 2025, 2028, 2030, 2031, 2032, 2050, 6009, 6020].

(2) Systems containing MnO, Mn₂O₃, CoO, NiO, PbO, ZnO with the major oxide components Al₂O₃, CaO, FeO, Fe₂O₃, MgO, SiO₂.

Revised: 3/3/2019

Documentation Module

Solution Databases

FACT oxide database - documentation - FactSage Browser - [FToxid_Documentation.htm]

File View About...

Search phase diagrams: + must contain: Found: 899

THE FACT FToxid OXIDE DATABASES

The FToxid solution database contains oxide solutions evaluated/optimized by the FACT group. The FToxid compound database contains all stoichiometric solid and liquid oxide compounds evaluated/optimized by the FACT group to be thermodynamically consistent with the FToxid solution database.

Systems and Components

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You should use the information provided here as a dictionary. When you are performing a calculation for a given system, check if the system has been optimized. You can also access the solution description in the Equilib and Phase Diagram Module (this will be shown later).

(1) M
All m
data 1
2031

(2) S
CaO, FeO, Fe₂O₃, MgO, SiO₂.

Done Revised: 3/3/2019

Documentation Module

[SGUN] – SGTE Unary database

SGTE Unary database - FactSage Browser - [SGUNbase.HTM]

File View About...

Search phase diagrams: + must contain: Found: 899

SGTE Unary database

The SGTE Unary database - reference data for the thermodynamic properties of the elements

The development and use of databanks for the calculation of complex multi-component phase equilibria has made it necessary to adopt standards for the critical assessment of data. The basis for the whole process is the definition of reference data for the thermodynamic properties of the elements (and other key components) in various phases in which they may occur or dissolve.

Through the years SGTE has determined and compiled such data in the form of Gibbs energies of the elements in various crystalline states and in the liquid state. This compilation has been used as the basis for very many assessments of binary and higher order alloy systems, initially by members of SGTE, meanwhile by many other scientists from the field. These subsystems can, thanks to the use of the same data for the component elements, be combined into higher order systems and thus make it possible to investigate real world alloys.

It is SGTE's general policy to make the data for the elements freely available to the scientific community. In case you want to set up a new database for the component data from SGUNBase while you are using the database, FCC_A1, BCC_A2 etc.

There is however one other case of use of the SGUNBase: When ChemSage *.DAT files have

Revised: 3/3/2019

Done

You need to download from [SGTE](#). Remember SGUN database provides the lattice stability for most elements.

Documentation Module

List of database files stored in \FACTDATA

6. Database Information

1. Database Files stored in \FACTDATA

To locate the \FACTDATA directory on your PC, at the top of the FactSage main menu click on 'Tools > FactSage version, directories, ...' and consult the *Data directory*. For most Standalone and Client Versions the databases are stored in \FactSage\FACTDATA .

In FACTDATA the data are stored as compounds (base.* files) and solutions (soln.* files). A protected public database (e.g. FToxid) may several files (e.g. FToxid53base.* where * = cdb, crf, iw0, iw1; FToxid53soln.* where * = fdb, idx, ini, iw0, iw1, rtf, sdc, sdi)

Screenshot showing the summary of public databases in FactSage 7.3.

Fact	FactSage	SGTE
<input type="checkbox"/> FactPS	<input type="checkbox"/> FScopp	<input type="checkbox"/> BINS
<input type="checkbox"/> FToxid	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGTE
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSupsi	<input type="checkbox"/> SGsold
<input type="checkbox"/> FThall		
<input type="checkbox"/> FTOxCN		
<input type="checkbox"/> FTfritz		
	Other	

- FactPS, ELEM and SGPS are compounds-only (pure substances) databases.
- FactPS, FToxid, FTsalt, FTmisc, FTOxCN, FTfritz, FThelg, FTpulp, ELEM and Ftdemo are included in the FACT package of databases. FTlite and FTnucl are special databases that are leased separately.
- FactPS, FToxid, FTsalt, FTlite, FScopp, FSlead, FSstel, SGPS, SGnobl and SpMCBN have been updated in FactSage 7.3.

Revised: 3/3/2019

Documentation Module: Private Databases

List of database files stored in \FACTDATA

The screenshot shows the 'List of Database Files - FactSage Browser - [LISTDATA.htm]' window. The left pane displays a tree view of database files, with 'List of database files stored in \FACTDATA' highlighted. The right pane shows a tutorial titled '4. Activating a Private Database – Adding it to the List'. A red box highlights the text: 'Wait for Chapter 5.4. Case Studies.' Another red box highlights the text: 'You will now see which databases are already on the List (see 'OK') and which are not but could be (see '>No<').' A third red box highlights the text: 'Two methods are offered for you to add databases to the List:'. The tutorial text describes how to add a private database to the FactSage List of databases.

Wait for Chapter 5.4. Case Studies.

4. Activating a Private Database – Adding it to the List

If a private database file is stored on your PC, in order to include it in FactSage calculations you must add it to the **List** of databases (i.e. tell FactSage what the database is and where it is stored). In the FactSage main menu click on 'View Data' - this opens the View Data module. Click on the 'Summary' button for a complete list and status of all the FactSage database files – specify the directory where your private files are stored (we recommend that you do not store private data in \FACTDATA). You will now see which databases are already on the List (see 'OK') and which are not but could be (see '>No<').

Now click on 'Add ...' – this opens a 'List of Databases' Window. (In the other FactSage modules clicking on 'Data Search > Databases ...' has the same effect.)

Two methods are offered for you to add databases to the **List**:

- Select the database type ('compound', 'solution', or 'both') click on 'Browse' and locate the \FACTDATA folder on your PC (not on the network) and 'Open' the particular database. Click on 'OK' to add it to the List of databases.
- Select the database type ('compound', 'solution', or 'both') click on 'Scan' and the program will list each database that is not on the **List**. Click on 'OK' to add it to the list of databases.

If the database is coupled (compound and solution databases with the same database nickname) you must add both databases to the **List**.

Revised: 3/3/2019

Documentation Module: FactSage References

List of references

FACT reference list - FactSage Browser - [FACT_reference_List.htm]

File View About...

Search phase diagrams: + must contain: Found: 899

FACTSAGE GENERAL REFERENCES – 2019

[0001] FACT, www.crct.polymtl.ca

[0002] C.W. Bale, P. Chartrand, S.A. Decterov, G. Eriksson, K. Hack, R. Ben Mahfoud, J. Melançon, A.D. Pelton and S. Petersen, "FactSage Thermochemical Software and Databases", Calphad Journal, **62**, 189-228 (2002).

[0003] C.W. Bale, A.D. Pelton and W.T. Thompson, "An Efficient Procedure for Computing Isothermal Predominance Diagrams", Can. Met. Quart., **25**, 107-112 (1986).

[0004] A.D. Pelton, W.T. Thompson, C.W. Bale and G. Eriksson, "FACT Thermochemical Databases for Calculations in Materials Chemistry at High Temperatures", High Temp. Science, **26**, 231-250 (1990).

[0005] C.W. Bale, W.T. Thompson, A.D. Pelton, G. Eriksson, P.K. Talley and J. Melancon, "Recent Developments in the FACT System", Proc. Int'l Symp. on Computer Databases, CIM, (1993).

[0008] I.-H. Jung, "Overview of the applications of thermodynamic database to steelmaking process",

Left pane contents:

- [FToxCN] - FACT high-T oxycarbonitride database:
- [FTfirtz] - FACT fertilizer database:
- [FThall] - FACT database for Hall aluminum process:
- [FThelg] - FACT aqueous (Helgeson) database:
- [FTpulp] - FACT pulp and paper database:
- [FTlite] - FACT Al-alloy and Mg-alloy databases:
 - (pdf) general description and list of optimized systems
 - list of compounds and solutions
 - phase diagrams
- [FTnuc] - FACT nuclear database for the nuclear industry:
- [FS Copp] - FactSage copper alloy database:
- [FSlead] - FactSage lead alloy database:
- [FSsteel] - FactSage steel alloy database:
- [FSupsil] - FactSage ultrapure silicon database:
- [SGsold] - SGTE solder alloy database:
- [SGTE] - SGTE 2011 alloy database:
- [SGTE] - SGTE 2014 alloy database:
- [SGTE] - SGTE 2017 alloy database:
- [BINS] - SGTE free binary alloy database:
- [SGUN] - SGTE unary database:
- [SGnobl] - SGTE noble metal alloy database:
- [SpMCBN] - Spencer Group carbide-nitride database:
- [TDmeph] - MEPHISTA database for heavy metal phase diagrams:
- [TDnuc] - NUCLEA nuclear database:
- List of database files stored in FACTDATA
- List of references

Text box: In the general description of a database, you might find some references used for the development of the database. These references are listed here.

Revised: 3/3/2019

Documentation Module: Summary

The Documentation Module should always be consulted before any compounds and solution phases are included in your calculations so that you are aware of the limitations of the databases and appropriate remedies.

The Documentation Module gives detailed descriptions about the databases of **COMPOUND** (i.e., elemental species and stoichiometric compounds) and **SOLUTIONS** (i.e., homogeneous mixture which are mixed on an atomic or molecular scale).

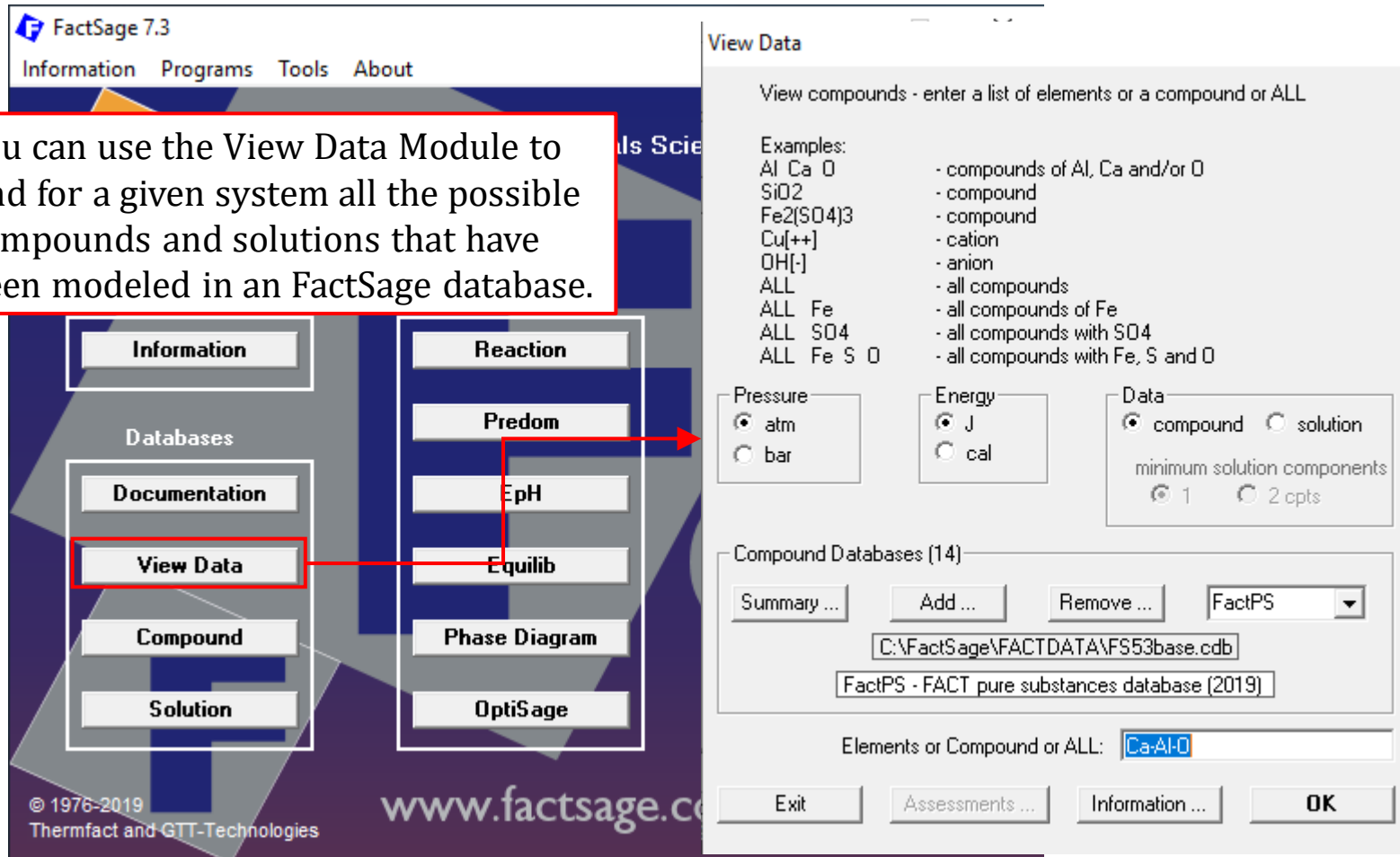
FactSage Practical

MSE302

Practical 1. View Data

View Data Module

You can use the View Data Module to find for a given system all the possible compounds and solutions that have been modeled in an FactSage database.



Run the "View Data" Module

View Data Module

For example, say we wish to know for the Al-Mg system the thermodynamic properties of all the compounds that have been modeled in the FTlite database...

The screenshot shows the 'View Data' window with the following components and annotations:

- Examples:** A list of input examples with their corresponding data types:
 - Al Ca O: compounds of Al, Ca and/or O
 - SiO2: compound
 - Fe2(SO4)3: compound
 - Cu[++]: cation
 - OH[-]: anion
 - ALL: all compounds
 - ALL Fe: all compounds of Fe
 - ALL SO4: all compounds with SO4
 - ALL Fe S O: all compounds with Fe, S and O
- Pressure:** Radio buttons for 'atm' (selected) and 'bar'.
- Energy:** Radio buttons for 'J' (selected) and 'cal'.
- Data:** Radio buttons for 'compound' (selected) and 'solution'.
- minimum solution components:** Radio buttons for '1' (selected) and '2 bpts'.
- Compound Databases (14):** A list of databases with 'FTlite' selected in the dropdown menu. Below the list, the path 'C:\FactSage\FACTDATA\FTlite60base.cdb' is shown, followed by 'FTlite - FACT Al-alloy and Mg-alloy compounds (2019)'.
- Elements or Compound or ALL:** A text input field containing 'Al Mg'.
- Buttons:** 'Exit', 'Assessments ...', 'Information ...', and 'OK'.

Annotations with red boxes and arrows point to the following elements:

- 'Examples:' label
- 'compound' radio button in the Data section
- 'Unit Selection.' text box pointing to the Pressure and Energy sections
- 'We wish to view compounds, not solutions.' text box pointing to the 'compound' radio button
- 'We wish to see what compounds are modeled in FTlite. If you wish to see how the Al-Mg compounds are modeled in other databases, you can choose other databases or ALL databases.' text box pointing to the database dropdown
- 'This permits the user to add a private database.' text box pointing to the database list
- 'Al Mg' text input field
- 'OK' button

View Data Module

For example, say we wish to know for the Al-Mg system the thermodynamic properties of all the compounds that have been modeled in the FTLite database...

You can save the list as a txt file by File\Save As...

File Edit Sort Compounds Summary Databases Units Atomic Wts. Table Graph Help << Back

5 compounds, 21 phases

FTlite - FACT Al-alloy and Mg-alloy compounds (2019)

Compounds ordered by alphabet (see 'Sort Compounds') - All Phases

Al	FTlite	S1	S2	S3	S4	S5	S6	S7	...	L1	L
Al30Mg23	FTlite	S									
Al3Mg	FTlite	S									
AlMg	FTlite	S									
Mg	FTlite	S1	S2	S3	S4	S5	S6	S7		L	

Double click...

All the possible compounds that are modeled in FTLite are listed, including different structures.

Note: we cannot edit the species stored in the public protected databases.

FactSage 7.3 | C:\FactSage\FACTDATA\FTlite60base.cdb 7.3 1703 compounds read-only

View Data Module

For example, say we wish to know for the Al-Mg system the thermodynamic properties of all the compounds that have been modeled in the FTlite database...

You can sort the compounds based on different properties.

Double click...

You can also set units here.

FactSage 7.3 | C:\FactSage\FACTDATA\FTlite60base.cdb 7.3 1703 compounds read-only

View Data Module

For example, say we wish to know for the Al-Mg system the thermodynamic properties of all the compounds that have been modeled in the FTlite database...

View Data Al Units: T(K) P(atm) Energy(J) Quantity(mol)

File Edit Sort Com Atomic Wts. Table Graph Help << Back

10 Phases

Phase summary of Al.

Phases Cp(T) H(T) G(T) S(T) Volume Magnetic Refs. Trans. Mol Wt.%

Name: Aluminum
Formula Weight: 26.9815386
Stoichiometric Compound: Al

Refs: 501 529

Basic Info of Al.

Reference used.

	Phase	Cp Range, K	Density, g/ml	Ref.
S1	fcc_a1	298.15 - 700.00 700.00 - 933.47 933.47 - 3900.00	2.69822	501
S2	hcp_a3	298.15 - 700.00 700.00 - 933.47 933.47 - 3900.00		
S3	hcp_zn	298.15 - 700.00 700.00 - 933.47 933.47 - 3900.00		
S4	cbcc_a12	298.15 - 700.00 700.00 - 933.47	2.702	

Number of Gibbs energy equations.

Phase abbreviation.

FactSage 7.3 C:\FactSage\FACTDATA\FTlite60base.cdb 7.3 1703 compounds read-only

View Data Module

For example, say we wish to know for the Al-Mg system the thermodynamic properties of all the compounds that have been modeled in the FTlite database...

View Data Al Units: T() c_p functions: molar heat capacity at constant pressure.

File Edit Sort Compounds Summary Databases Units Atomic Wts. Table Graph Help << Back

10 Phases FTlite - FACT Al-alloy and Mg-alloy compounds (2019)

Phases **Cp(T)** H(T) G(T) S(T) Volume Magnetic Refs. Trans. Mol Wt.%

Name: Aluminum

$$C_p = \sum_{i=1}^8 C_{(i)} T^{P(i)}$$

Cp range: T(min) - T(max).
When T < T(min), Cp(T) is extrapolated.
When T > T(max), Cp(T) at T(max) is used.

Meyer-Kelley Equation.

	DH(298.15) (J/mol)	S(298.15) (J/mol-K)	C(i)	P(i)	C(i)	P(i)	Cp (K)
S1	0.00	28.299997	24.367198	0	3.76932400E-03	1	298 - 700
			-148184.00	-2	5.26598400E-06	2	
S1			38.584430	0	-3.70639640E-02	1	700 - 933
			-148184.00	-2	3.45853620E-05	2	
S1			31.748192	0	1.10747160E+30	-10	933 - 3900
S2	5481.00	30.099997	24.367198	0	3.76932400E-03	1	298 - 700
			-148184.00	-2	5.26598400E-06	2	
S2			38.584430	0	-3.70639640E-02	1	700 - 933
			-148184.00	-2	3.45853200E-05	2	
S2			31.748192	0	1.10747160E+30	-10	933 - 3900

Recall from Chapter 2.2 the Gibbs energy equation.

FactSage 7.3 C:\FactSage\FACTDATA\FTlite60base.cdb 7.3 1703 compounds read-on

View Data Module

For example, say we wish to know for the Al-Mg system the thermodynamic properties of all the compounds that have been modeled in the FTLite database...

Other functions can be calculated from $c_p(T)$ page.

These values are absolute G (not Delta G)
- click on 'Help' for an explanation.

Explanation next page.

The Gibbs energy of a pure compound at 1 atm depends on temperature only.

	G(T)			T(K)
S1	-7976.14806	+137.093038 T	-1.884662000E-03 T ²	298 - 700
	+74092.0000 T ⁻¹	-8.776640000E-07 T ³	-24.3671976 T ln(T)	
S1	-11276.2371	+223.048445 T	+1.853198200E-02 T ²	700 - 933
	+74092.0000 T ⁻¹	-5.764227000E-06 T ³	-38.5844296 T ln(T)	
S1	-11278.3762	+188.684153 T	-1.230524000E+28 T ⁻⁹	933 - 3900
	-31.7481920 T ln(T)			
S2	-2495.15000	+135.293038 T	-1.884662000E-03 T ²	298 - 700
	+74092.0000 T ⁻¹	-8.776640000E-07 T ³	-24.3671976 T ln(T)	
S2	-5795.23426	+221.248435 T	+1.853198200E-02 T ²	700 - 933
	+74092.0000 T ⁻¹	-5.764220000E-06 T ³	-38.5844296 T ln(T)	
S2	-5797.38475	+186.884161 T	-1.230524000E+28 T ⁻⁹	933 - 3900

View Data Module

For example, say we wish to know for the Al-Mg system the thermodynamic properties of all the compounds that have been modeled in the FTlite database...

Explanation of H, G and S

H(T), G(T) and S(T) are absolute values - not the delta values.
 Absolute S(T) are calculated from the 3rd law:

$$S(T) = \int_{298.15}^T \frac{C_p(T)}{T} dT$$
 or
$$S(T) = S(298.15 \text{ K}) + \int_{298.15}^T \frac{C_p(T)}{T} dT$$

 Absolute H(T) and G(T) are given by:

$$H(T) = \Delta H(\text{formation}, 298.15 \text{ K}) + \int_{298.15}^T C_p(T) dT$$

$$G(T) = H(T) - T \cdot S(T)$$

The standard Gibbs energy of formation Delta G (and Delta H) for a reaction is obtained by combining the G(T) (and H(T)) expressions for the reactants and products.

For example, the formation of Fe3C(s):

$$3 \text{ Fe(s)} + \text{C(s)} = \text{Fe}_3\text{C(s)}$$

$$\Delta G(\text{formation}) = G(T)(\text{Fe}_3\text{C}) - 3 G(T)(\text{Fe}) - G(T)(\text{C})$$

$$\Delta H(\text{formation}) = H(T)(\text{Fe}_3\text{C}) - 3 H(T)(\text{Fe}) - H(T)(\text{C})$$

 where G(T)(Fe3C), H(T)(Fe3C), etc. are the expressions of G(T) and H(T) are listed here in the tables.

For tabular values of H(T)-H(298) click on 'Table > all phases ...'.
 For tabular values of Delta H etc. use the Reaction module.

Quantity(mol)

bases Units Atomic Wts. Table Graph Help << Back

Al-alloy and Mg-alloy compounds (2019)

S(T) Volume Magnetic Refs.

J/mol - 1 atm

These values are absolute G (- click on 'Help' for an explanation)

G(T)

G(T)	T(K)
137.093038 T	298 - 700
76640000E-07 T^3	298 - 700
223.048445 T	700 - 933
54227000E-06 T^3	700 - 933
188.684153 T	933 - 3900
135.293038 T	298 - 700
76640000E-07 T^3	298 - 700
221.248435 T	700 - 933
54220000E-06 T^3	700 - 933
186.884161 T	933 - 3900

OK

Package 7.3 C:\factSage\FACTDATA\thermo\base.cdb 7.3 1703 compounds read-only

View Data Module

For example, say we wish to know for the Al-Mg system the thermodynamic properties of all the compounds that have been modeled in the FTLite database...

View Data Al Units: T(K) P(atm) Energy(J) Quantity(mol)

File Edit Sort Compounds Summary Databases Units Atomic Wts. Table Graph Help << Back

10 Phases FTlite - FACT Al-alloy and Mg-alloy compounds (2019)

Phases Cp(T) H(T) G(T) S(T) **Volume** Magnetic Refs. Trans. Mol Wt. %

Name: Aluminum
Volume data

Non-ideal gas properties
(-none-)

Expansivities / Compressibilities / Derivative of Bulk

Expansivity [1/K] = a + bT + c/T + d/T^2

	a	bT	c/T	d/T^2
S1	3.43290E-05	+ 7.62280E-08 T	+ 3.58254E-03 /T	+ 8.57216E-03 /T^2
S2	3.43290E-05	+ 7.62280E-08 T	+ 3.58254E-03 /T	+ 8.57216E-03 /T^2
L1	6.70917E-05	- 3.57128E-09 T	+ 5.98336E-02 /T	+ 0.00000E+00 /T^2

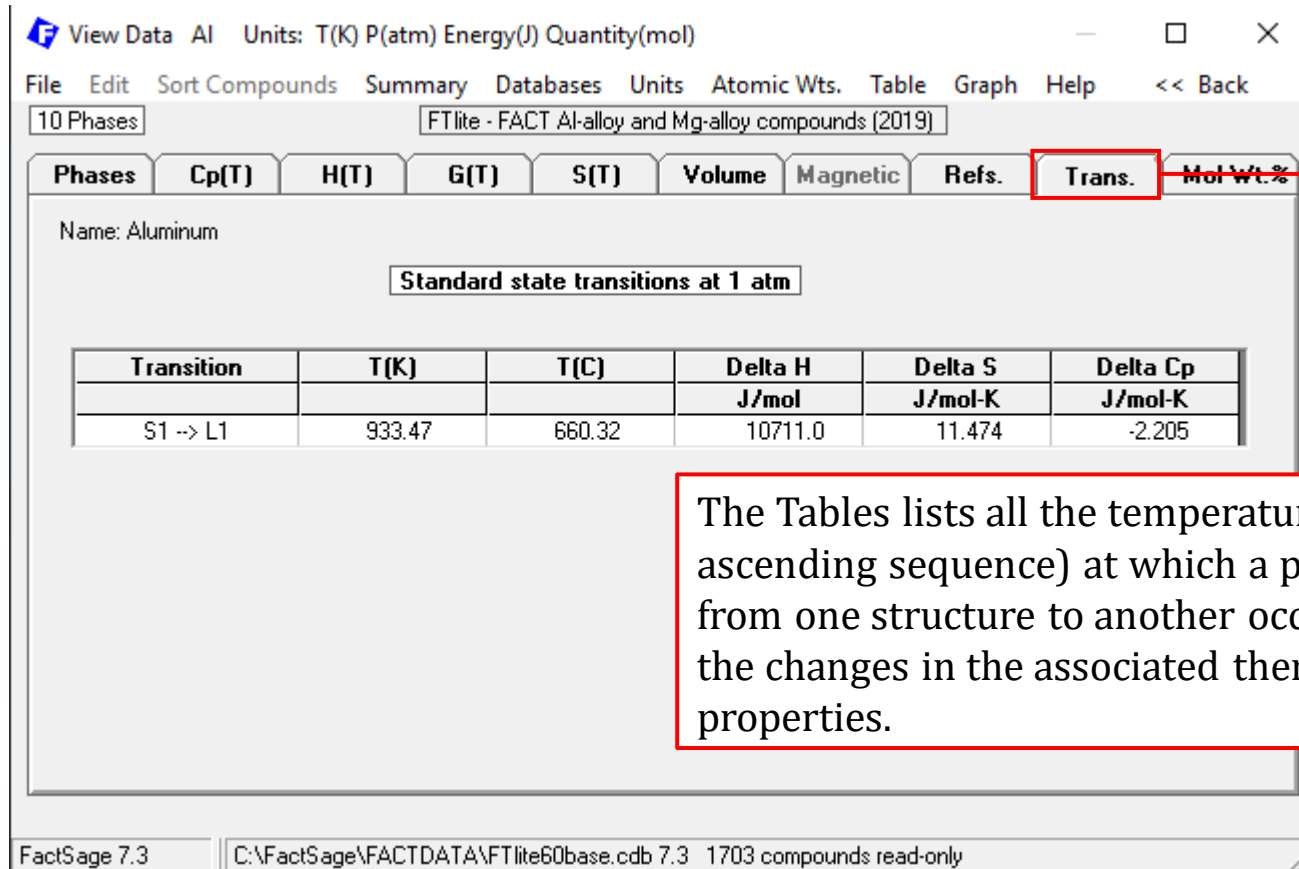
FactSage 7.3 C:\FactSage\FACTDATA\FTlite60base.cdb 7.3 1703 compounds read-only

Although in many cases of MSE302 we are not interested in the volume properties, the temperature dependence of volume is described by the Expansivity.

$$\alpha_V = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_P$$

View Data Module

For example, say we wish to know for the Al-Mg system the thermodynamic properties of all the compounds that have been modeled in the FTlite database...



View Data Al Units: T(K) P(atm) Energy(J) Quantity(mol)

File Edit Sort Compounds Summary Databases Units Atomic Wts. Table Graph Help << Back

10 Phases FTlite - FACT Al-alloy and Mg-alloy compounds (2019)

Phases Cp(T) H(T) G(T) S(T) Volume Magnetic Refs. **Trans.** Mol Wt. %

Name: Aluminum

Standard state transitions at 1 atm

Transition	T(K)	T(C)	Delta H J/mol	Delta S J/mol-K	Delta Cp J/mol-K
S1 -> L1	933.47	660.32	10711.0	11.474	-2.205

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The Tables lists all the temperatures (in an ascending sequence) at which a phase transition from one structure to another occurs and also the changes in the associated thermodynamic properties.

View Data Module

The thermodynamic properties including $c_{P,i}(T)$, $h_i(T)$, $g_i(T)$, and $s_i(T)$ against temperature for all phases/structures can be plotted.

The screenshot shows the FactSage 7.3 View Data module. The main window displays the 'Graph' menu, which is open, showing options for plotting thermodynamic properties. The 'Plot (all phases)' option is selected, and the 'TK limits (300 - 2000 K) ...' option is also visible. The 'Phases' sub-menu is open, showing options for 'Cp vs T', 'H vs T', 'G vs T', and 'S vs T'. A red box highlights the 'Graph' menu and the 'TK limits (300 - 2000 K) ...' option. A red arrow points from the 'Graph' menu to the 'TK limits (300 - 2000 K) ...' option. Another red arrow points from the 'TK limits (300 - 2000 K) ...' option to the 'T(K):' dialog box. The dialog box is titled 'T(K):' and contains the text 'Enter temperature limits, K (range 100 to 20000):'. Below this text is a text input field with the value '300 2000 100'. The dialog box also has 'OK' and 'Cancel' buttons. A red box highlights the 'min max step' text in the input field. A red arrow points from the 'min max step' text to the 'min max step' text in the input field. The main window also shows a table of thermodynamic properties for Aluminum (Al) and a summary of the data.

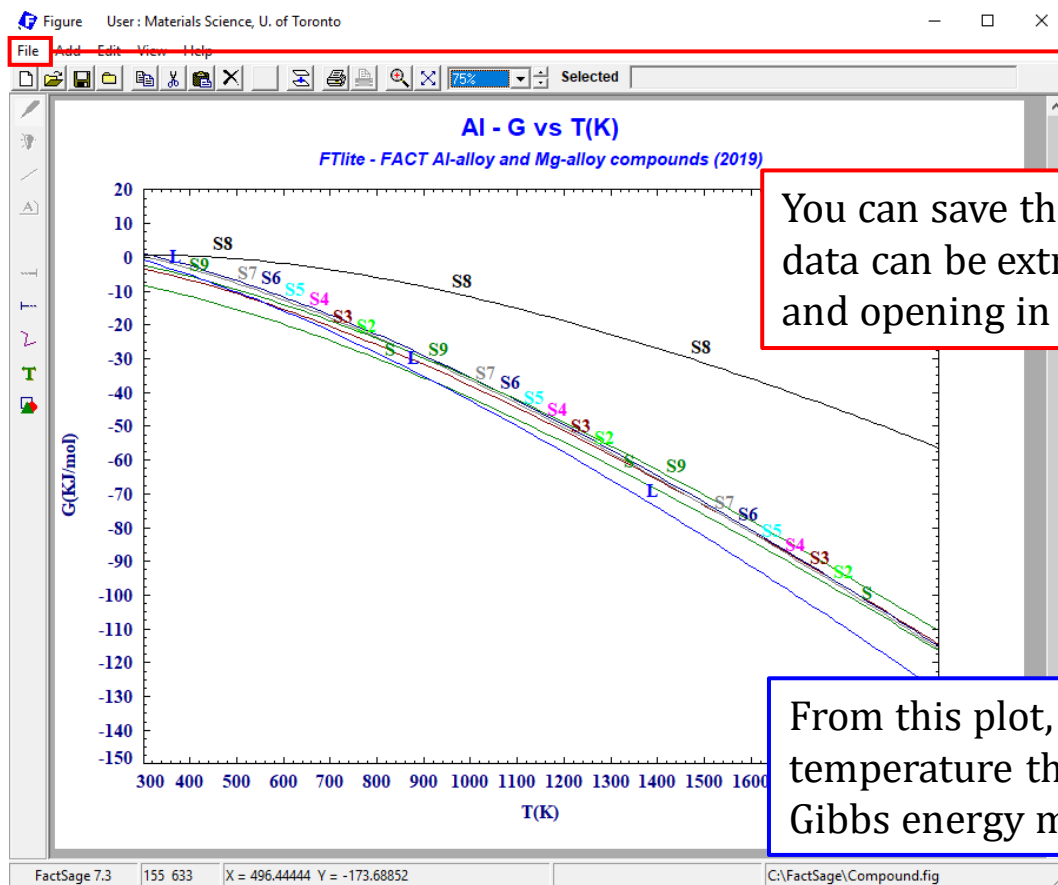
You can choose to plot the thermodynamic properties for (i) one phase or (ii) all phases. You can also adjust the temperature range.

Element	mol	mol wt	mol wt	mol wt
Al	1	100.00000	26.98154	100.00000
Total	1	100	26.98154	100

T(K):
Enter temperature limits, K (range 100 to 20000):
'min max step'
Click on "Cancel" for the default values 300 2000 100
300 2000 100

View Data Module

The thermodynamic properties including $c_{P,i}(T)$, $h_i(T)$, $g_i(T)$, and $s_i(T)$ against temperature for all phases/structures can be plotted.



You can save the plot in the ".fig" format. The data can be extracted by changing the file to ".txt" and opening in the Notepad.

From this plot, you can determine at any given temperature the most stable structure based on the Gibbs energy minimization principle.

View Data Module

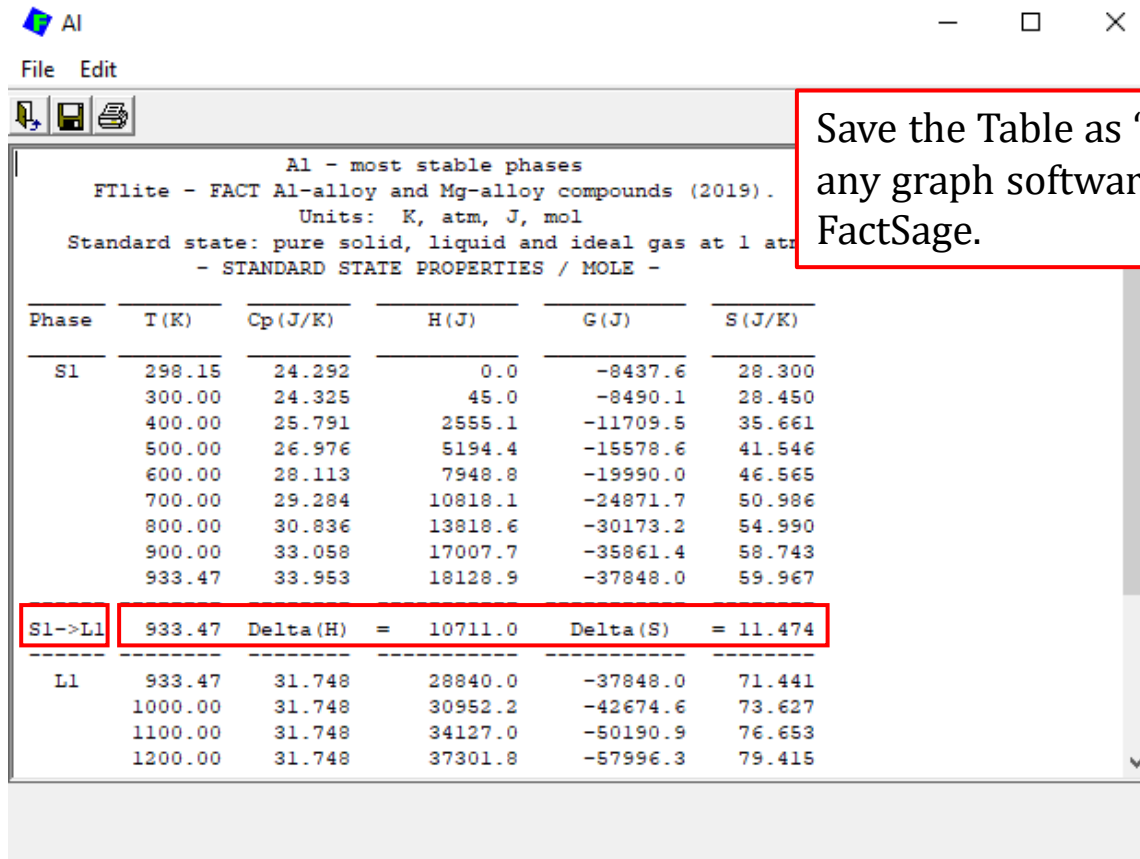
We can also tabulate the most stable phase only under a given temperature range. To do this, we need to set “Table\Phases\most stable”.

The screenshot shows the FactSage 7.3 View Data module for Aluminum. The 'Table' menu is open, and the 'Phases' option is selected. The 'most stable' option is checked in the 'all phases' list. The main window displays a table of phase data for Aluminum.

	Phase	Cp Range, K	Density, g/ml	Ref.
S1	fcc_a1	298.15 - 700.00	2.69822	501
		700.00 - 933.47		
		933.47 - 3900.00		
S2	hcp_a3	298.15 - 700.00		
		700.00 - 933.47		
		933.47 - 3900.00		
S3	hcp_zn	298.15 - 700.00	2.702	
		700.00 - 933.47		
		933.47 - 3900.00		
S4	cbcc_a12	298.15 - 700.00		
		700.00 - 933.47		

View Data Module

We can also tabulate the most stable phase only under a given temperature range. To do this, we need to set “Table\Phases\most stable”.



The screenshot shows the FactSage View Data Module window. The title bar is "Al". The menu bar has "File" and "Edit". The toolbar has icons for opening, saving, and printing. The main window displays the following text:

Al - most stable phases
FTlite - FACT Al-alloy and Mg-alloy compounds (2019).
Units: K, atm, J, mol
Standard state: pure solid, liquid and ideal gas at 1 atm
- STANDARD STATE PROPERTIES / MOLE -

Phase	T(K)	Cp(J/K)	H(J)	G(J)	S(J/K)
Sl	298.15	24.292	0.0	-8437.6	28.300
	300.00	24.325	45.0	-8490.1	28.450
	400.00	25.791	2555.1	-11709.5	35.661
	500.00	26.976	5194.4	-15578.6	41.546
	600.00	28.113	7948.8	-19990.0	46.565
	700.00	29.284	10818.1	-24871.7	50.986
	800.00	30.836	13818.6	-30173.2	54.990
	900.00	33.058	17007.7	-35861.4	58.743
	933.47	33.953	18128.9	-37848.0	59.967
Sl->Ll	933.47	Delta(H)	= 10711.0	Delta(S)	= 11.474
Ll	933.47	31.748	28840.0	-37848.0	71.441
	1000.00	31.748	30952.2	-42674.6	73.627
	1100.00	31.748	34127.0	-50190.9	76.653
	1200.00	31.748	37301.8	-57996.3	79.415

Save the Table as “.txt” file. You can then plot using any graph software, or use the Figure Module in FactSage.

View Data Module

Now, let us view the thermodynamic data for a magnetic species: Fe.

View Data

View compounds - enter a list of elements or a compound or ALL

Examples:

Al Ca O	- compounds of Al, Ca and/or O
SiO2	- compound
Fe2(SO4)3	- compound
Cu[++]	- cation
OH[-]	- anion
ALL	- all compounds
ALL Fe	- all compounds of Fe
ALL SO4	- all compounds with SO4
ALL Fe S O	- all compounds with Fe, S and O

Pressure
☒ atm
☐ bar

Energy
☒ J
☐ cal

Data
☒ compound ☐ solution
minimum solution components
☒ 1 ☐ 2 cpts

Compound Databases (17)

Summary ... Add ... Remove ... FTlite

C:\FactSage\FACTDATA\FTlite60base.cdb

FTlite - FACT Al-alloy and Mg-alloy compounds (2019)

Elements or Compound or ALL: Fe

Exit Assessments ... Information ... OK

View Data Module

Now, let us view the thermodynamic data for a magnetic species: Fe.

Four model parameters are required to describe the magnetic contribution.

View Data Fe Units: T(K) P(atm) Energy(J) Quantity(mol)

File Edit Sort Compounds Summary Databases Units Atomic Wts. Table Graph Help << Back

8 Phases FTlite - FACT Al-alloy and Mg-alloy compounds (2019)

Phases Cp[T] H[T] G[T] S[T] Volume **Magnetic** Refs. Trans. Mol Wt. %

Name: Iron

Magnetic Properties

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

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

when $\tau \leq 1$

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

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

	Critical Temp. Tc (K)	Magnetic Moment B	P Factor	Structure Factor
S1	1043.00 (Curie)	2.2200	0.40000	1.0000
S2	67.00 (Neel)	0.7000	0.28000	0.3333

FactSage 7.3 C:\FactSage\FACTDATA\FTlite60base.cdb 7.3 1703 compounds read-only

For magnetic species, both lattice and magnetic contributions have to be considered:

$$g_i = {}^{\text{lattice}}g_i + {}^{\text{magnetic}}g_i$$

Model parameters for magnetic species.

View Data Module

The View Data Module also permits us to view the **solution phases**. Back to the Al-Mg system. (You could wait for Chapter 4 & 5)

View Data

View solutions - enter a list of elements or ALL

Examples:
Ca Al O S - solutions with Ca, Al, O and/or S
H O Fe S - solutions (including aqueous) of H, O, Fe and/or S
ALL - ALL solutions

Pressure
☒ atm
☐ bar

Energy
☒ J
☐ cal

Data
☐ compound ☒ solution
minimum solution components
☒ 1 ☐ 2 cpts

Solution Databases (16)
Summary ... Add ... Remove ... FTlite
C:\FactSage\FACTDATA\FTlite60soln.sdc
FTlite - FACT Al-alloy and Mg-alloy solutions (2019)

Elements or ALL: Al Mg

Exit Assessments ... Information ... OK

View Data Module

The View Data Module also permits us to view the **solution** phases. Back to the Al-Mg system. (You could wait for Chapter 4 & 5)

View Data Al-Mg - FTlite datasets

File Edit Sort Solutions Summary Databases Units Atomic Wts. Table Graph Help << Back

8 Solutions FTlite - FACT Al-alloy and Mg-alloy solutions (2019) 1/33

Solutions sorted by phase number [see 'Sort Solutions']

Phase	Name & End-members EMs	Information
1. FTlite-Liqu	Liquid	metal [I]
	2 EMs 2 elements #99	
	Al Mg	
2. FTlite-A1	FCC-A1	Prototype-Cu Strukturbericht = A1; Pe
	2 EMs 2 elements #12	C, N, B and H interstitial (Pearson = c
	Al Mg	
3. FTlite-A2	BCC-A2	Prototype-W Strukturbericht = A2; Pearson = cI2; Space Group =
	2 EMs 2 elements #12	C, H, N and B interstitial on tetrahedral sites
	Al Mg	
4. FTlite-A3	HCP-A3	Prototype-Mg Strukturbericht = A3; Pearson = hP2; Space group =
	2 EMs 2 elements #12	with M2X-hcp carbides, nitrides, borides, hydrides and oxides
	Al2Va Mg2Va	
	CBCC-A12;Prototype-Mn	Strukturbericht = A12; Pearson = cI58; Space group = I-43m (217)

FactSage 7.3 C:\FactSage\FACTDATA\FTlite60soln.sdc 7.3 read-only

Of course, if you choose other alloy solution databases, the solutions which are modeled might be different.

View Data Module

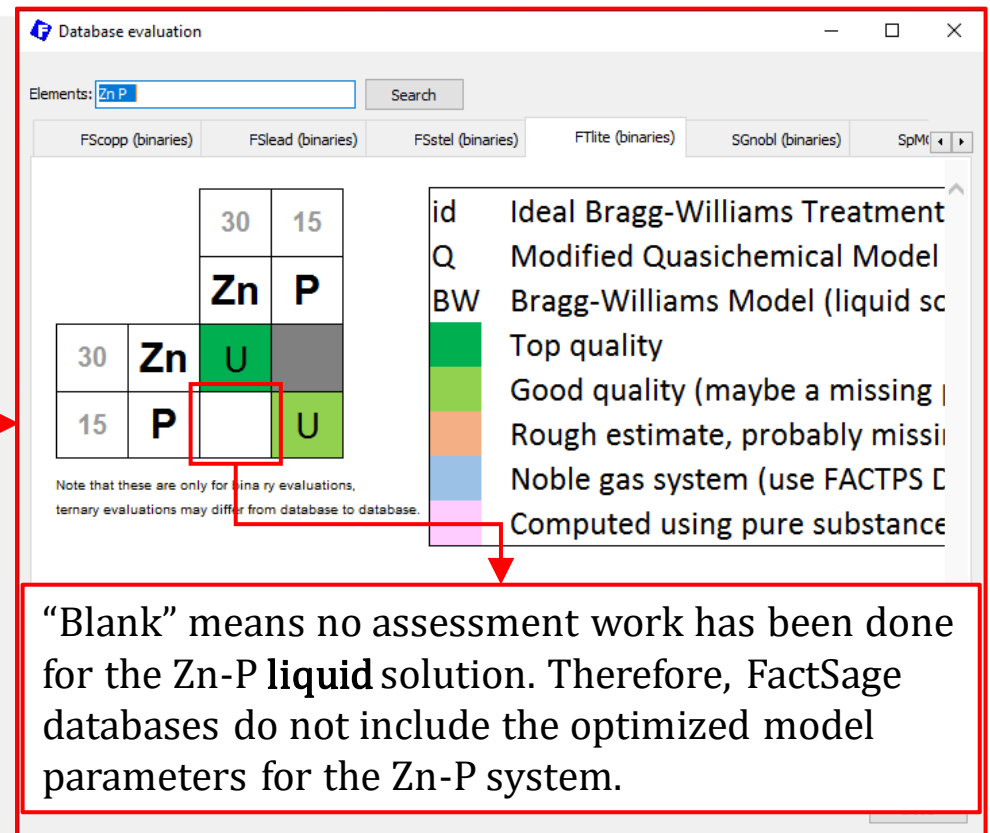
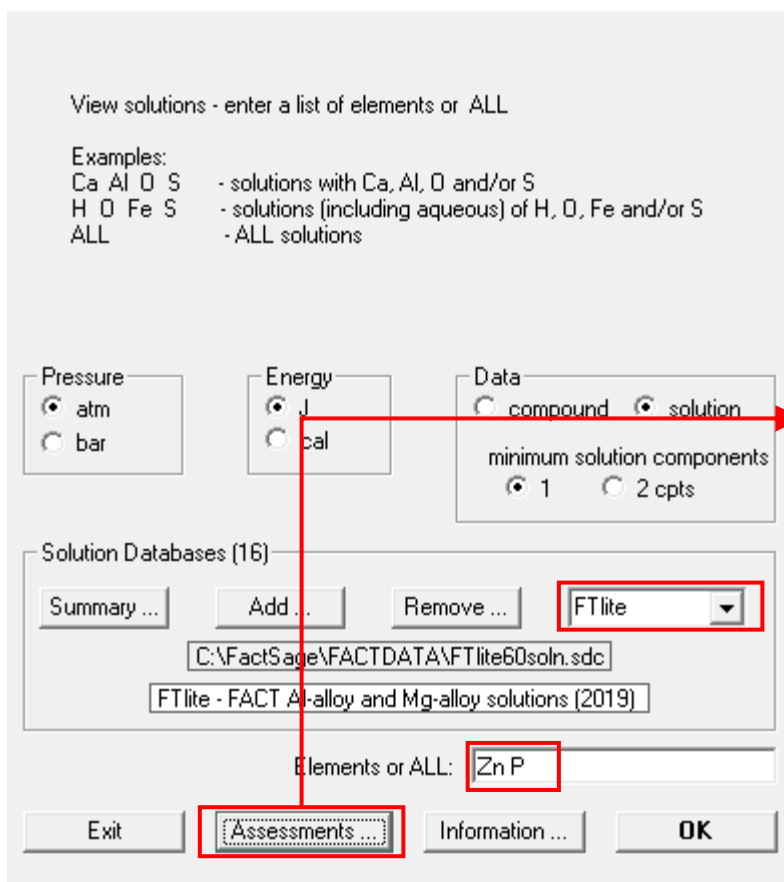
We check the **solution** phases for the system under investigation because this will increase our confidence to choose the correct database and solutions when performing a thermodynamic calculation.

Remember that FactSage will not calculate correctly in cases where data are not available.

View Data Module

The View Data Module can also help us determine if a binary system has been optimized by FactSage databases. Again, we use the Zn-P system.

View Data



FactSage Practical

MSE302

Practical 1. Compound

Compound Module

Using the **View Data** Module, we can view the thermodynamic functions of $c_{P,i}(T)$, $h_i(T)$, $g_i(T)$, and $s_i(T)$ in the Table/Graph. The **Compound Module** not only permits us to view the thermodynamic functions, but also administer a **private** database, i.e., enter, edit, or delete pure substance data in the database.

Here, we will use SGUN database as an example to show you how to view and edit a thermodynamic COMPOUND database.

(**Note:** SGUN database represents the SGTE Unary database, and is the basis for thermodynamic modeling of binary, ternary, and multi-component systems)

Compound Module

Download from the Quercus page: “SGUNbase.cdb”. This database was originally downloaded from [the SGTE website](#) and then converted by FactSage using the Equilib or Phase Diagram Module.

Next, create a new **folder** under the directory C:\FactSage**NAMEDATA** (for example, “FENGDATA”), and copy and paste “SGUNbase.cdb” to this folder.

Then in the Compound Module, click on File and Open Database.

Type “Zn” in the formula, and Enter. Check the thermodynamic properties of Zn for all possible structures shown in the SGUN database (refer to your course slides and see if you are able to view and edit the data). Also, for magnetic species Fe, compare the thermodynamic data of bcc-Fe shown in FactPS and SGUN.

Note: we will use the Compound Module in Chapter 5 (CALPHAD) when building the thermodynamic models for a binary system.

In-Class Exercise

Question.

Use the View Data Module to plot the Gibbs energy curves for solid, liquid and gaseous Al.

Note: choose FactPS database.

Use the generated graph to determine the stable phase at 1000 °C? Also, what is the melting temperature of Al? Explain how you find the melting temperature.