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

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: **F**acility for the **A**nalysis of **C**hemical **T**hermodynamics – 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)

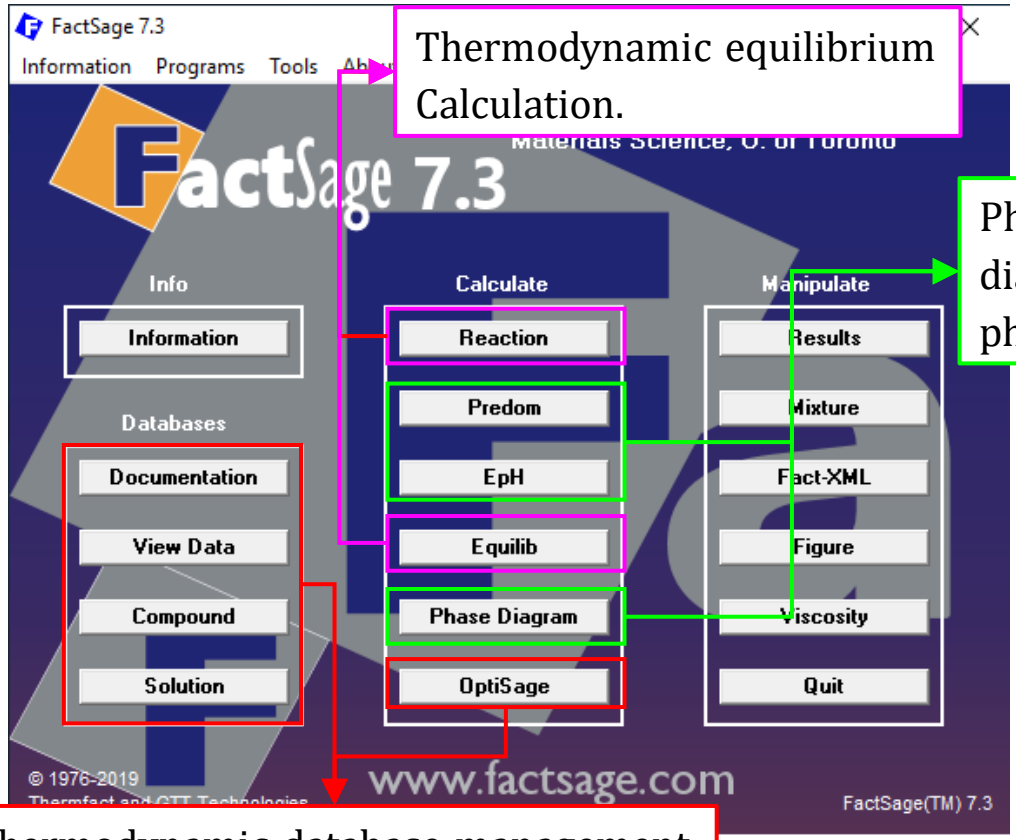
FactSage Overview: What can FactSage do?

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.

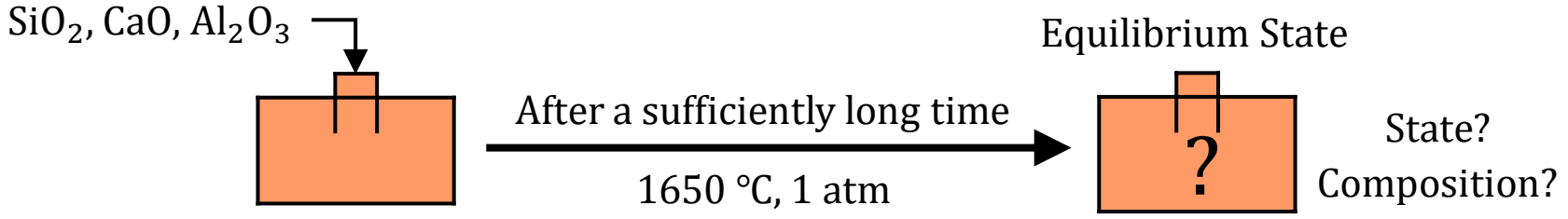
Phase Diagram Calculation (Phase diagram is graphical representation of phase equilibria).

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

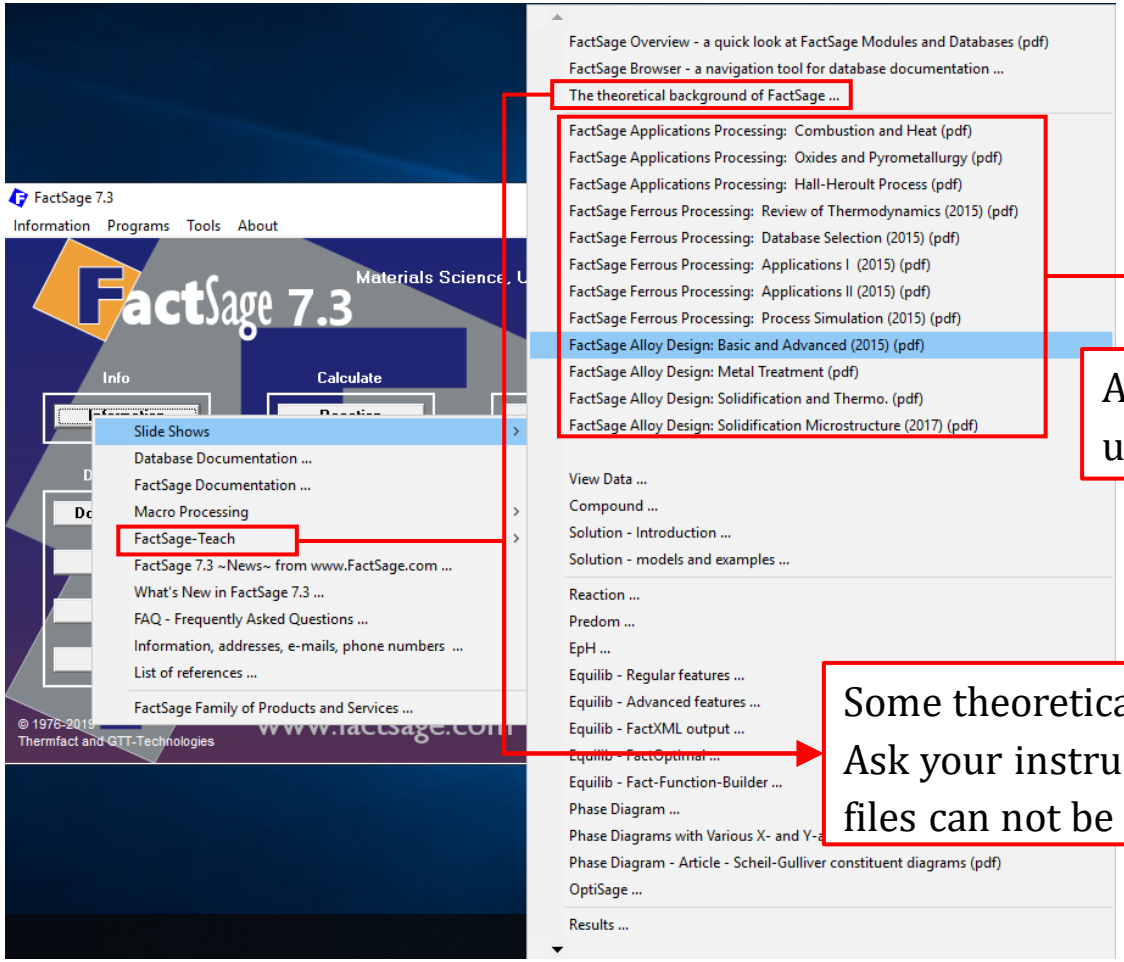
What thermodynamic properties/diagrams can be calculated in FactSage?

With critically assessed thermodynamic databases…	
Reliable Estimation	**Good Estimation**
✓ Equilibrium composition, partial pressure, activity ✓ Equilibrium phase diagram (stable/metastable phases) ✓ Melting and boiling point, phase transition temperatures ✓ Adiabatic combustion temperature ✓ Gibbs energy, Enthalpy, Entropy, heat capacity	✓ Viscosity of molten slag/glass ✓ Viscosity of molten alloy ✓ Thermal conductivity ✓ Density and volume

Properties that can not be calcualted	N/A
× Mechanical properties (strength, hardness, etc.) × Electrical conductivity × Permittivity × Crystallographic parameters × Magnetic susceptibility…	× First principle calculation × Diffusion analysis × Fluid dynamic analysis

Information Module

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



Advanced application examples using FactSage.

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

Directory Settings

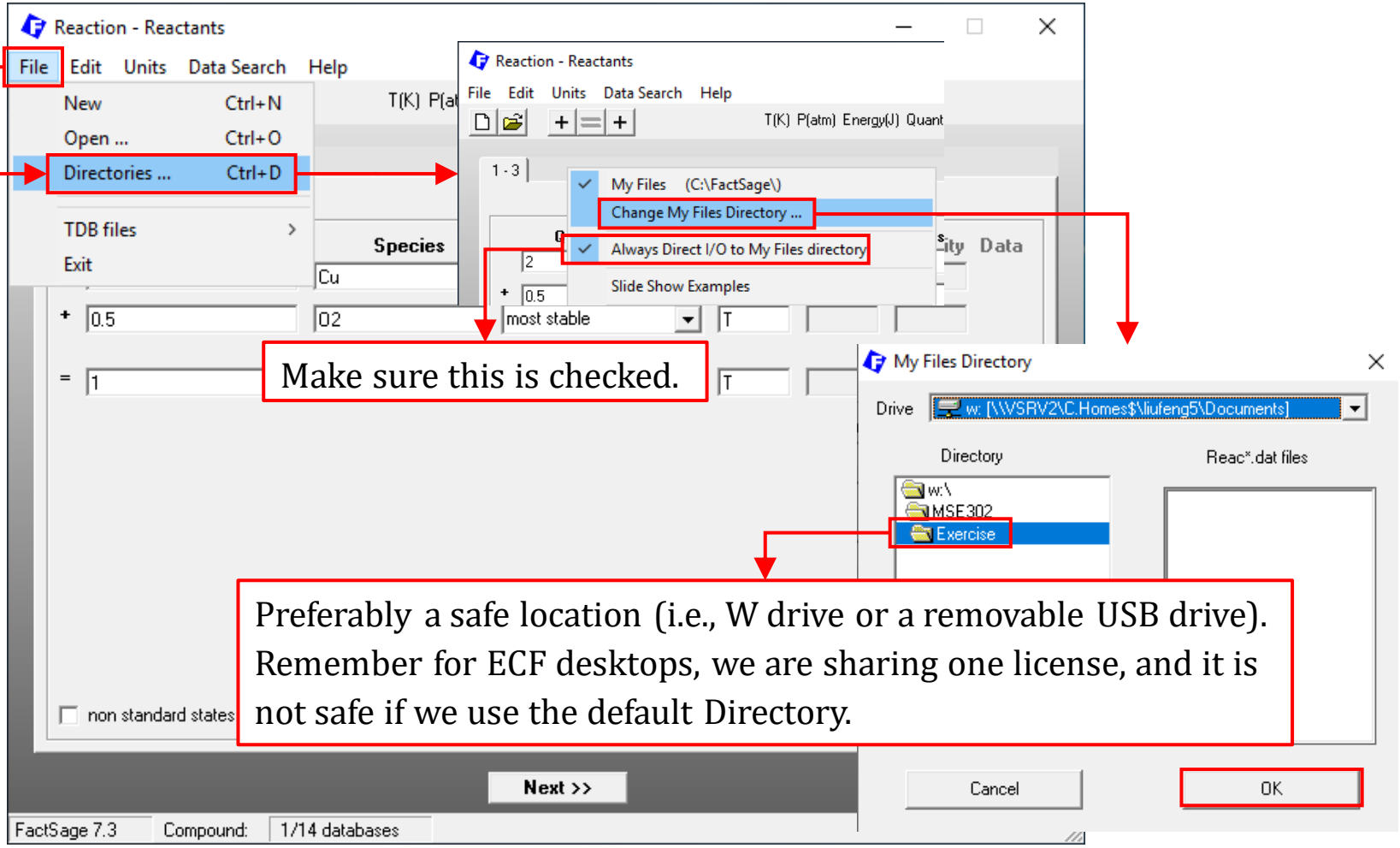
Before we carry out any thermodynamic calculations (in the Reaction, Predom, EpH, Equilib, Phase Diagram Module), we need to create a Directory. That can be on any hard drive or a movable USB.

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

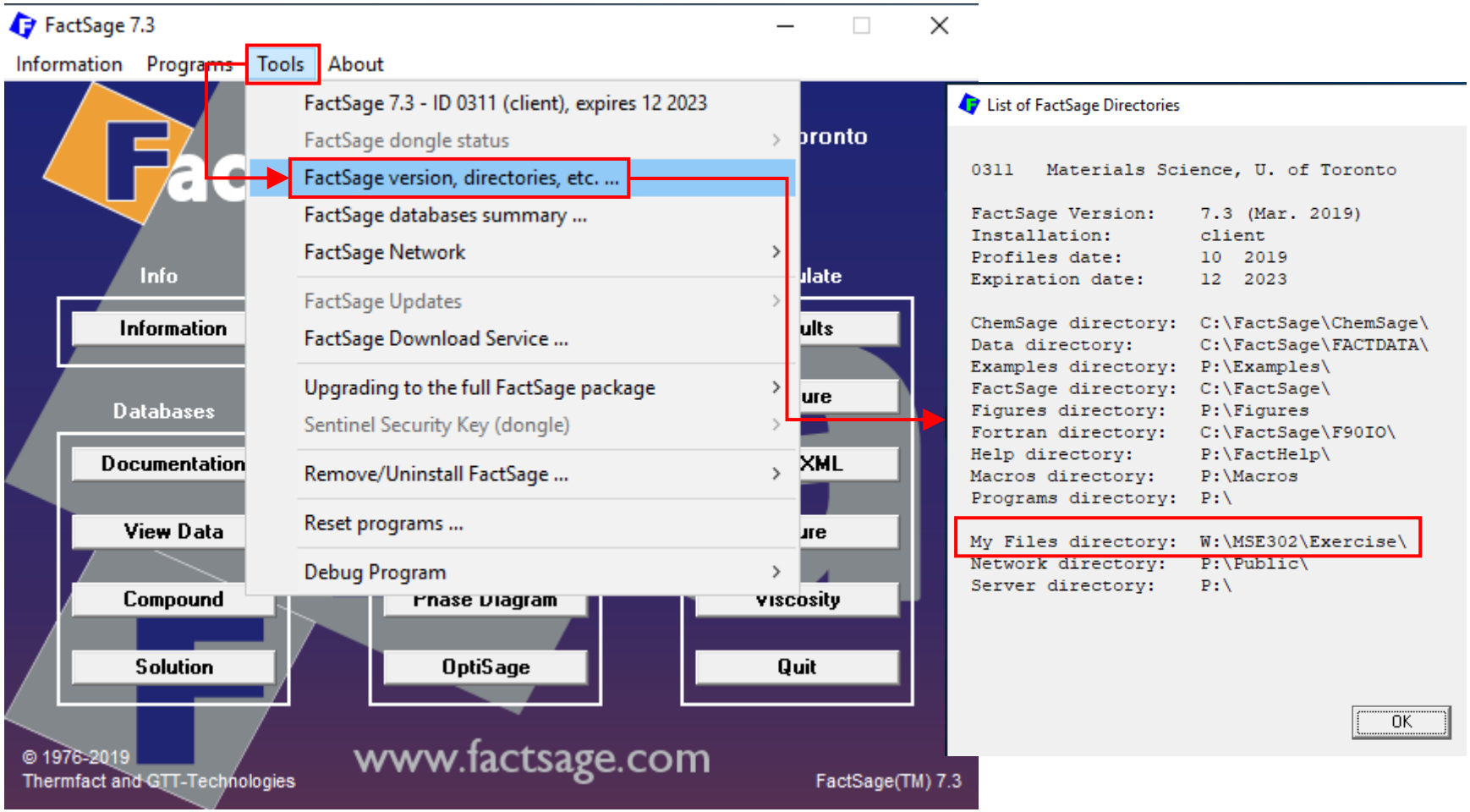
Now, if you run other modules, you should find that the Directory for these modules has also been changed.

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

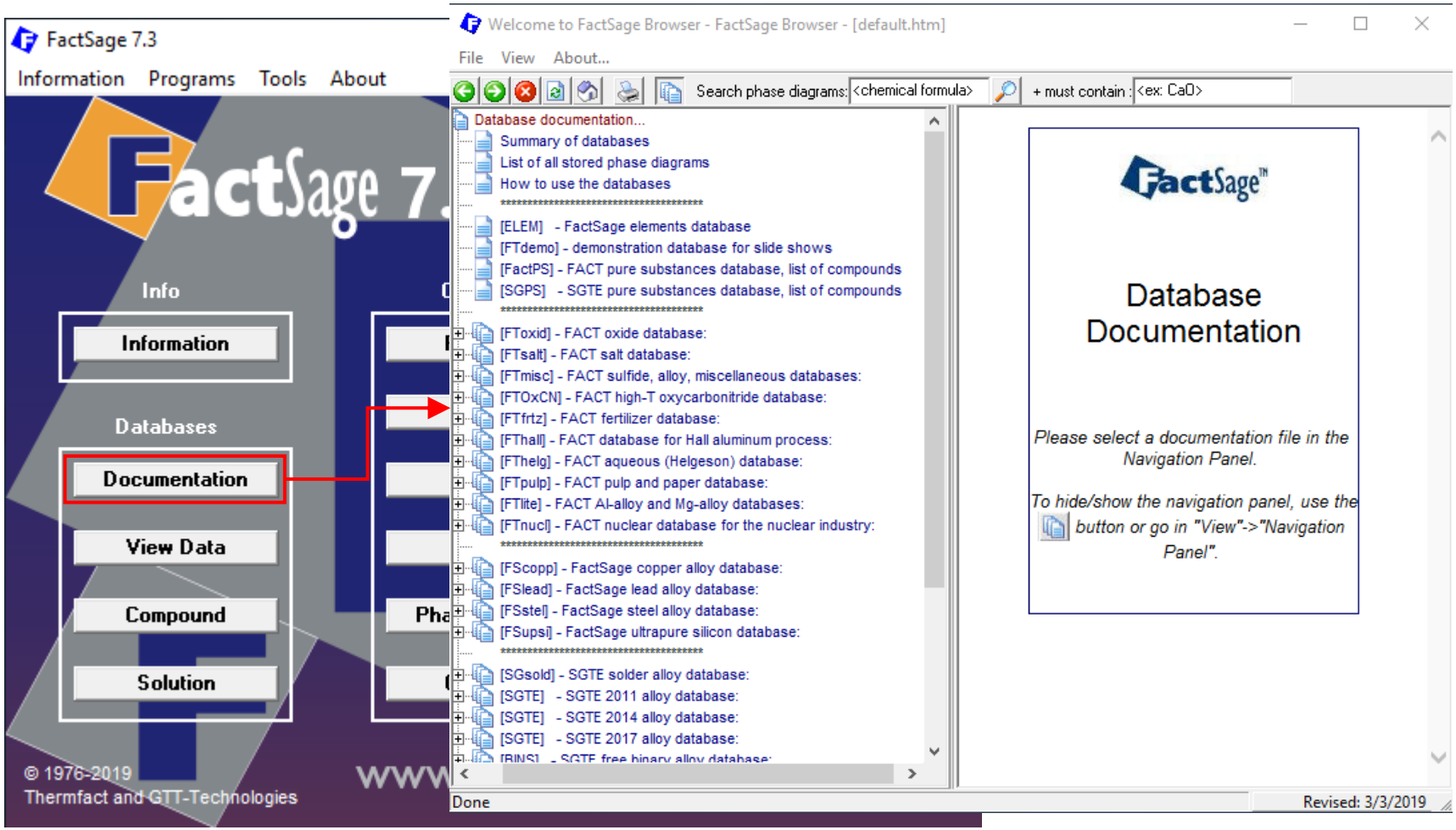


Documentation Module

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.

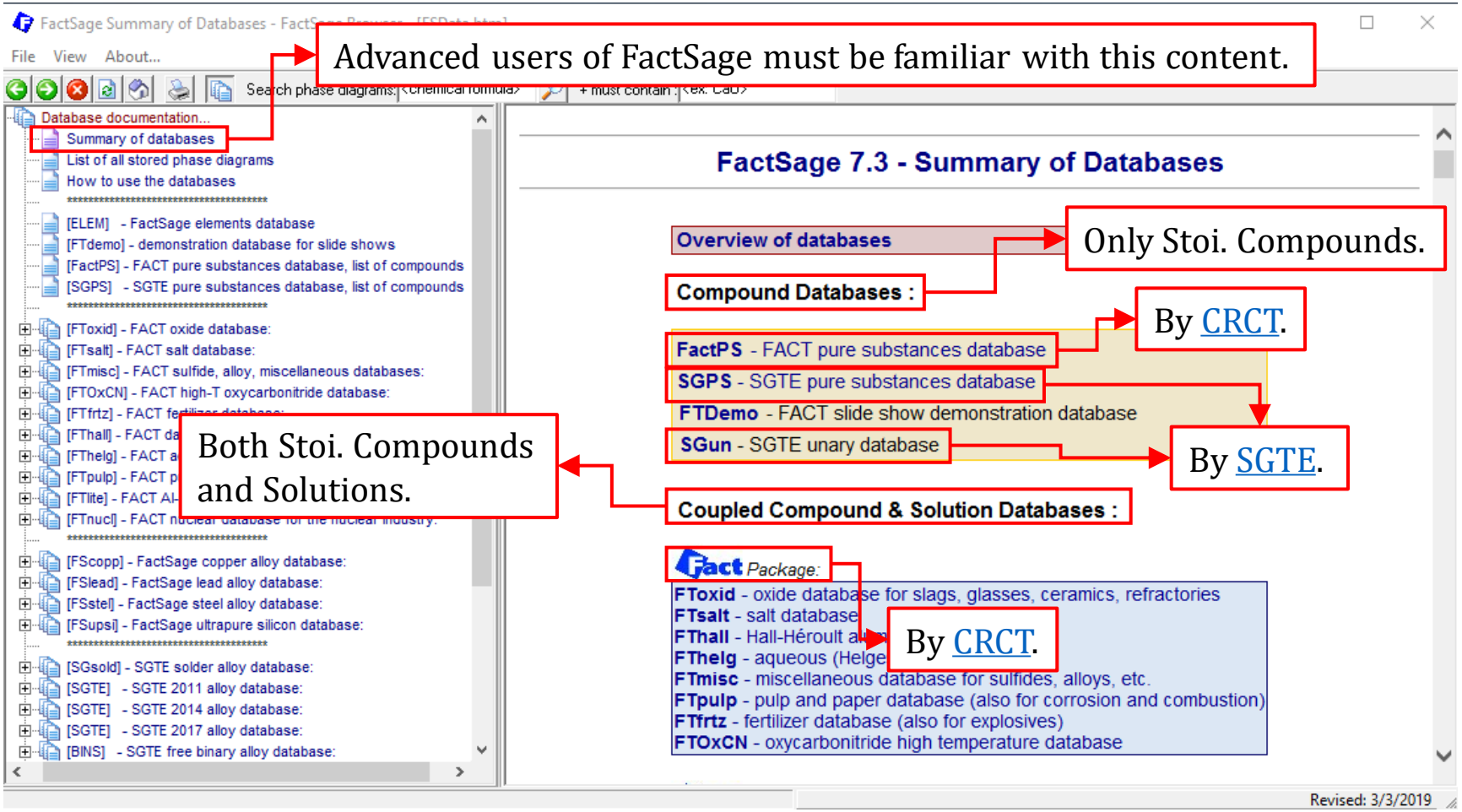
Documentation Module



Run the "Documentation" Module

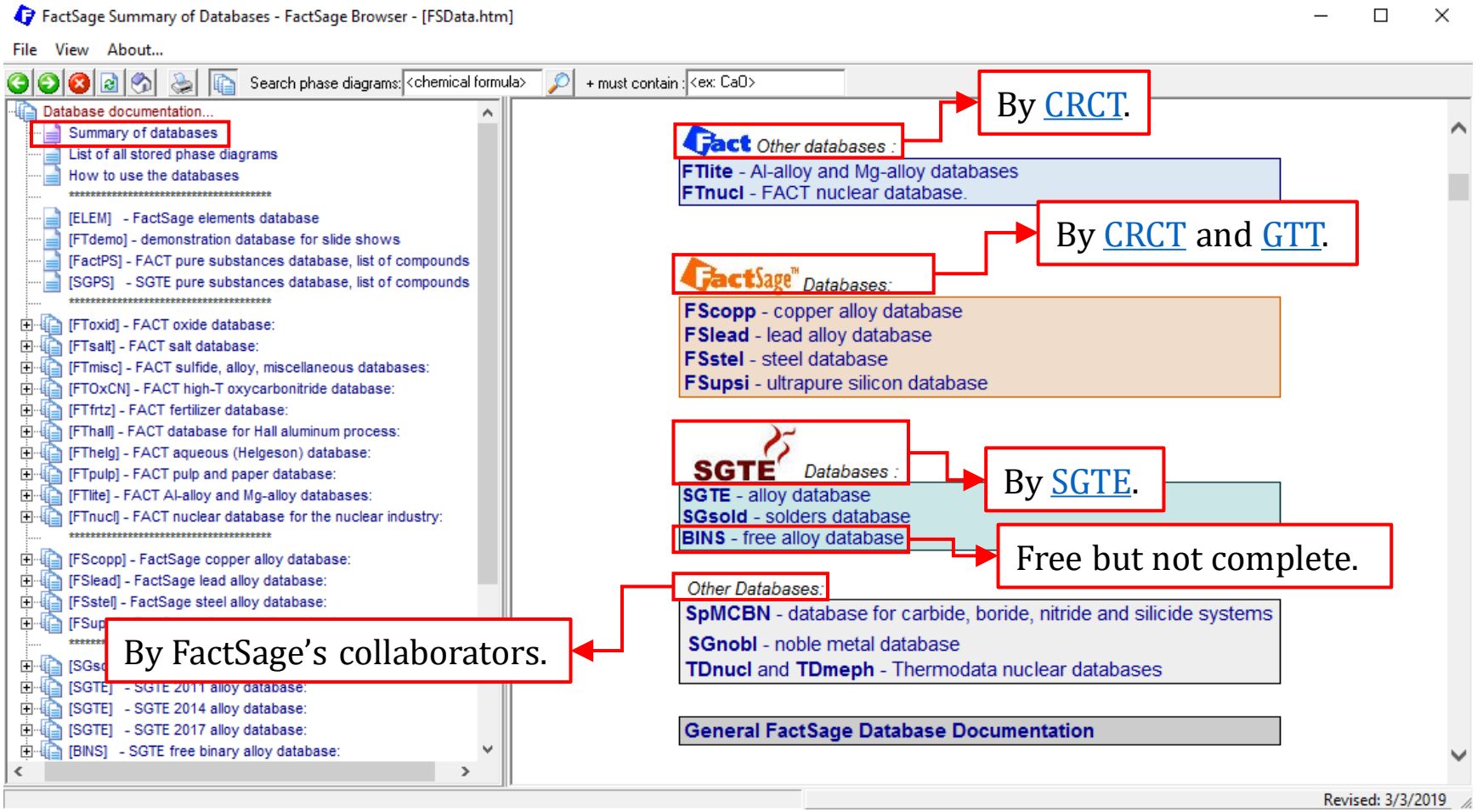
Documentation Module

Summary of Databases



Documentation Module

Summary of Databases



Documentation Module

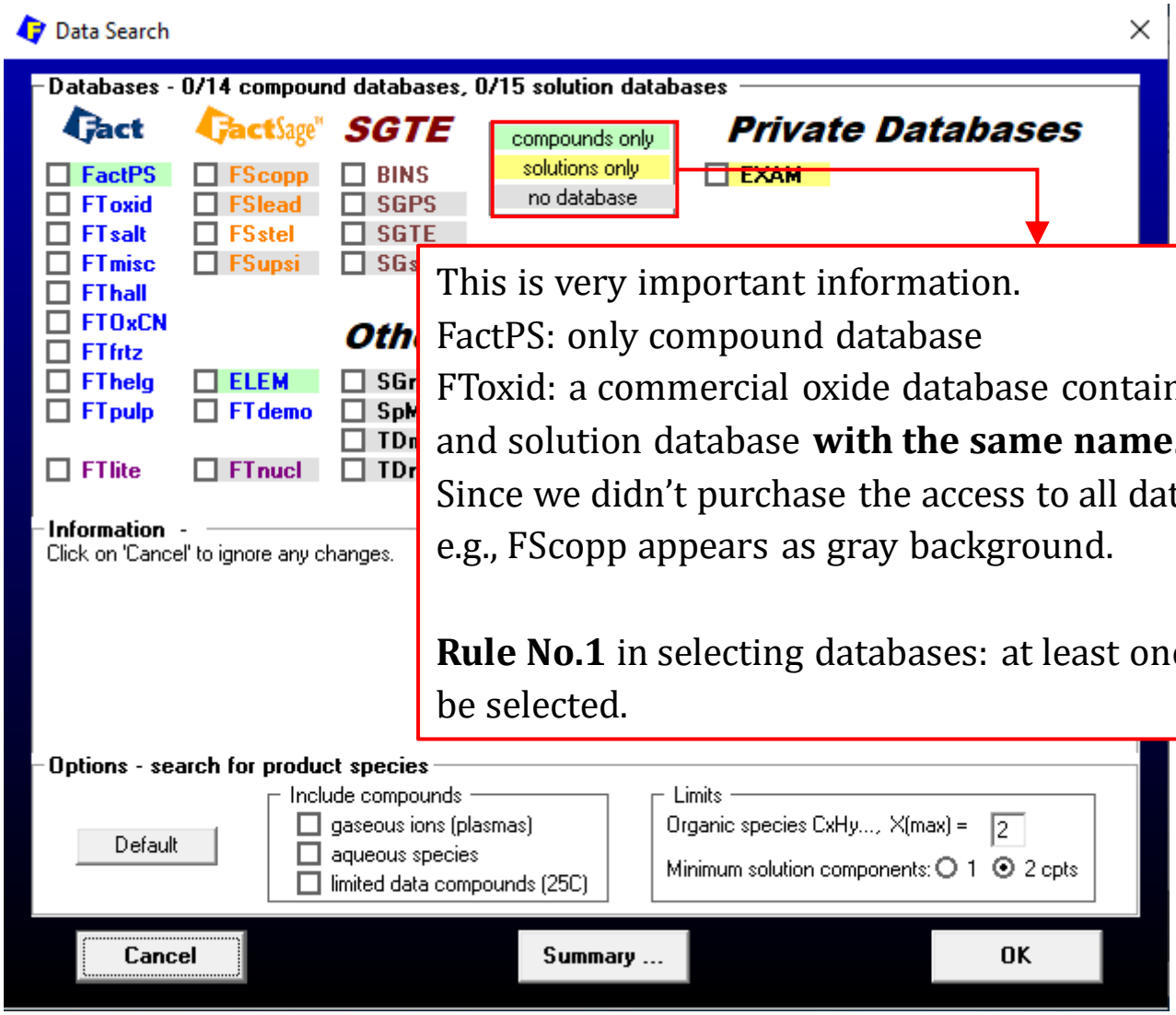
Compound Database	
FactPS	FACT compound database
SGPS	SGTE compound database

Compound Database & Solution Database (FACT)	
FToxid	Oxide (slag, glass, ceramics, refractory)
FTsalt	Salt
FThall	Hall-Héroult method (aluminum smelting)
FThelg	Dilute solution
FTmisc	Molten steel (main components are Fe, Cu, Ti, Pb, etc.), sulfur/sufide 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



This is very important information.

FactPS: only compound database

FToxid: a commercial oxide database contains both compound database and solution database **with the same name**.

Since we didn't purchase the access to all databases, some databases, e.g., FScopp appears as gray background.

Rule No.1 in selecting databases: at least one compound database must be selected.

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.

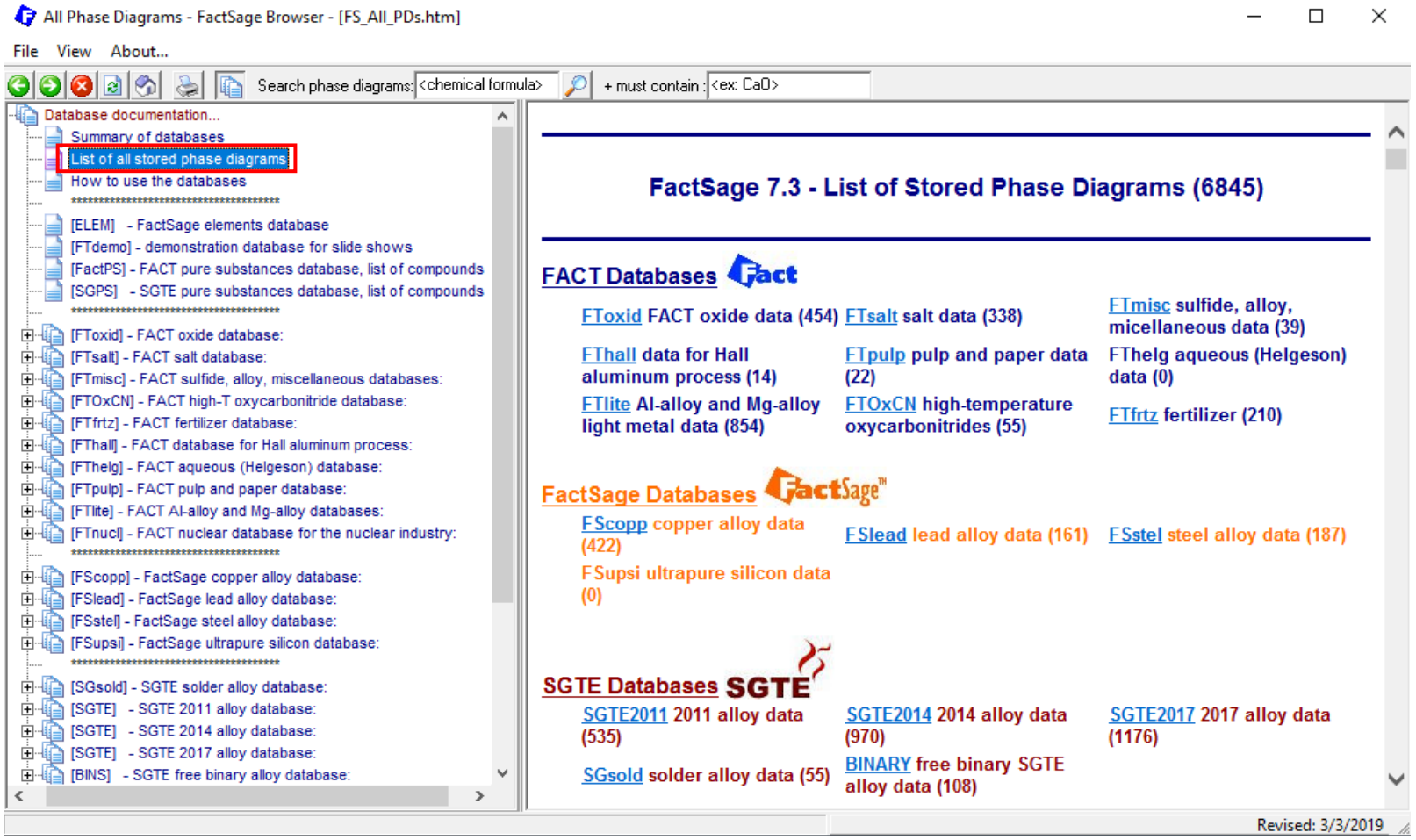
Documentation Module

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.

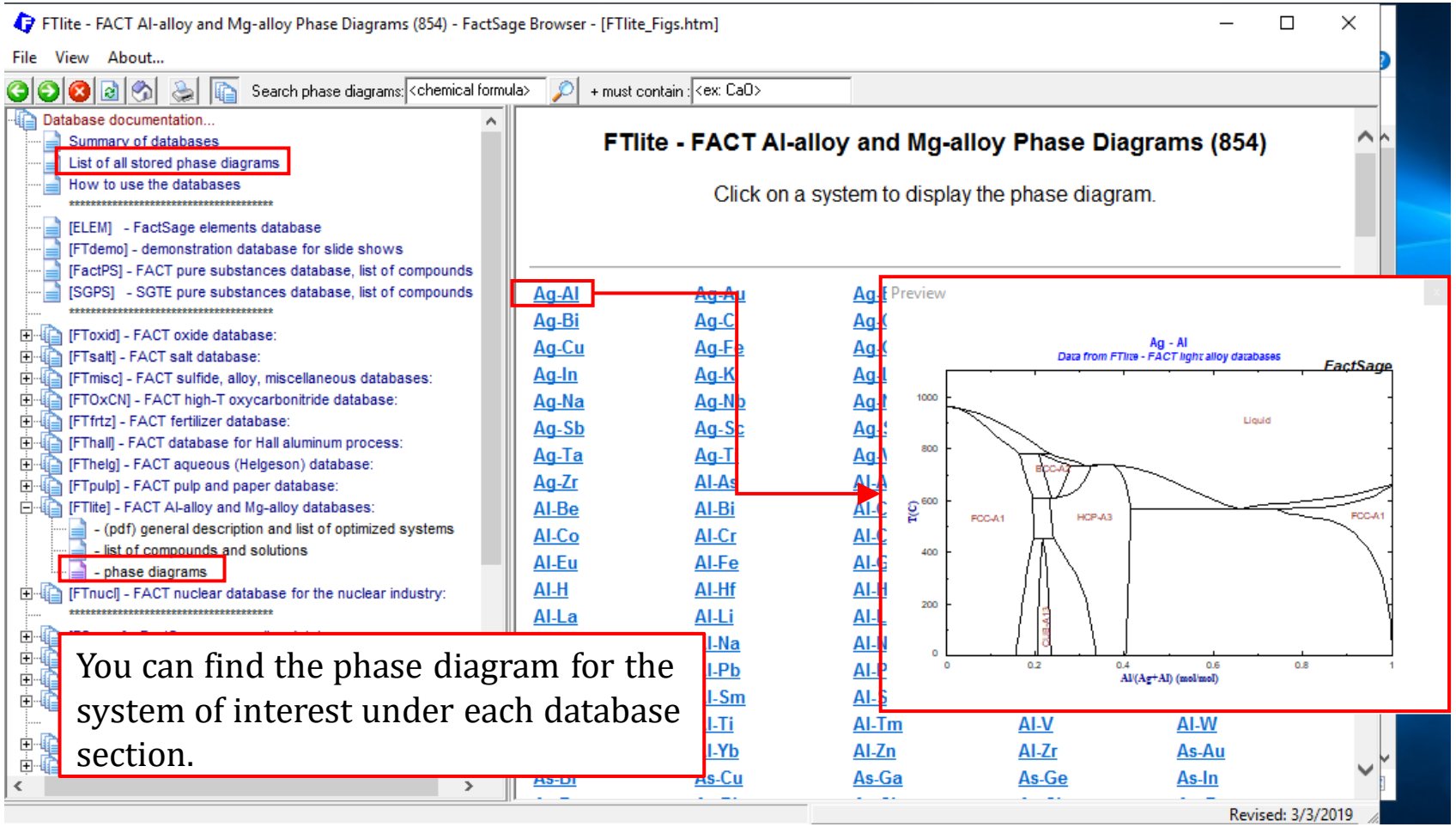
Documentation Module

List of All Stored Phase Diagrams



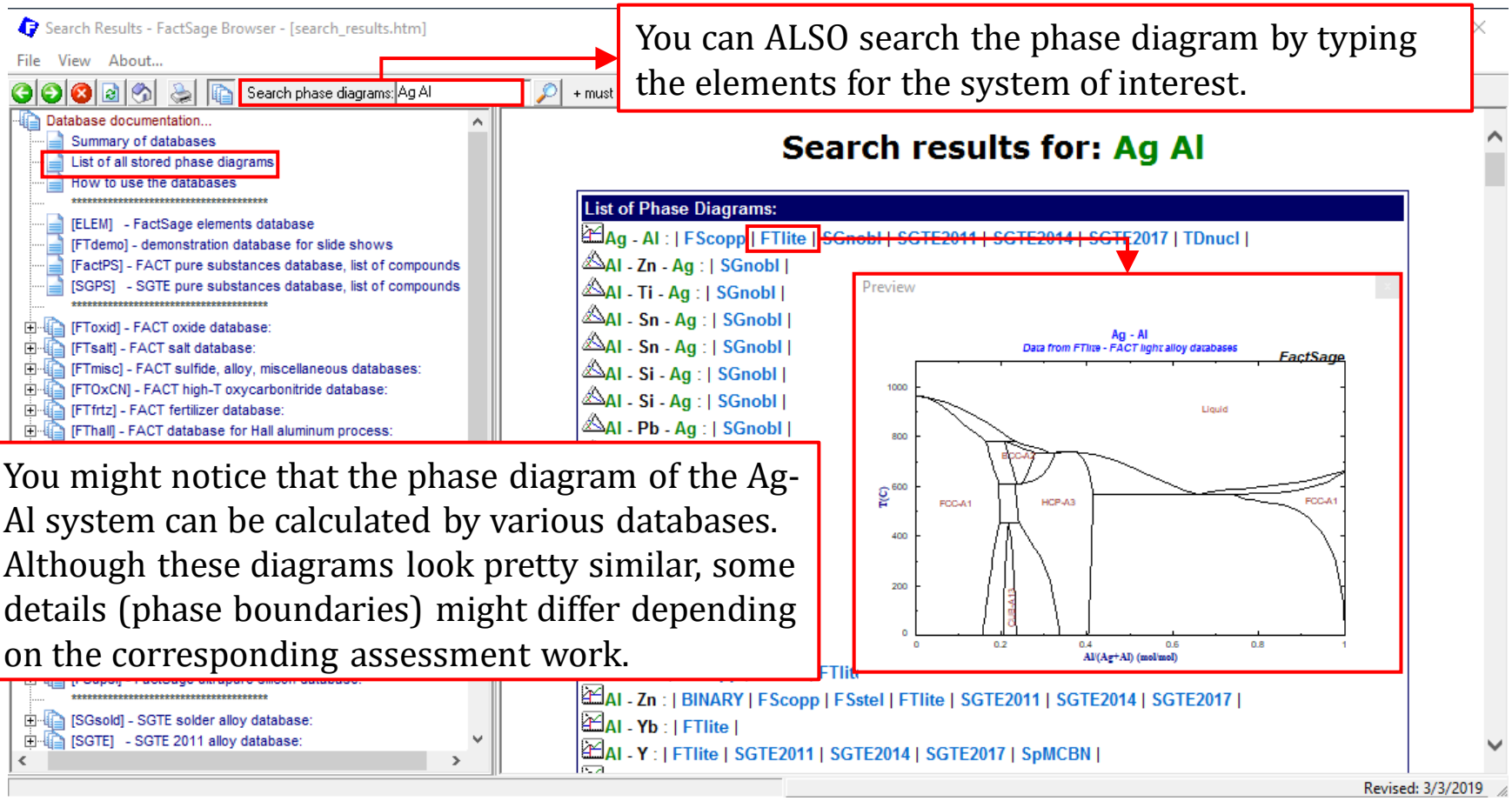
Documentation Module

List of All Stored Phase Diagrams



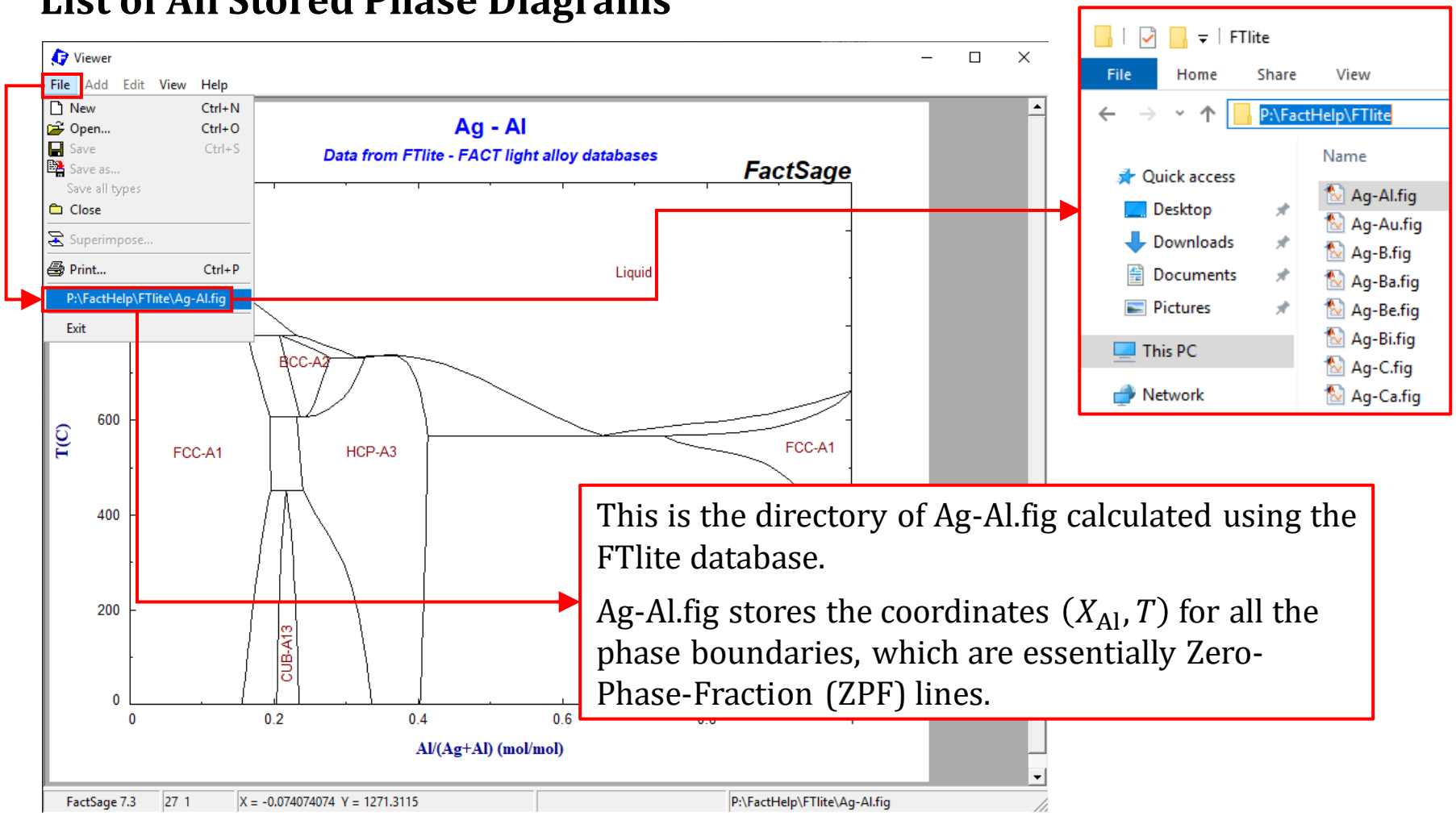
Documentation Module

List of All Stored Phase Diagrams



Documentation Module

List of All Stored Phase Diagrams

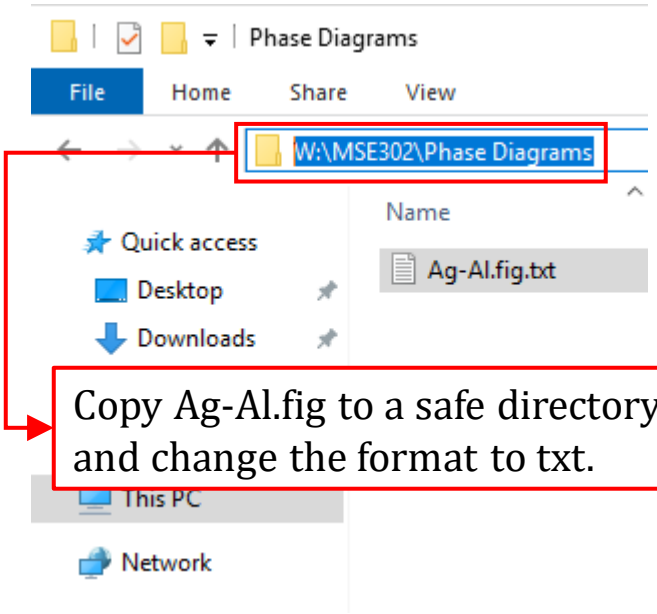


This is the directory of Ag-Al.fig calculated using the FTlite database.

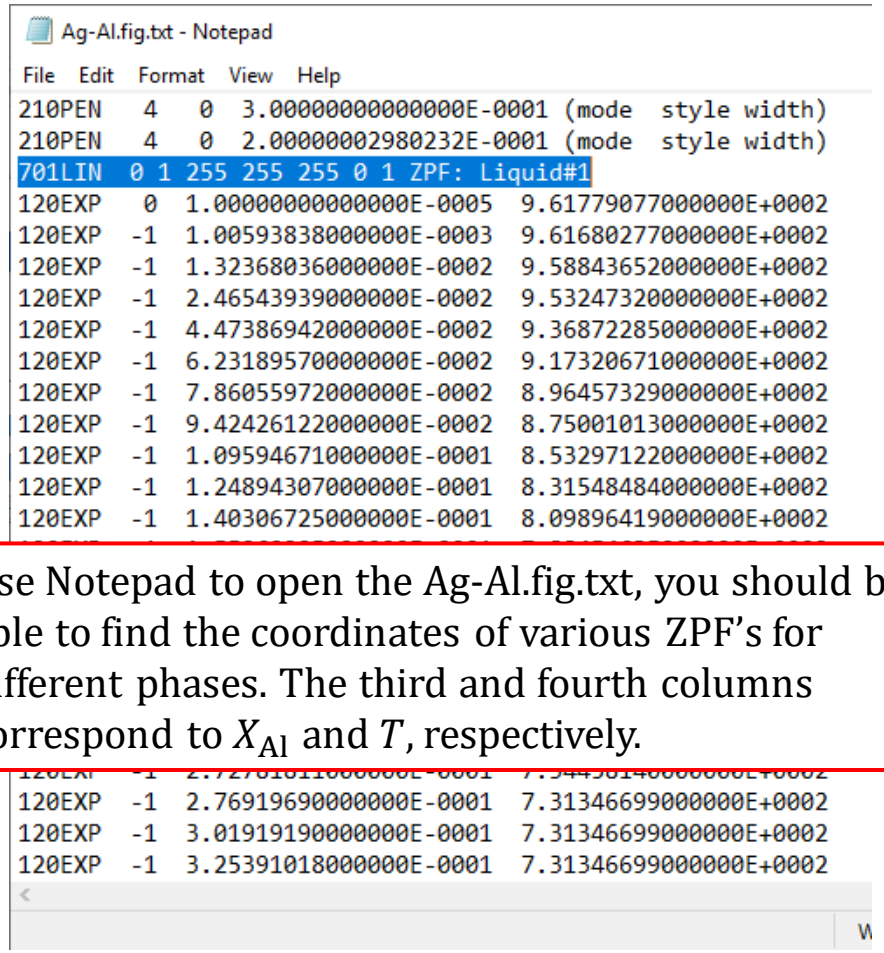
Ag-Al.fig stores the coordinates (X_{Al}, T) for all the phase boundaries, which are essentially Zero-Phase-Fraction (ZPF) lines.

Documentation Module

List of All Stored Phase Diagrams



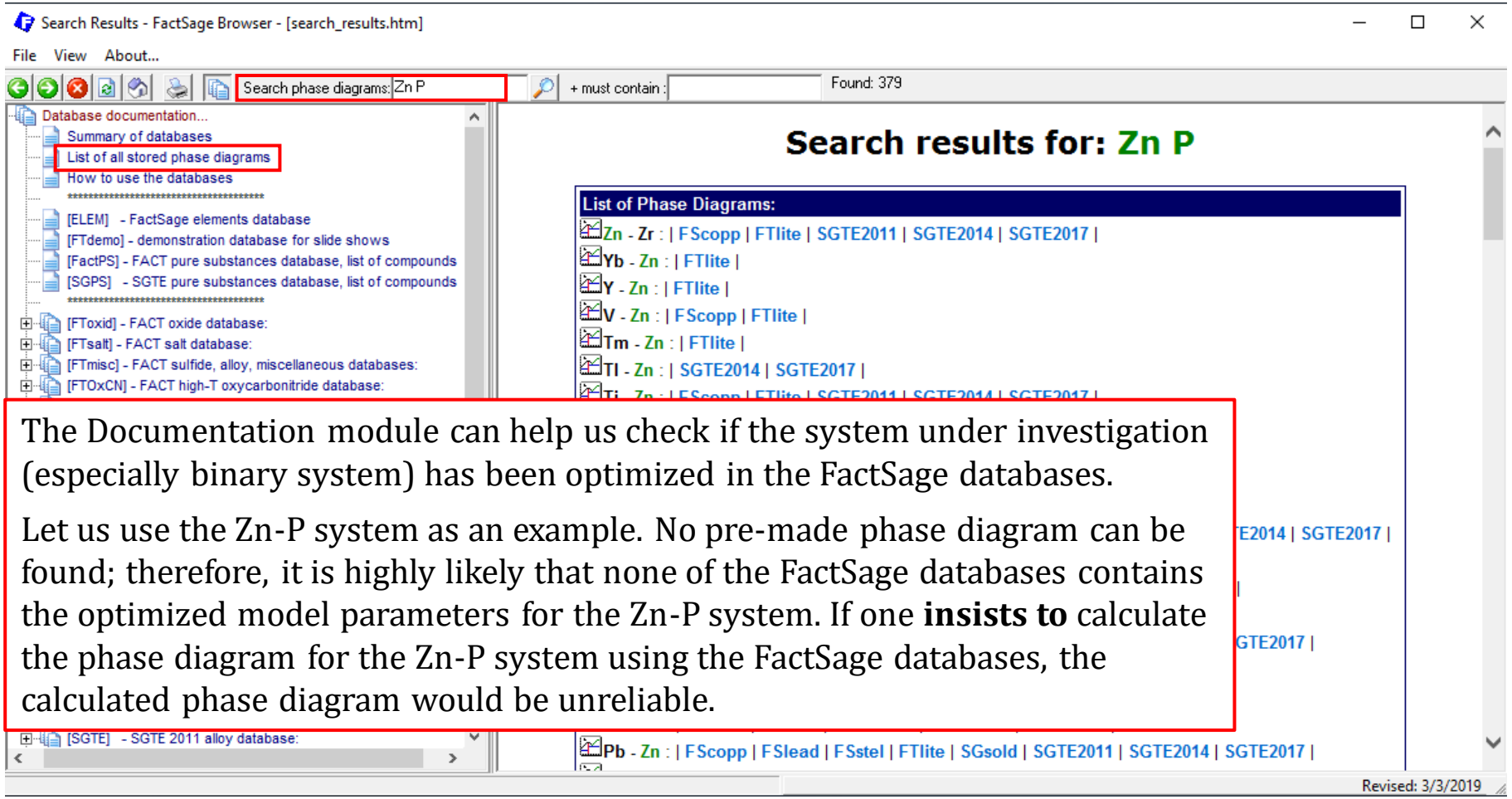
Copy Ag-Al.fig to a safe directory and change the format to txt.



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.

Documentation Module

List of All Stored Phase Diagrams

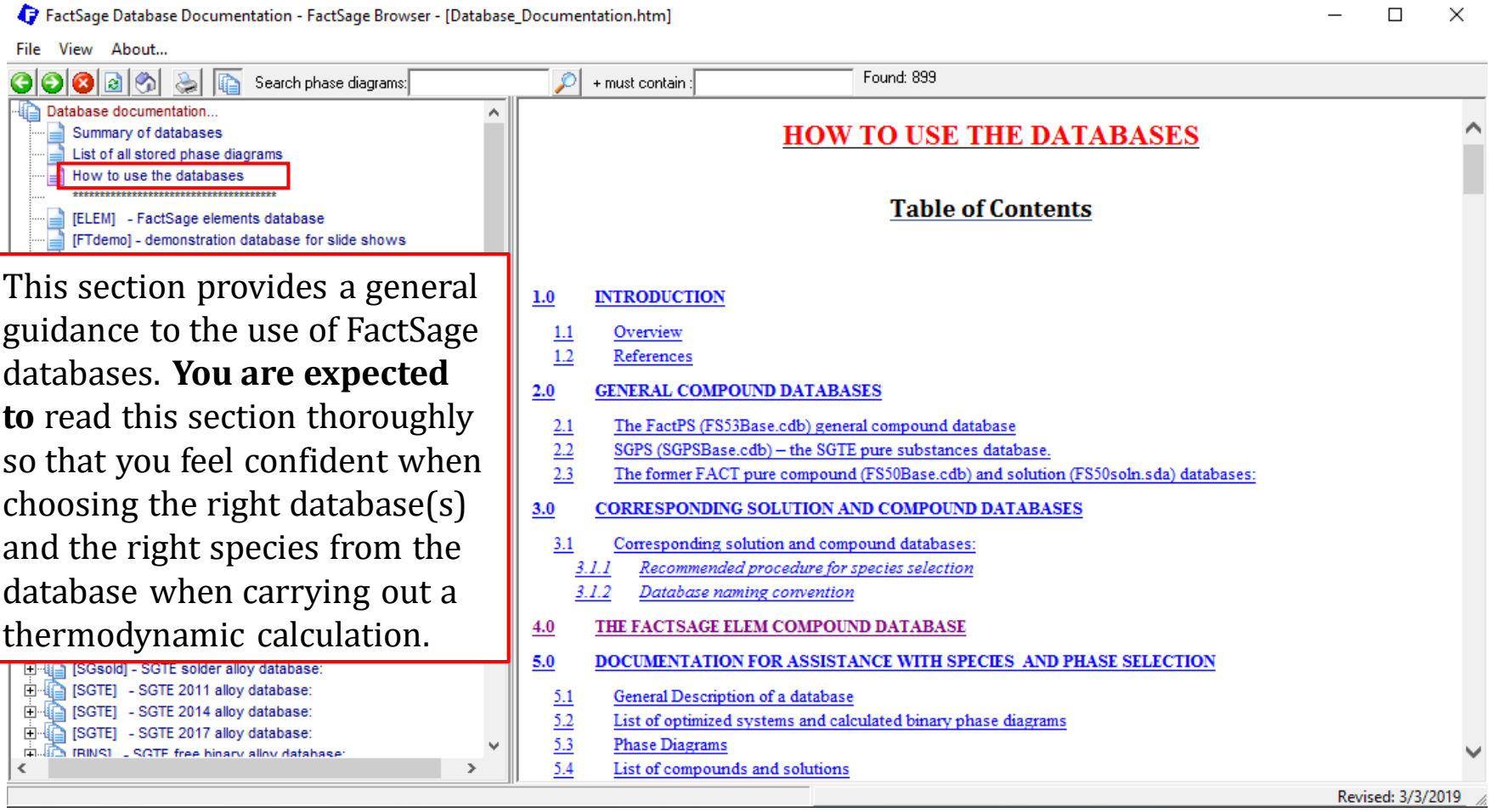


The Documentation module can help us check if the system under investigation (especially binary system) has been optimized in the FactSage databases.

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

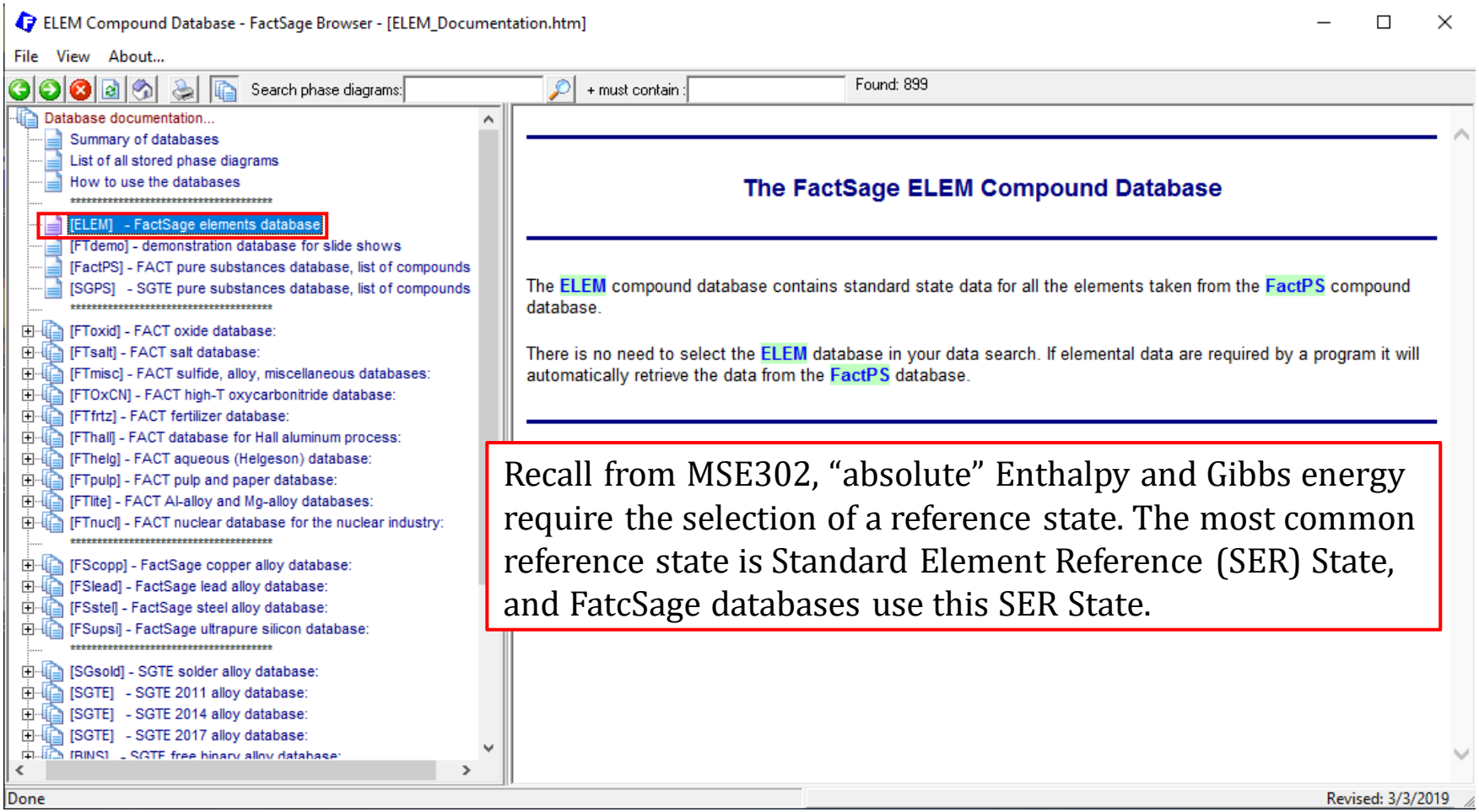
How to use the databases?



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.

Documentation Module

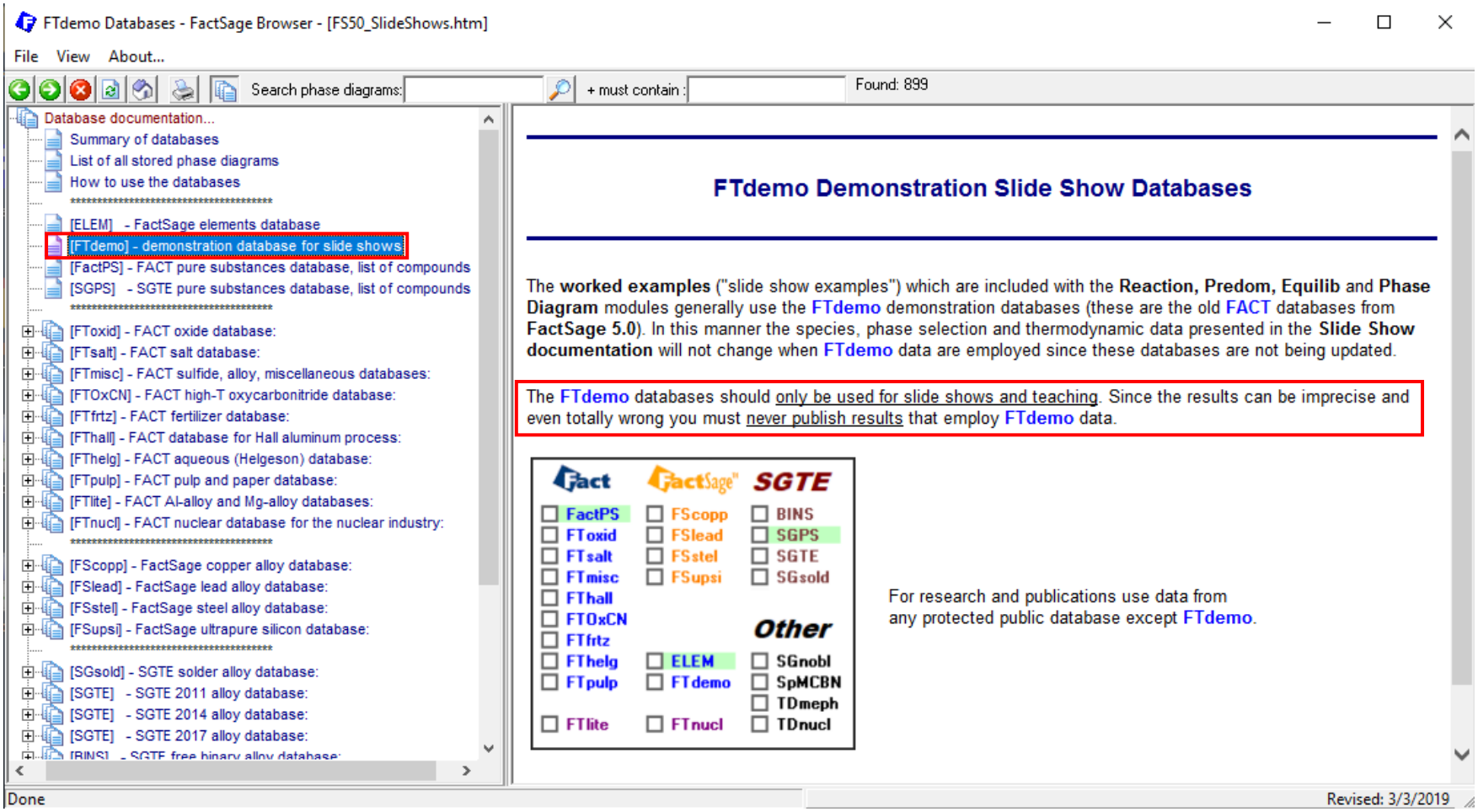
[ELEM] – FactSage elements database



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 FatcSage databases use this SER State.

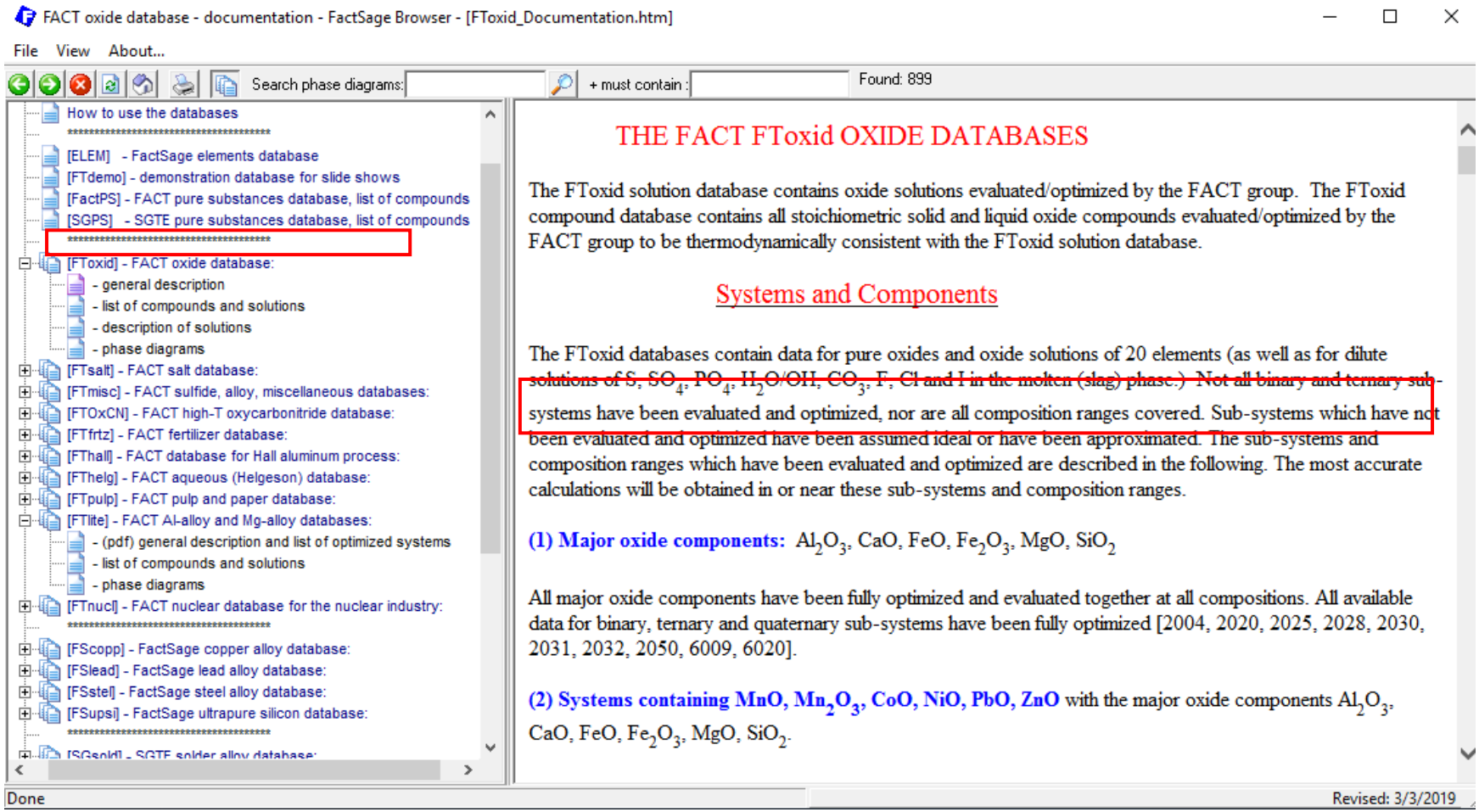
Documentation Module

[FTdemo] – demonstration database for slide shows



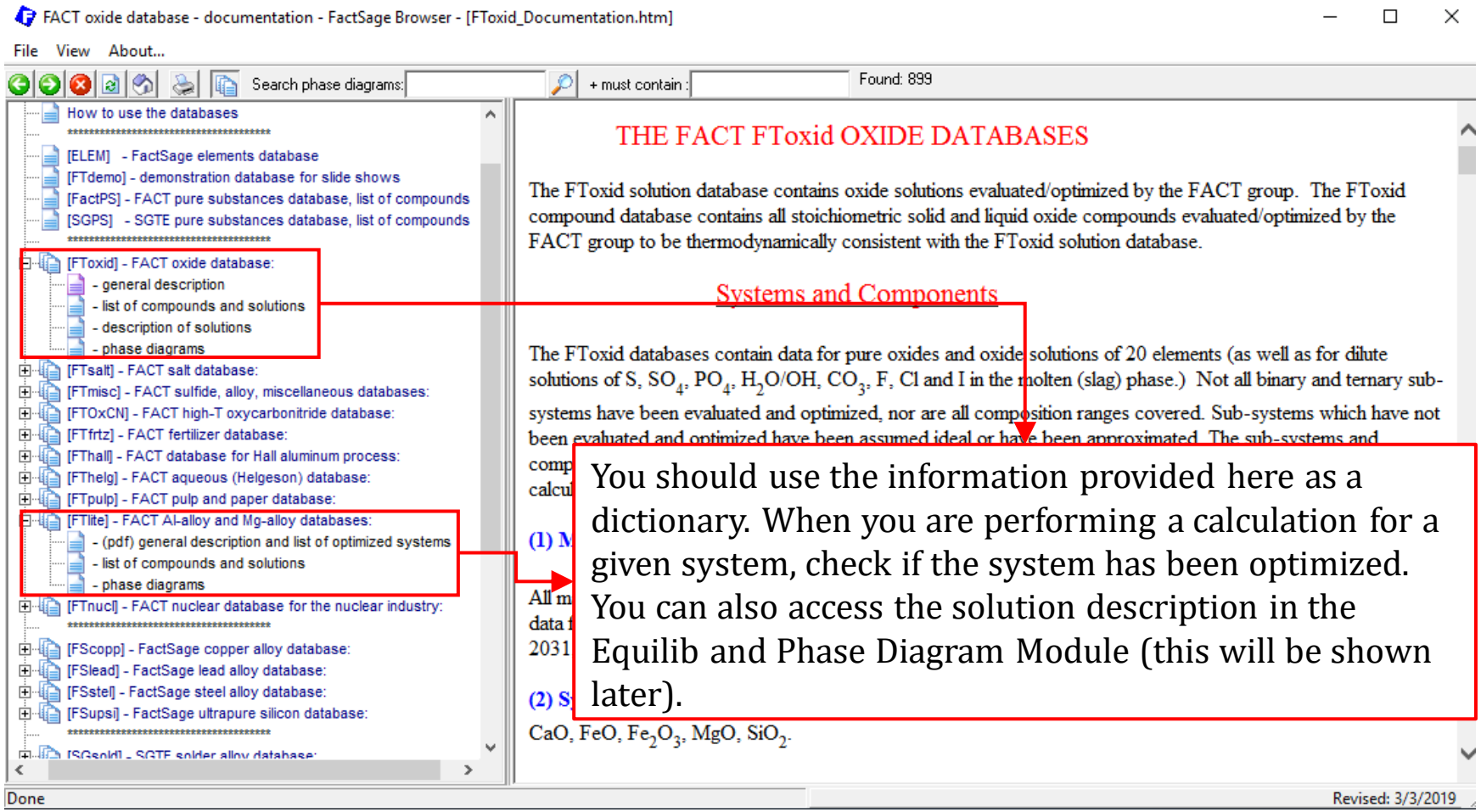
Documentation Module

[FTdemo] – demonstration database for slide shows



Documentation Module

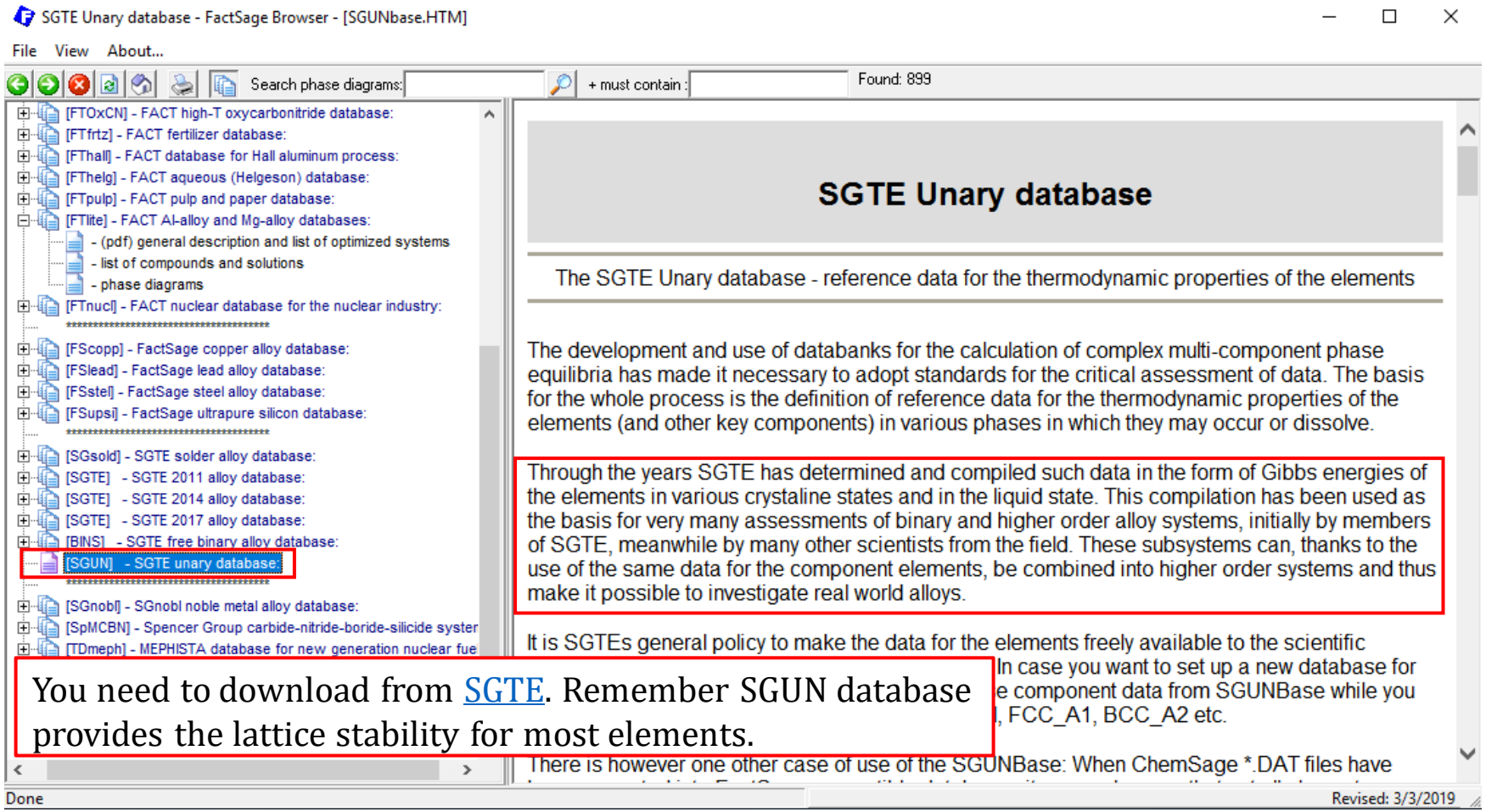
Solution Databases



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).

Documentation Module

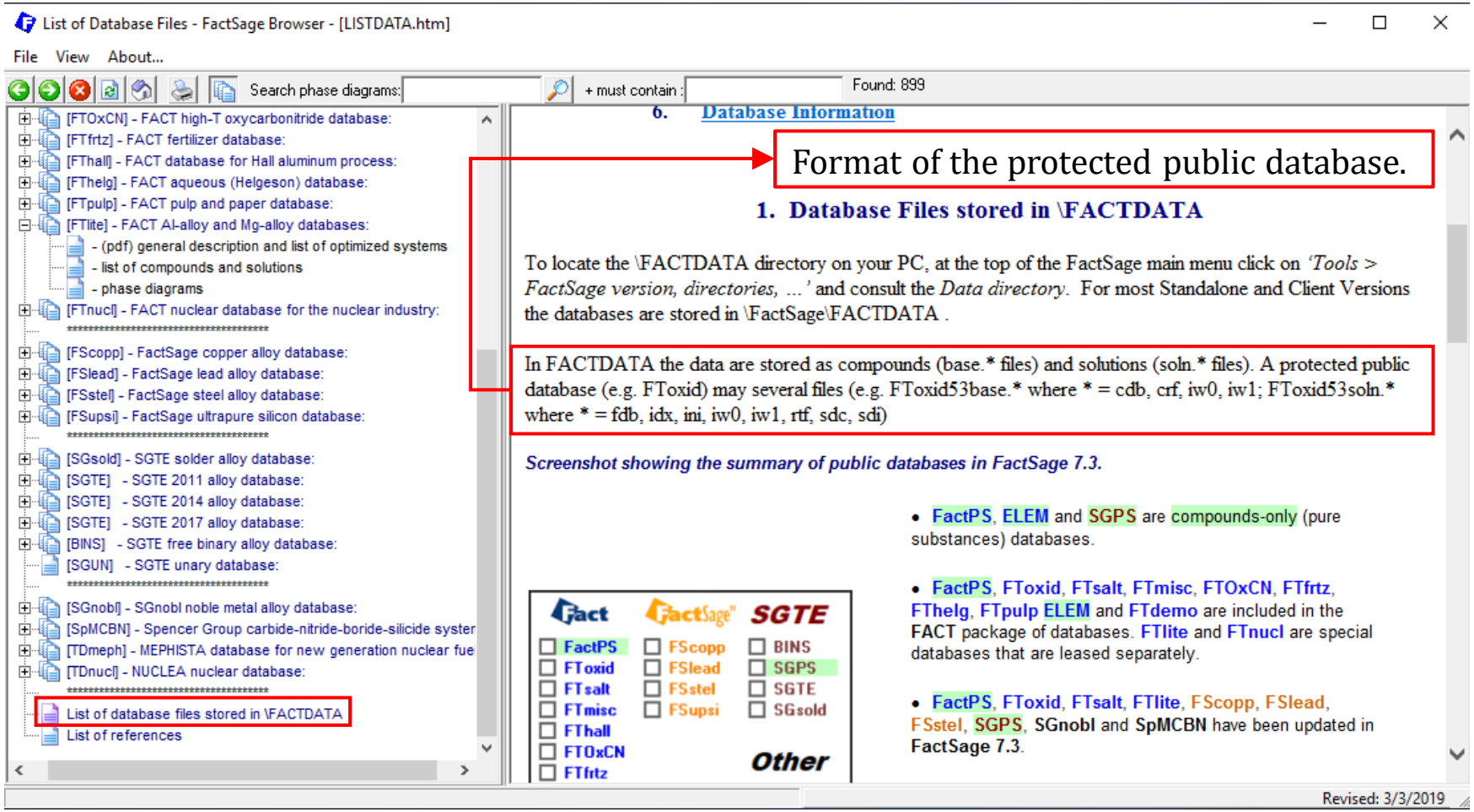
[SGUN] – SGTE Unary database



You need to download from SGTE. Remember SGUN database provides the lattice stability for most elements.

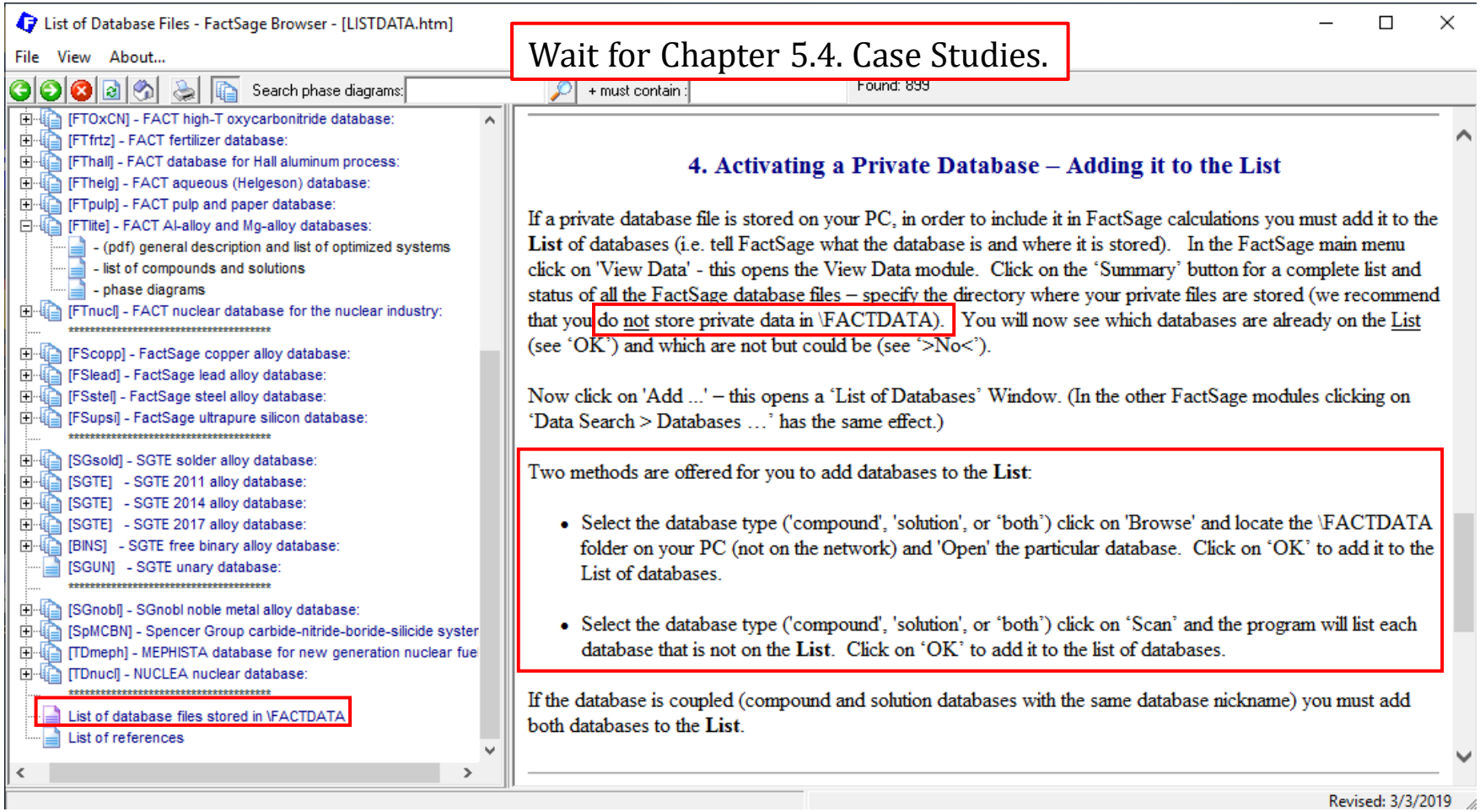
Documentation Module

List of database files stored in \FACTDATA



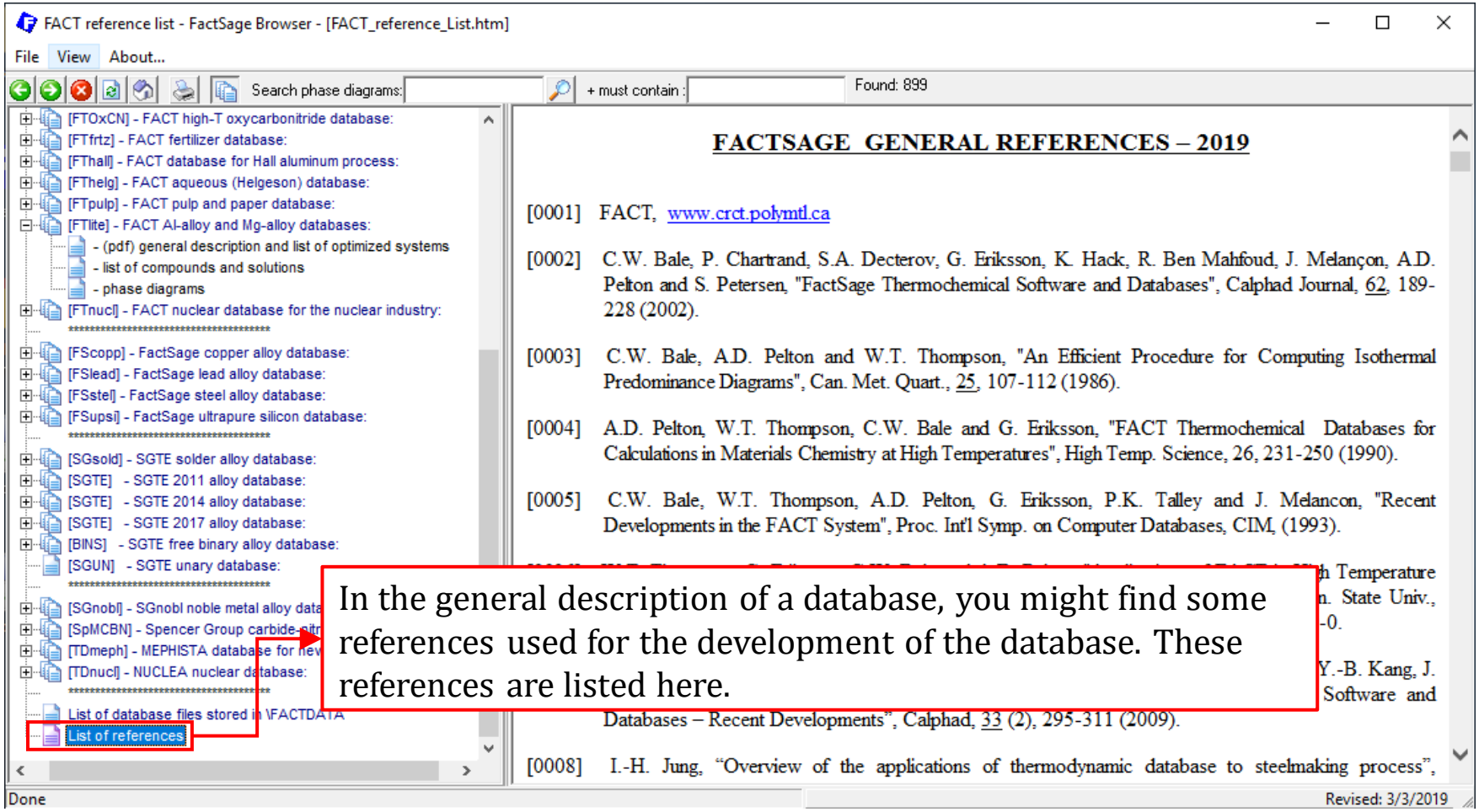
Documentation Module: Private Databases

List of database files stored in \FACTDATA



Documentation Module: FactSage References

List of references



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.

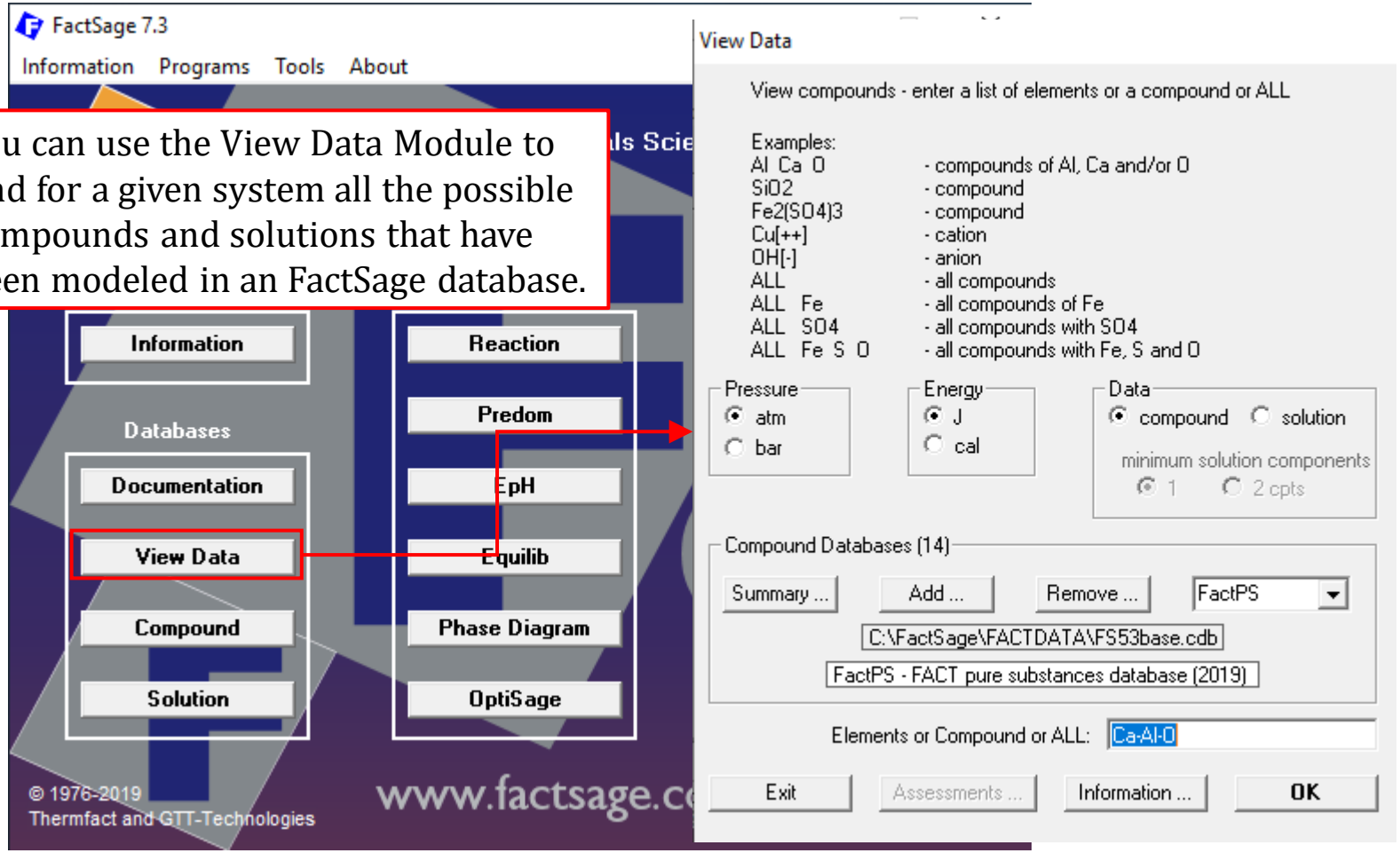
The Documentation Module gives detailed descriptions about the databases of **COMPOUND** (i.e., elemental species and stoichiometric compounds) and **SOLUTIONS** (i.e., homogeneous mixture which are mixed on an atomic or molecular scale).

FactSage Practical
MSE302

Practical 1. View Data

View Data Module

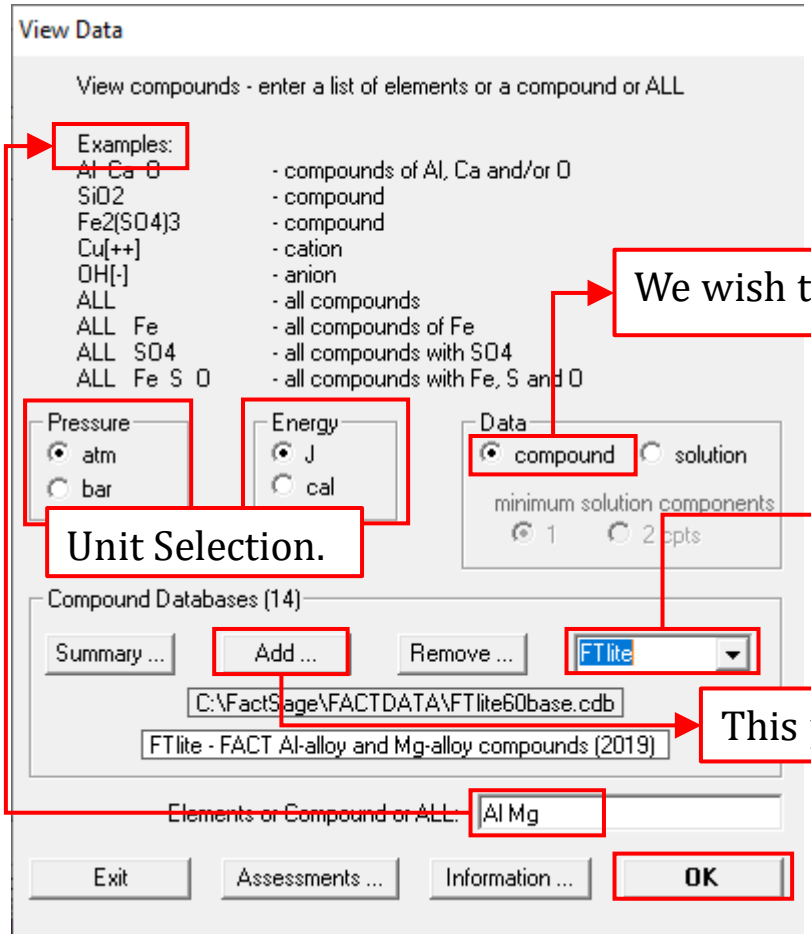
You can use the View Data Module to find for a given system all the possible compounds and solutions that have been modeled in an FactSage database.



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…



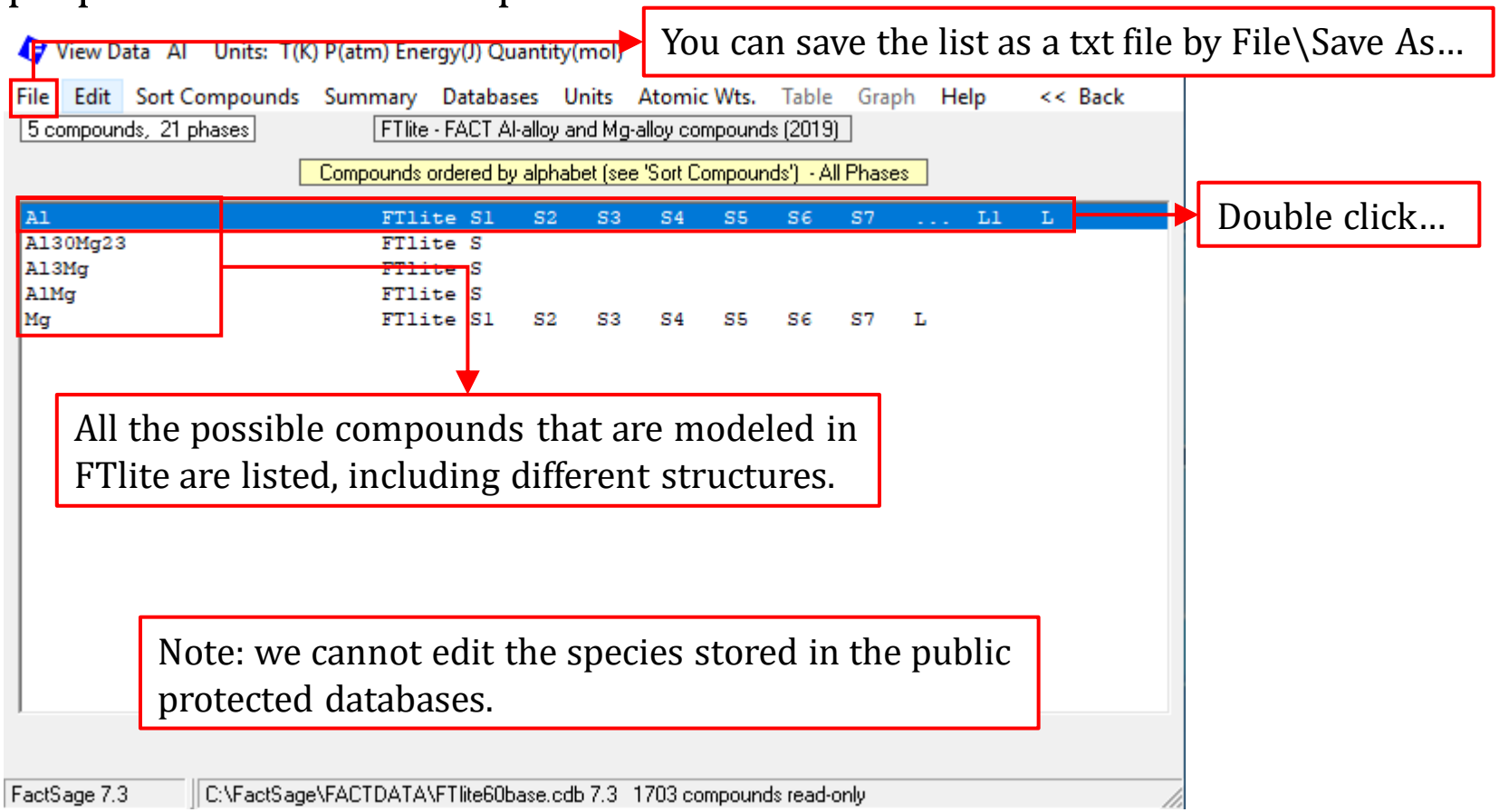
We wish to view compounds, not solutions.

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.

This permits the user to add a private database.

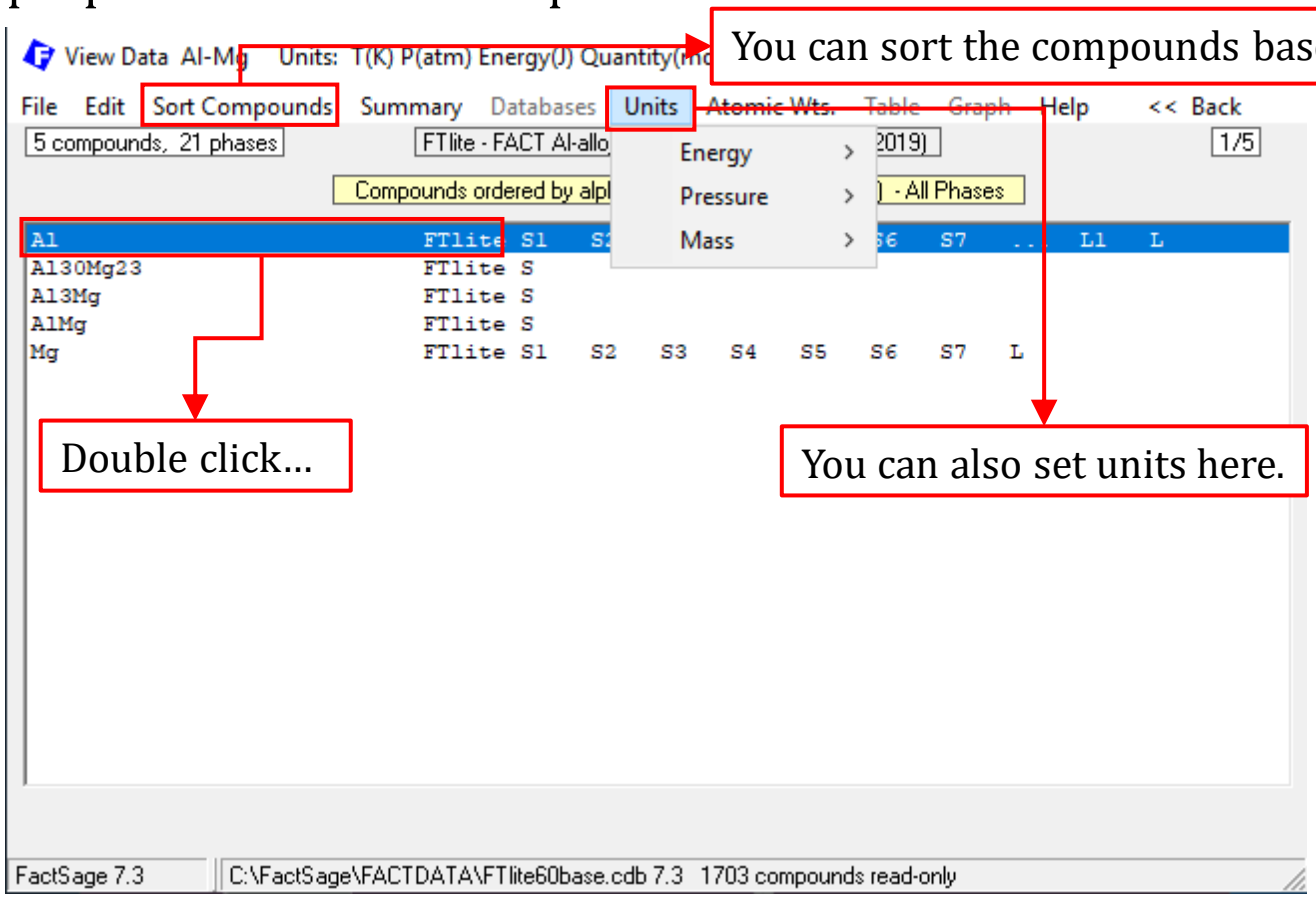
View Data Module

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 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…



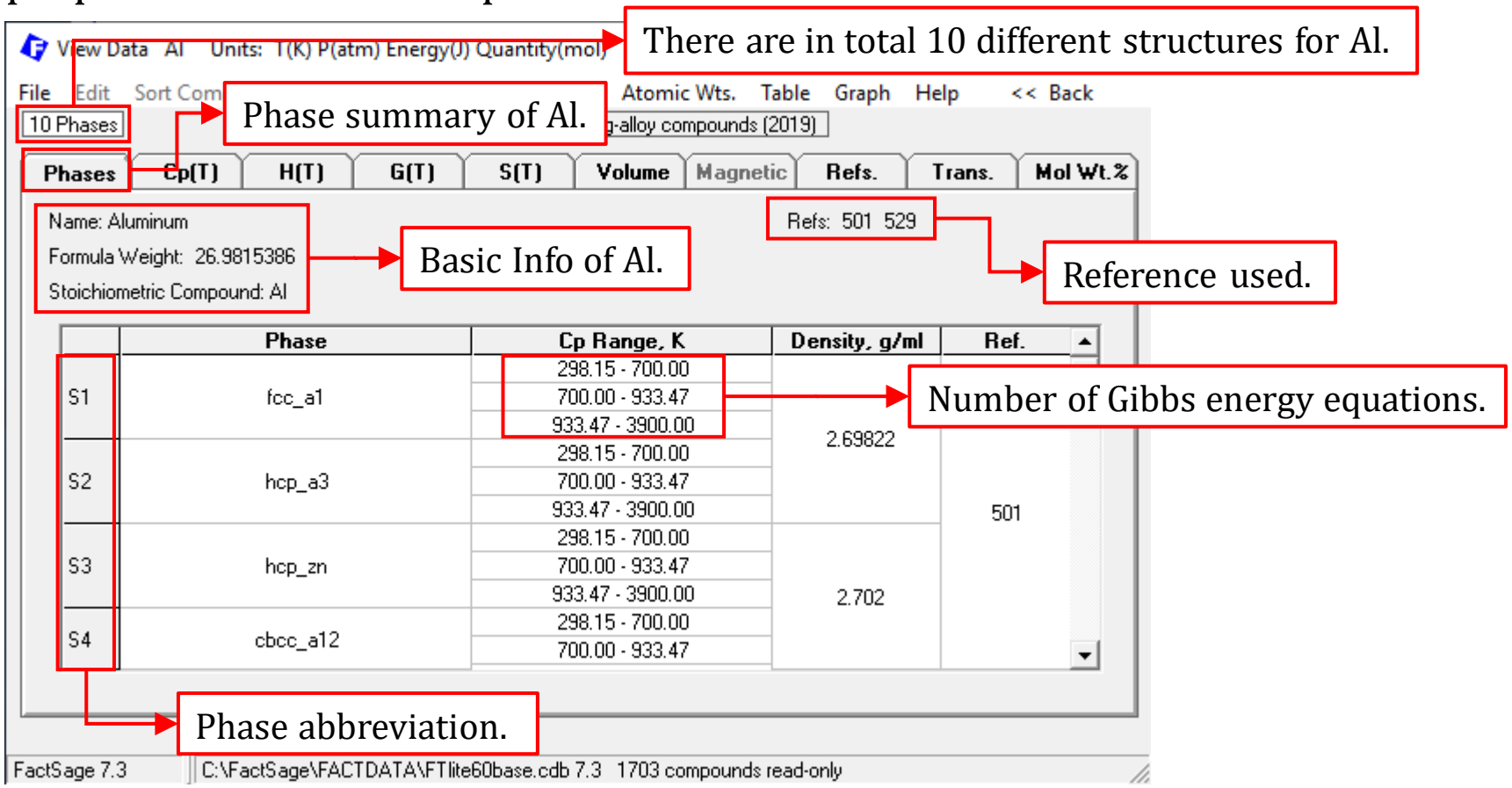
You can sort the compounds based on different properties.

Double click…

You can also set units here.

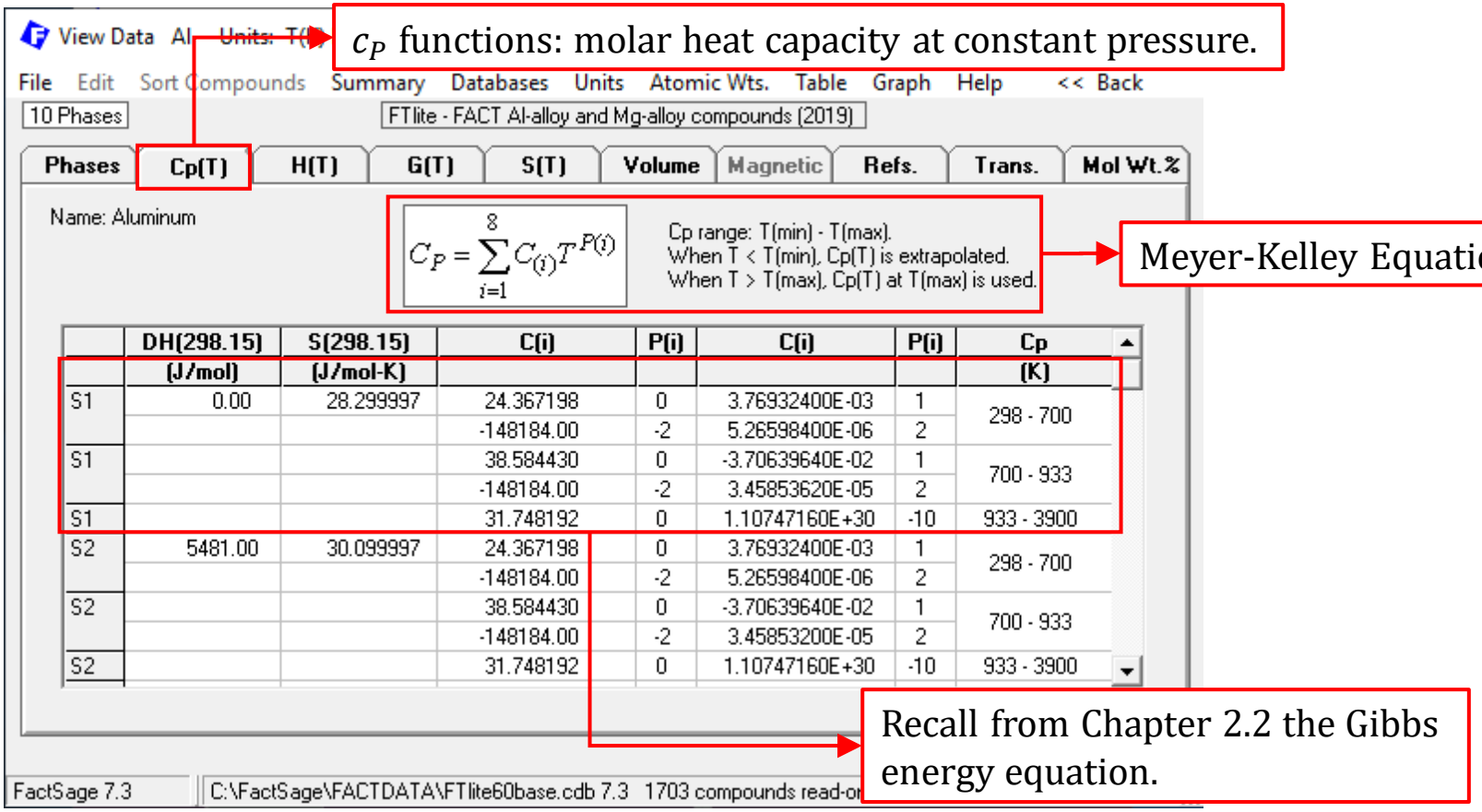
View Data Module

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 Module

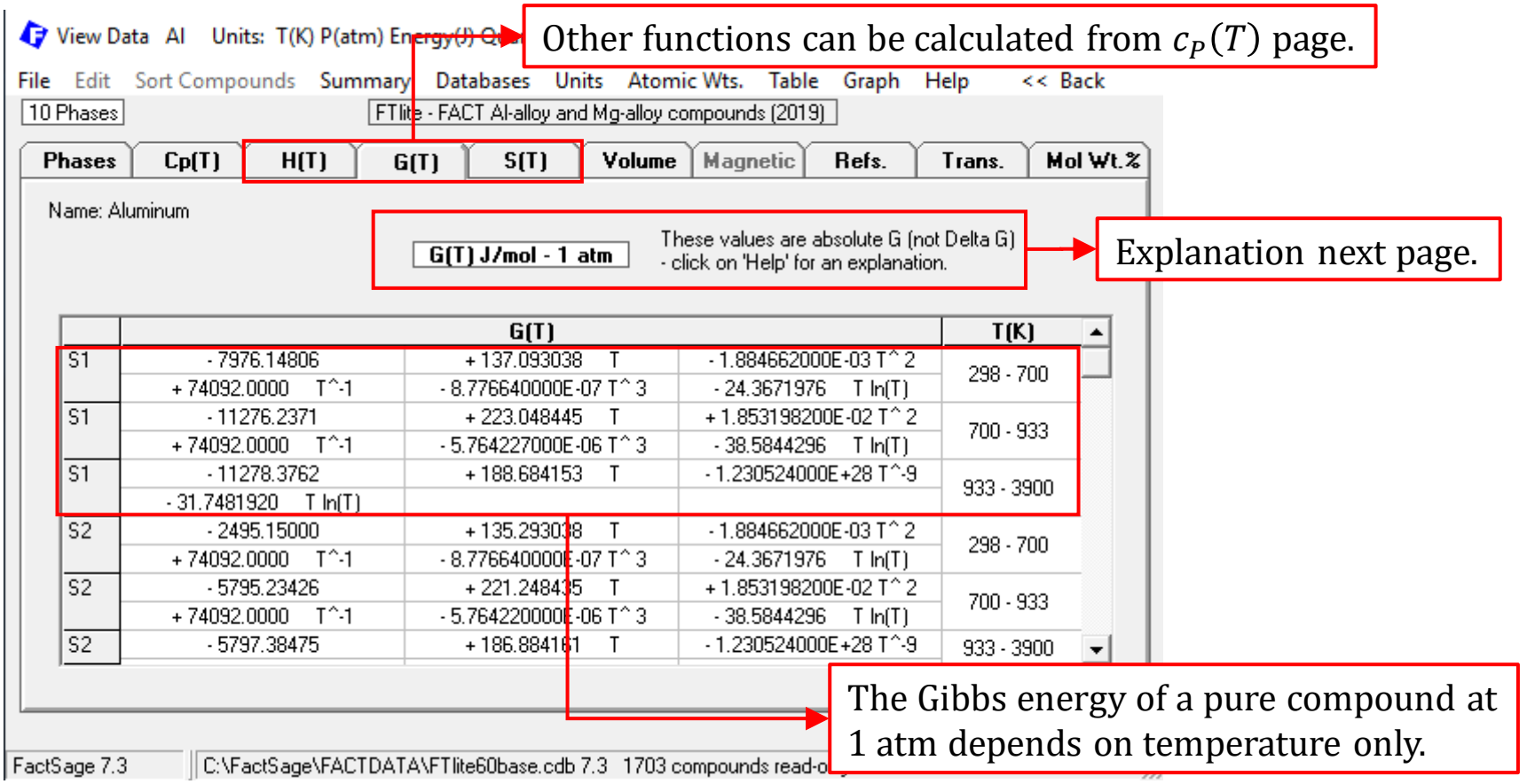
For example, say we wish to know for the Al-Mg system the thermodynamic properties of all the compounds that have been modeled in the FTlite database…



	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

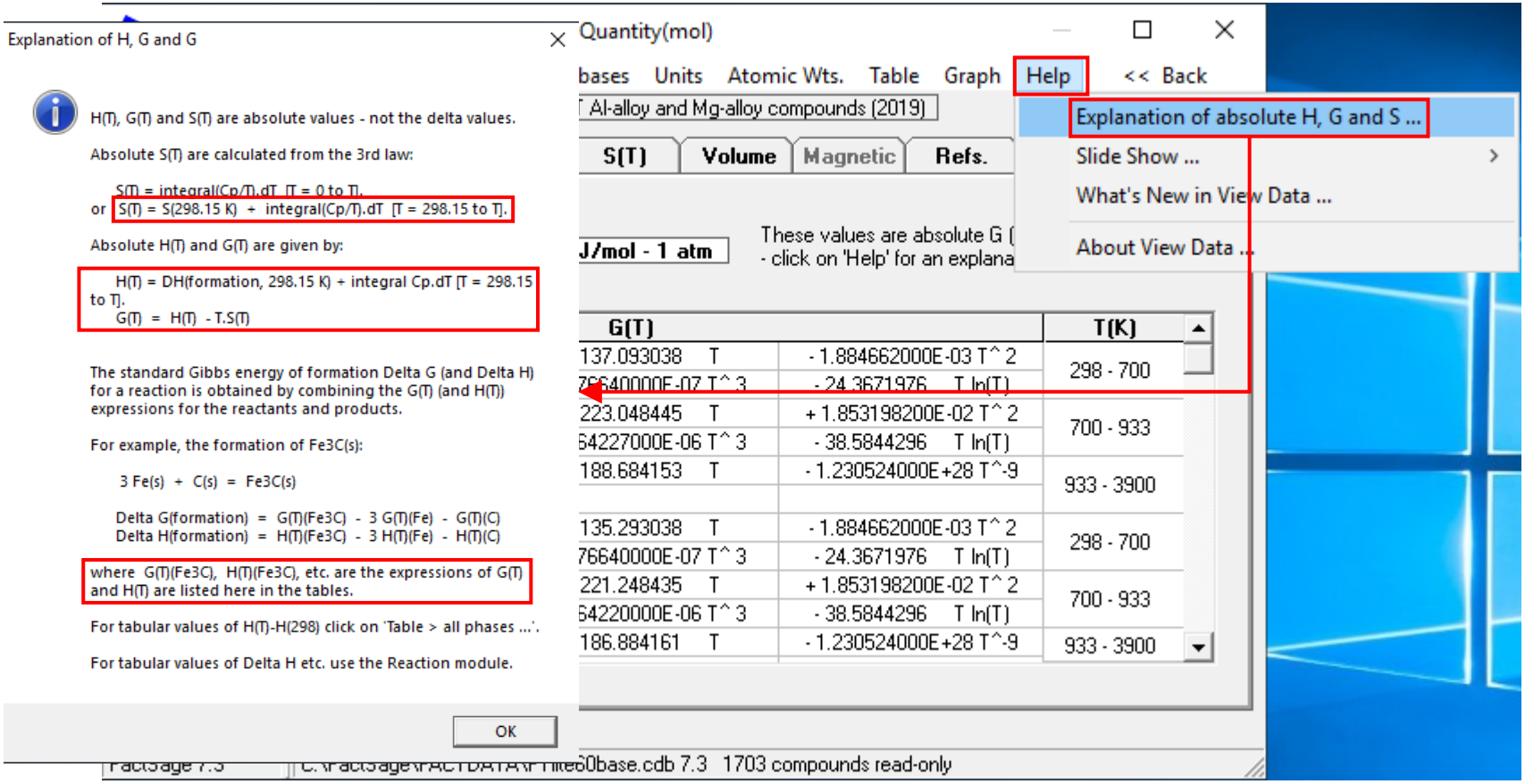
View Data Module

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…



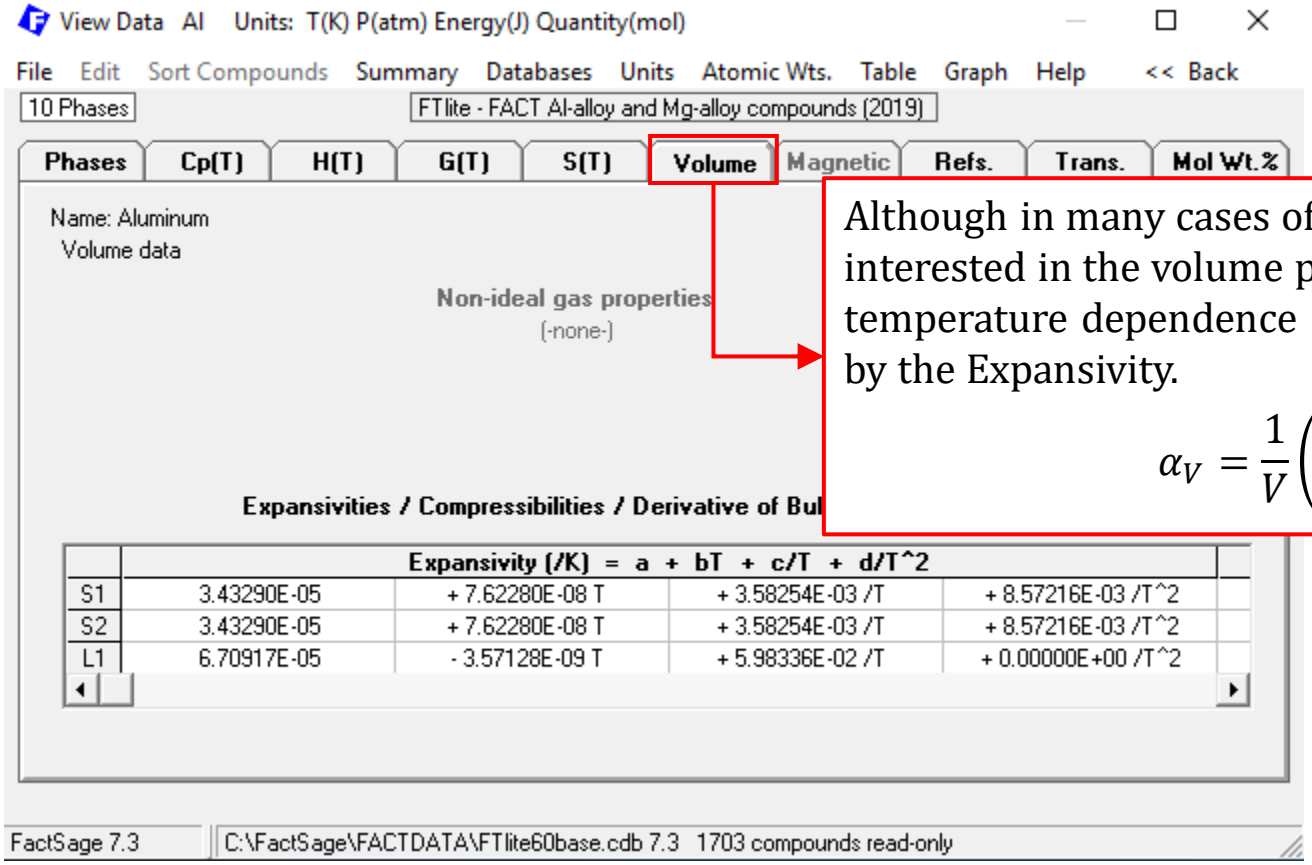
View Data Module

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 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…

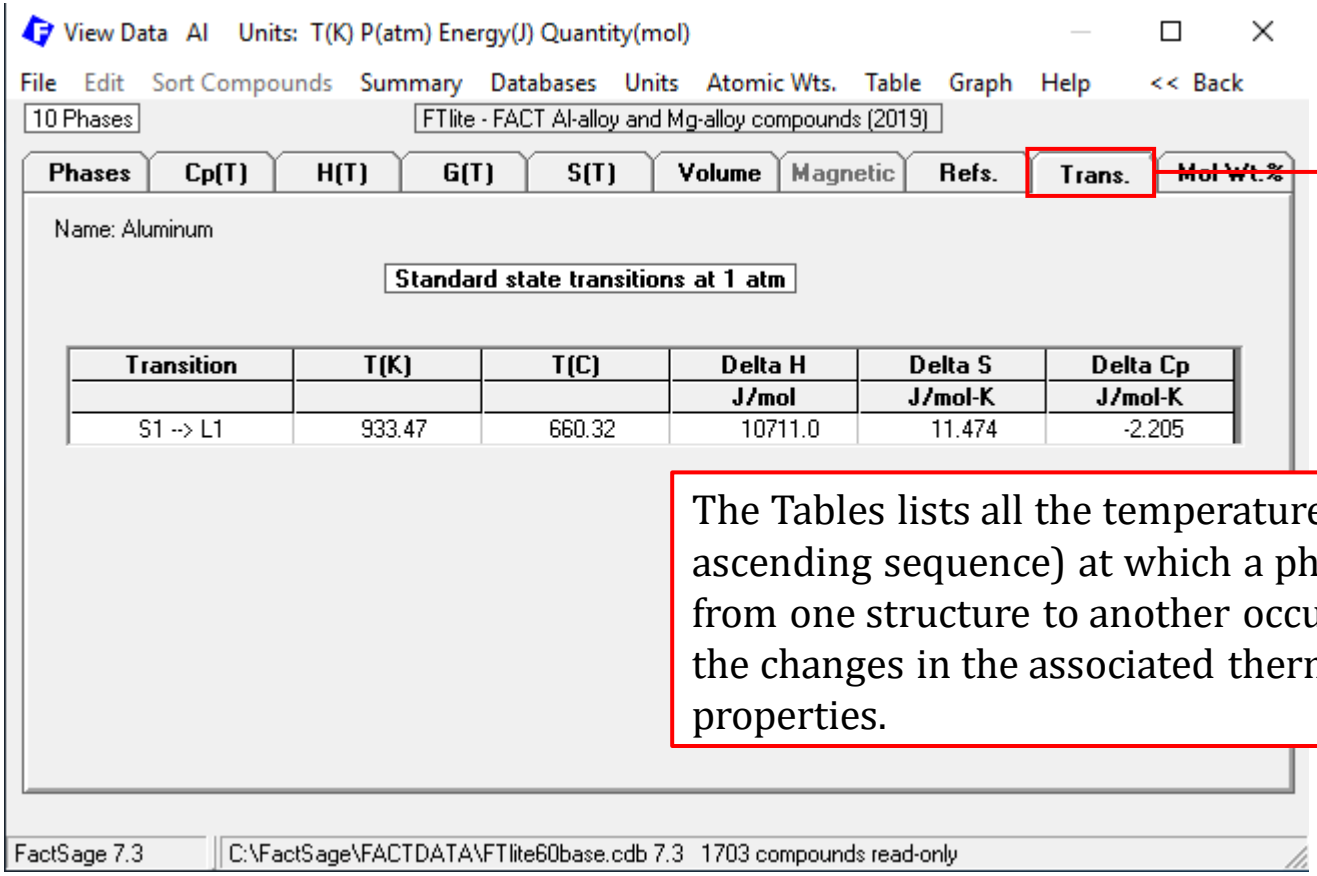


Although in many cases of MSE302 we are not interested in the volume properties, the temperature dependence of volume is described by the Expansivity.

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

View Data Module

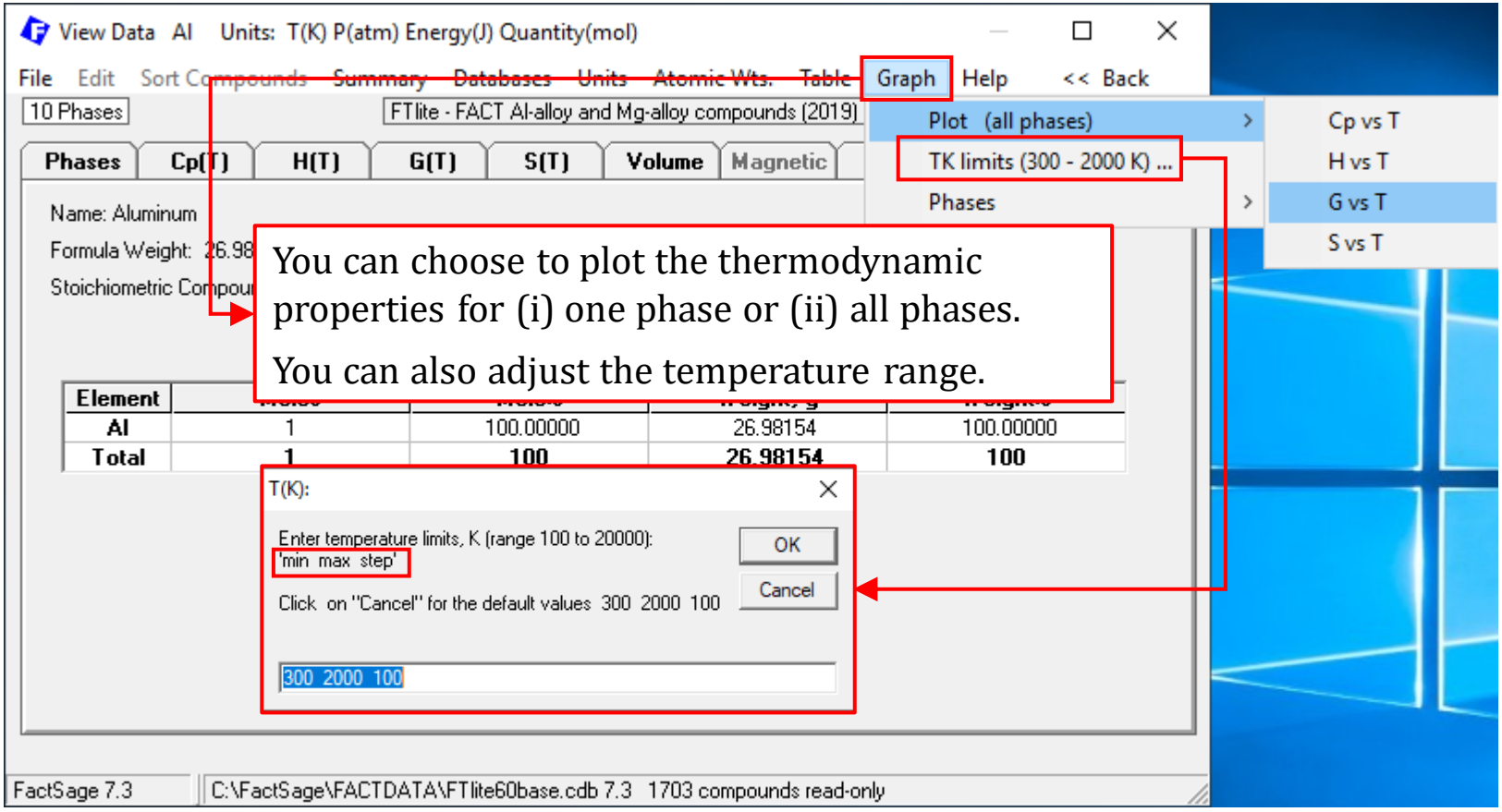
For example, say we wish to know for the Al-Mg system the thermodynamic properties of all the compounds that have been modeled in the FTlite database…



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.

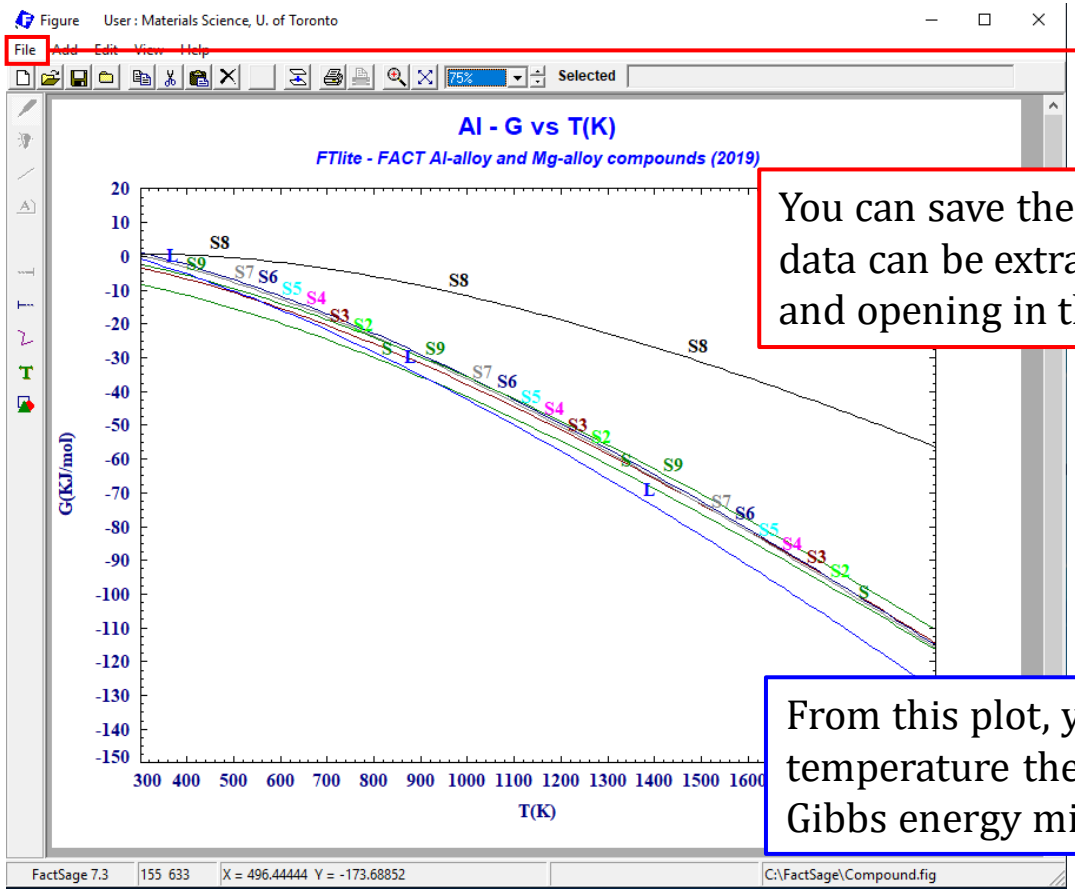
View Data Module

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.



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.

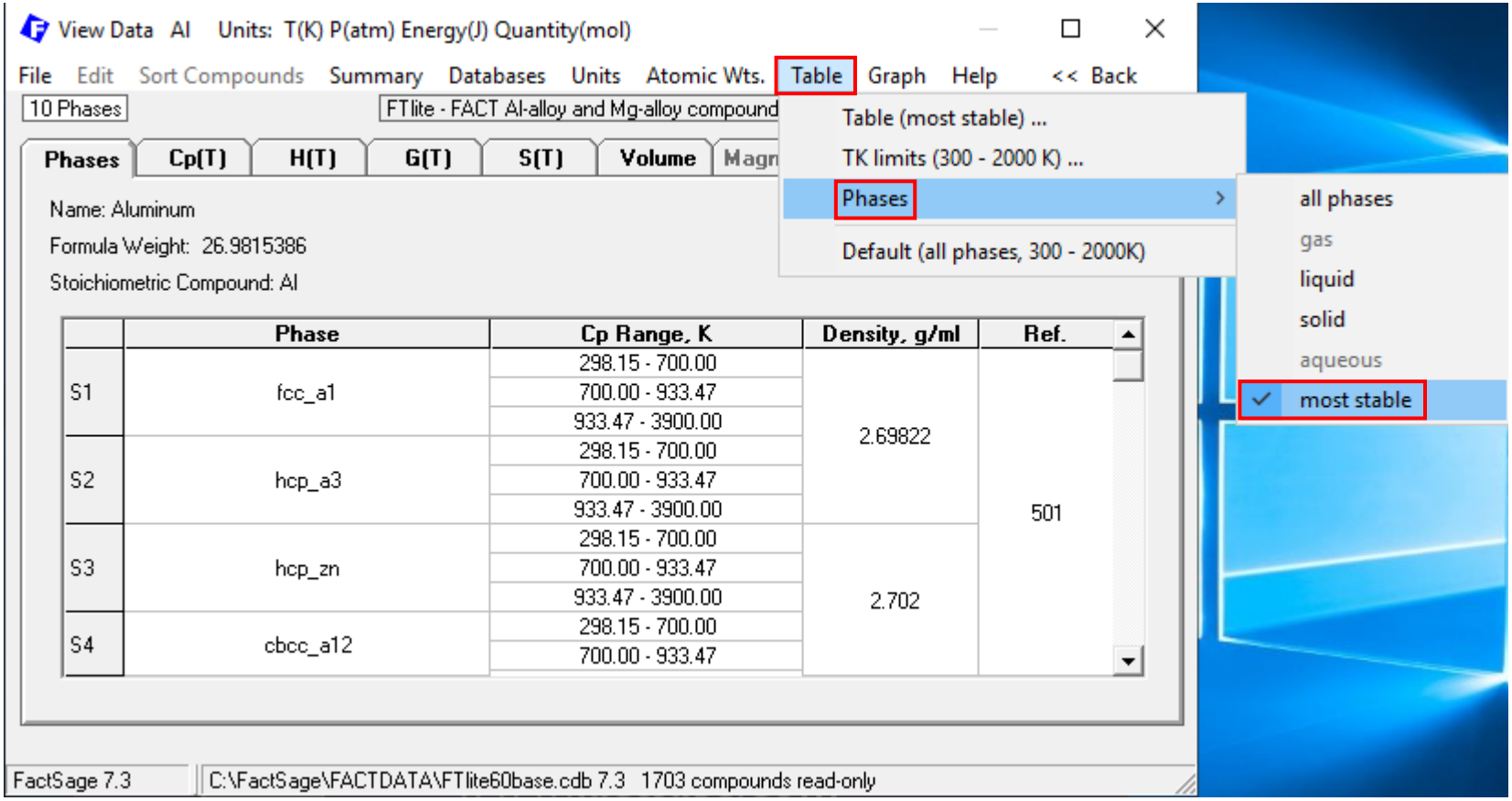


You can save the plot in the ".fig" format. The data can be extracted by changing the file to ".txt" and opening in the Notepad.

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

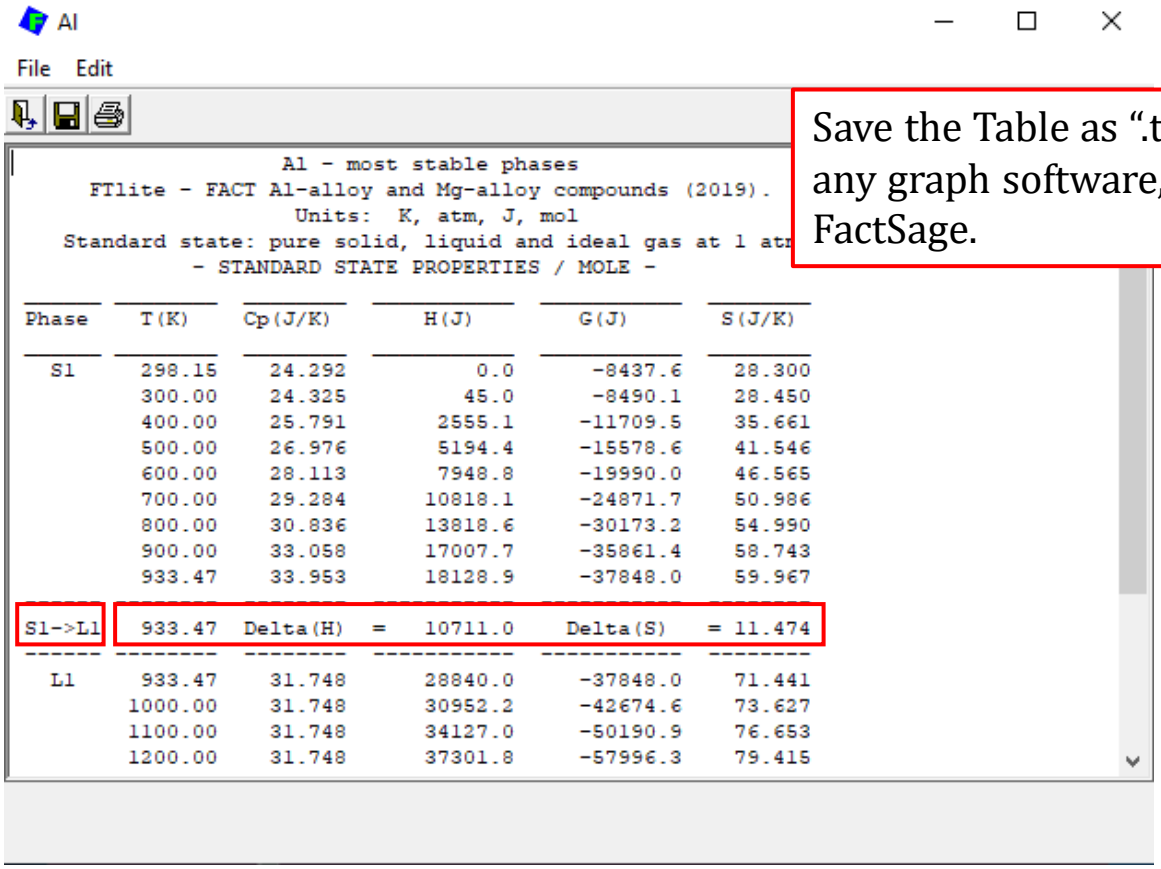
View Data Module

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”.



View Data Module

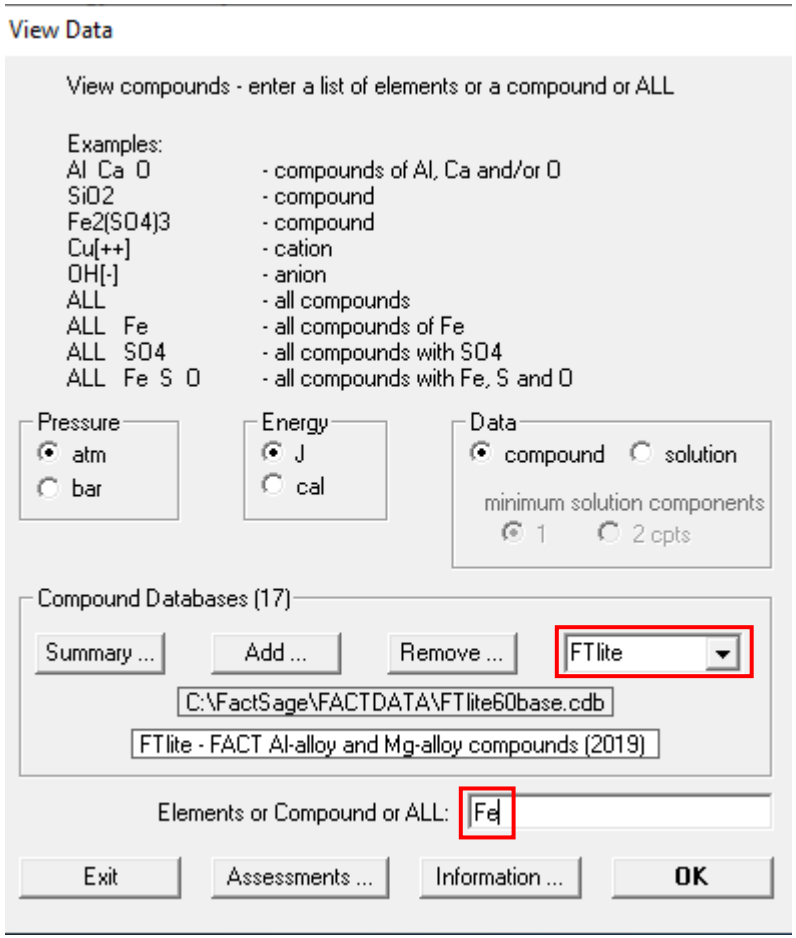
We can also tabulate the most stable phase only under a given temperature range. To do this, we need to set “Table\Phases\most stable”.



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

View Data Module

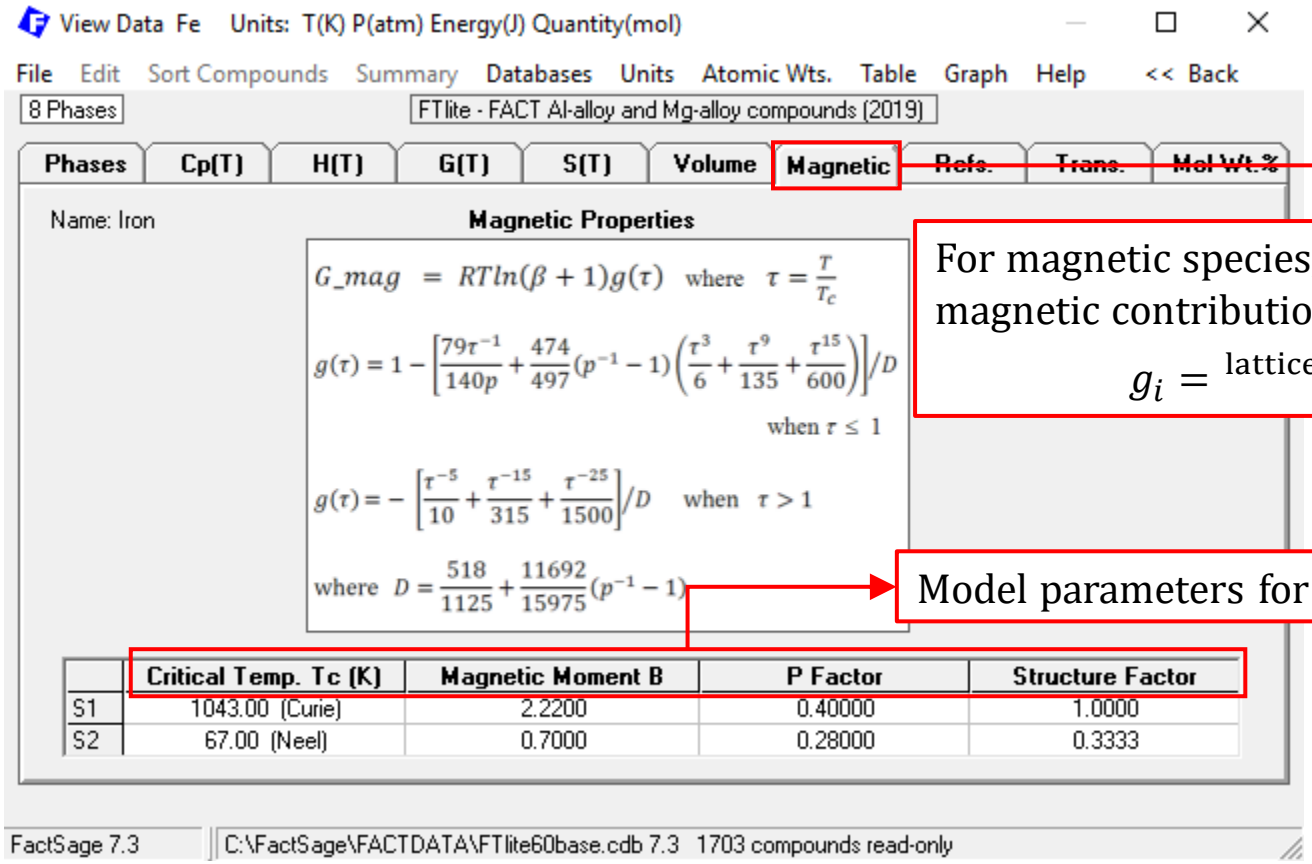
Now, let us view the thermodynamic data for a magnetic species: Fe.



View Data Module

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

Four model parameters are required to describe the magnetic contribution.



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

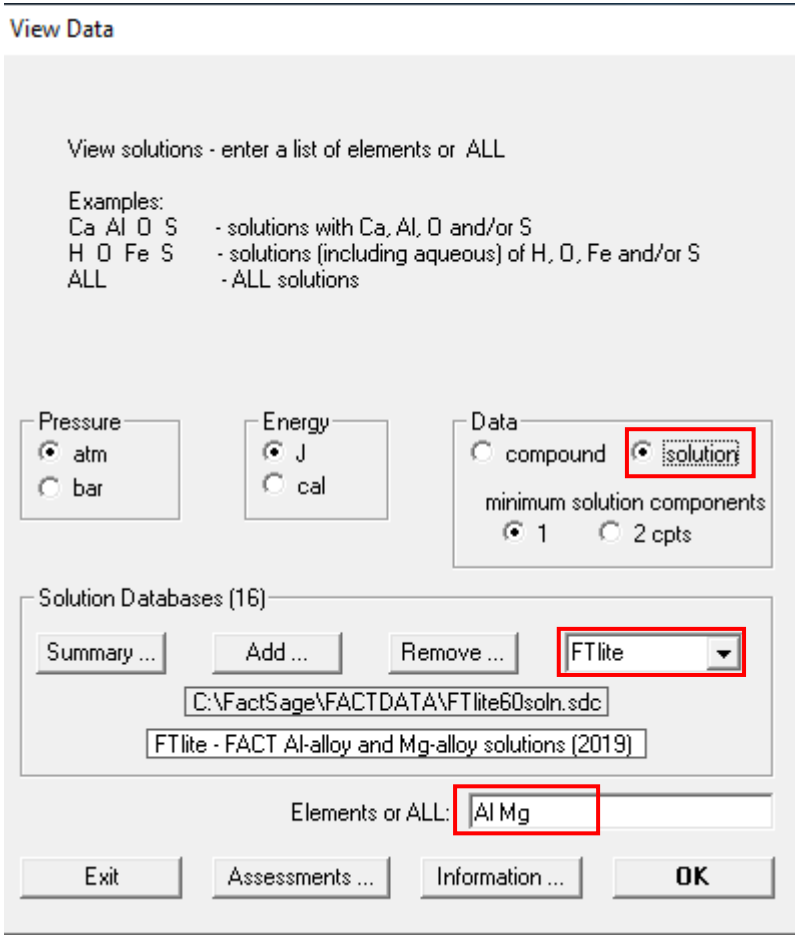
$$g_i = {}^{\text{lattice}}g_i + {}^{\text{magnetic}}g_i$$

Model parameters for magnetic species.

Pelton, Phase Diagrams and Thermodynamic Modeling of Solutions (Chapter 10)

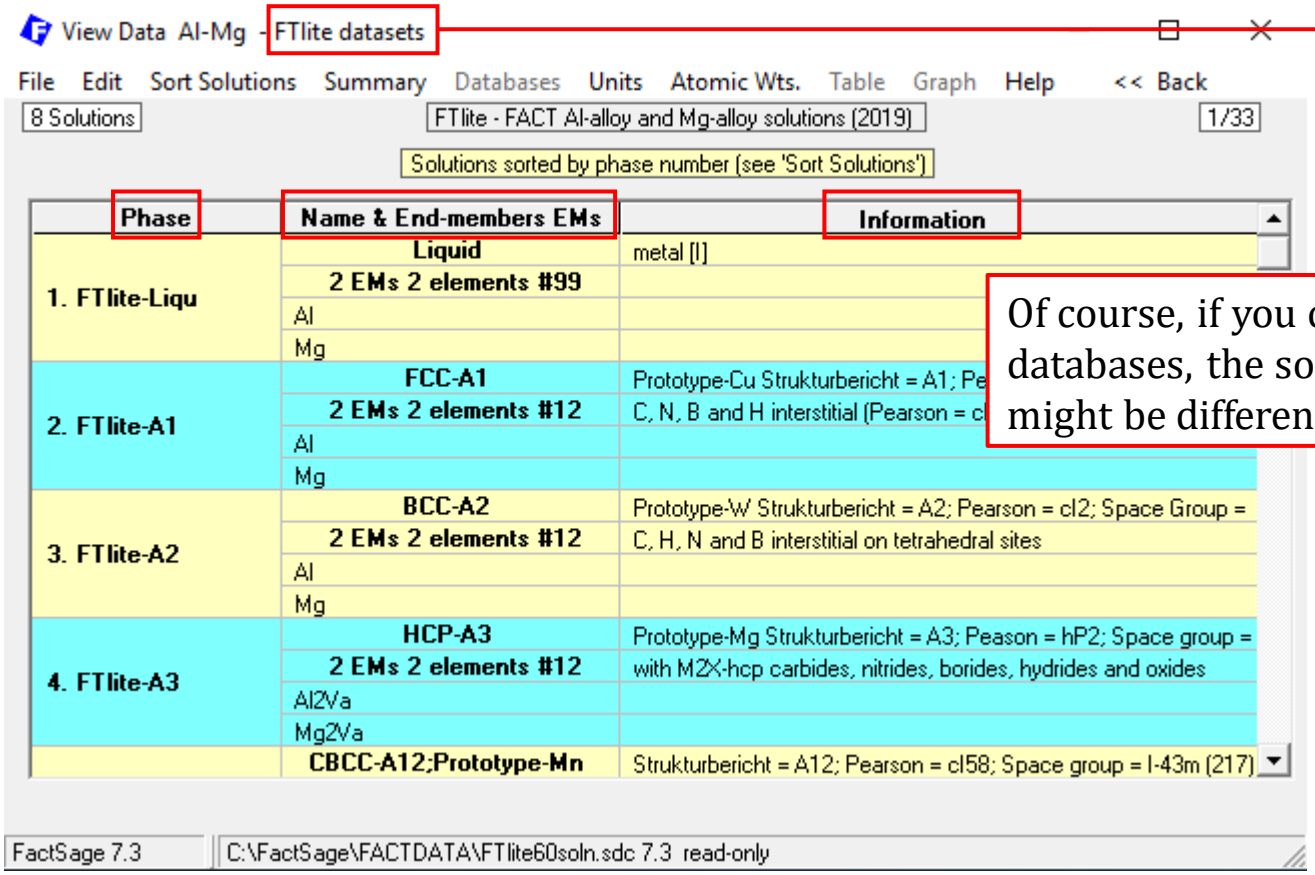
View Data Module

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 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)



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

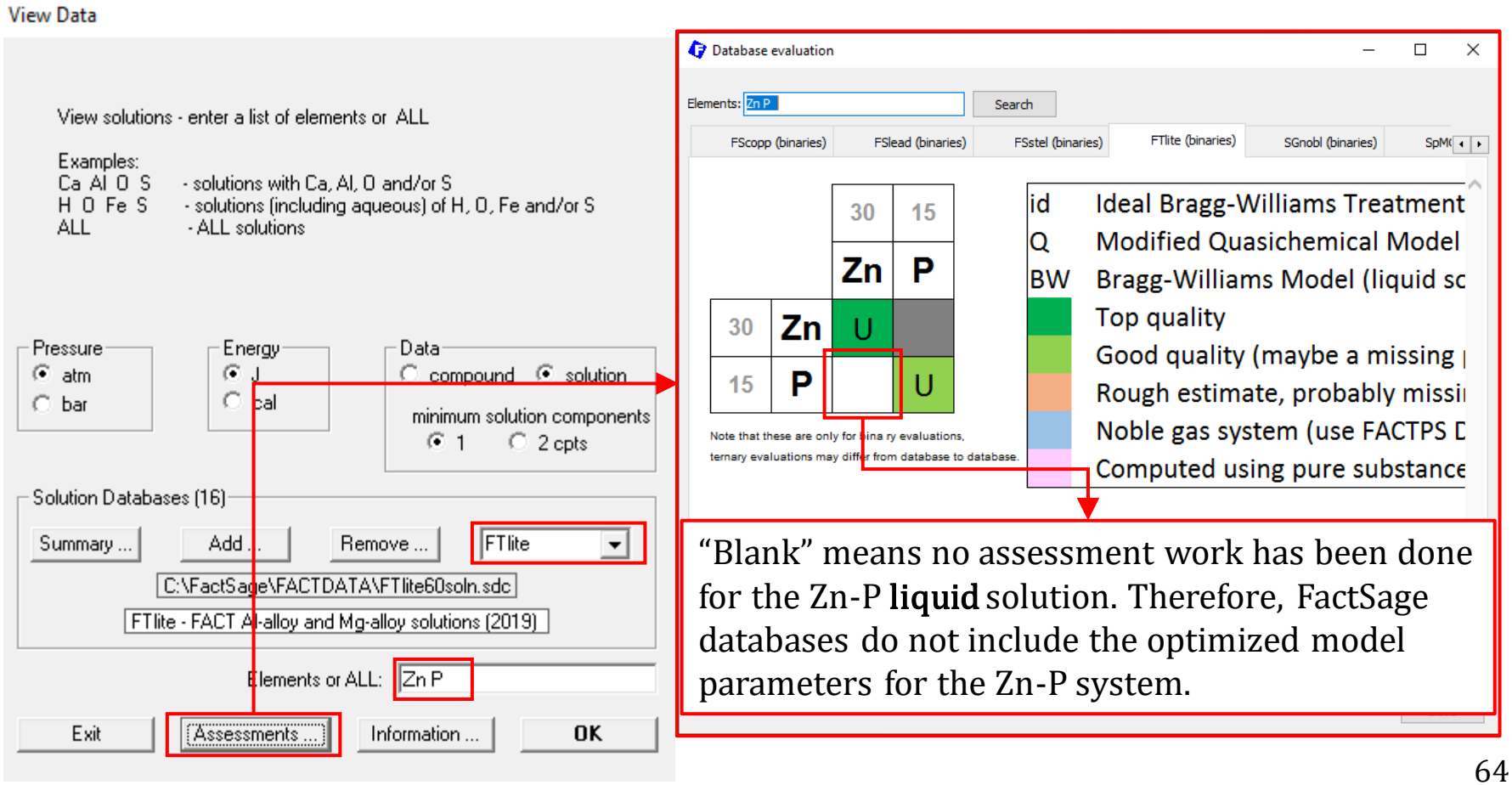
View Data Module

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.



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*NAME*DATA (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.