How to use
RCCM Gibbs energy Database for FactSage

Research Center of Computational Mechanics, Inc.
FactSage Support Team

Preface

RCCM Gibbs energy Database for FactSage (GeDb) is a collection of thermodynamic databases for FactSage. All of them are distributed free of charge.

GeDb can be used in FactSage Education package. Although FactSage Education package contains some public databases (FTlite, FToxid *etc*.), GeDb allows you to calculate equilibrium and phase diagram with the system that is not included these databases such as Nb-Re, Bi-Se, Ce-Pt.

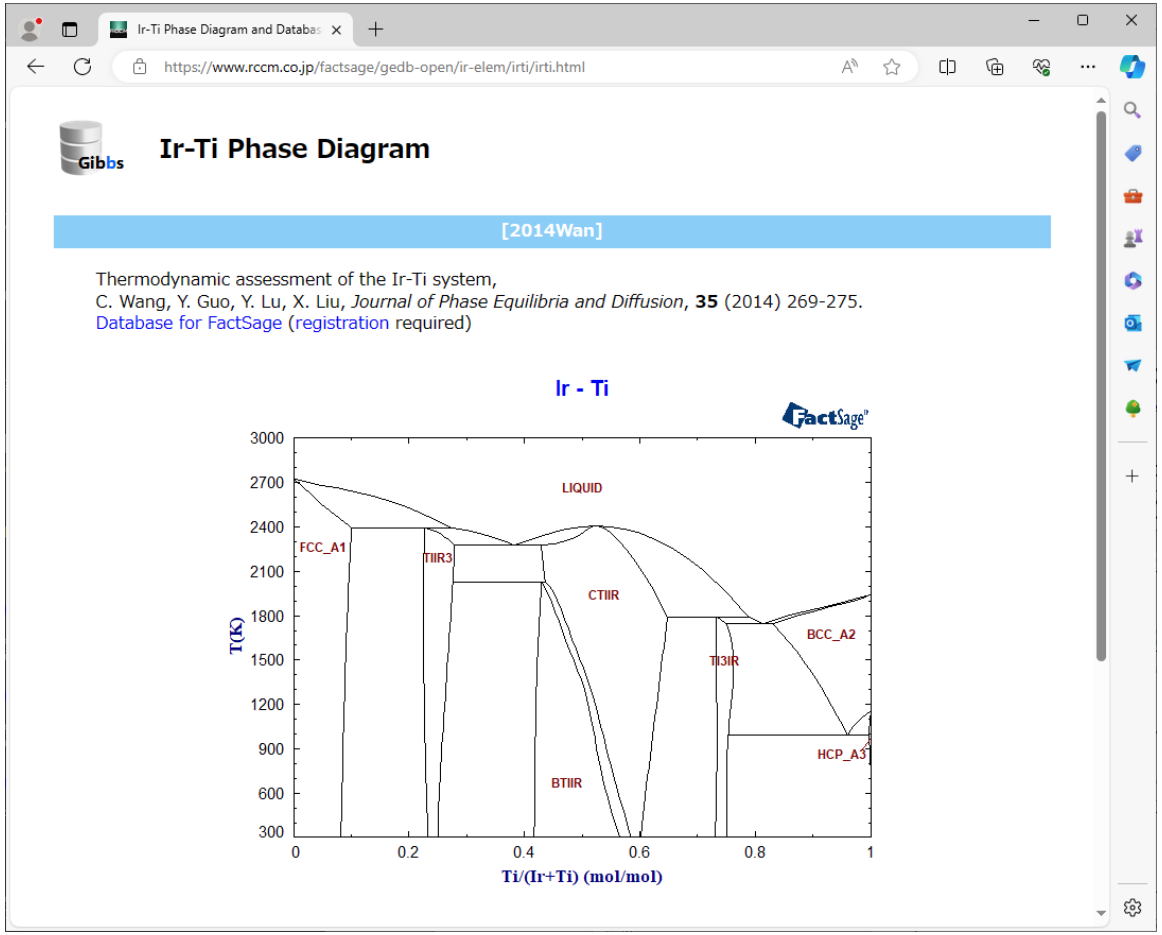
Furthermore, you can edit parameters in the databases using Compound and Solution apps in FactSage Education. By changing the parameters, please look at the changes in the calculated phase diagram. This will give you a deeper understanding of the thermodynamic database.

RCCM FactSage Support Team

1. Installing the Thermodynamic Database

Installing the Thermodynamic Databases

Download the Ir-Ti system database from GeDb to your desktop in advance.
Here after, the steps is shown to add this database to FactSage Education.
Of course, the same procedure is applicable for the full FactSage package.



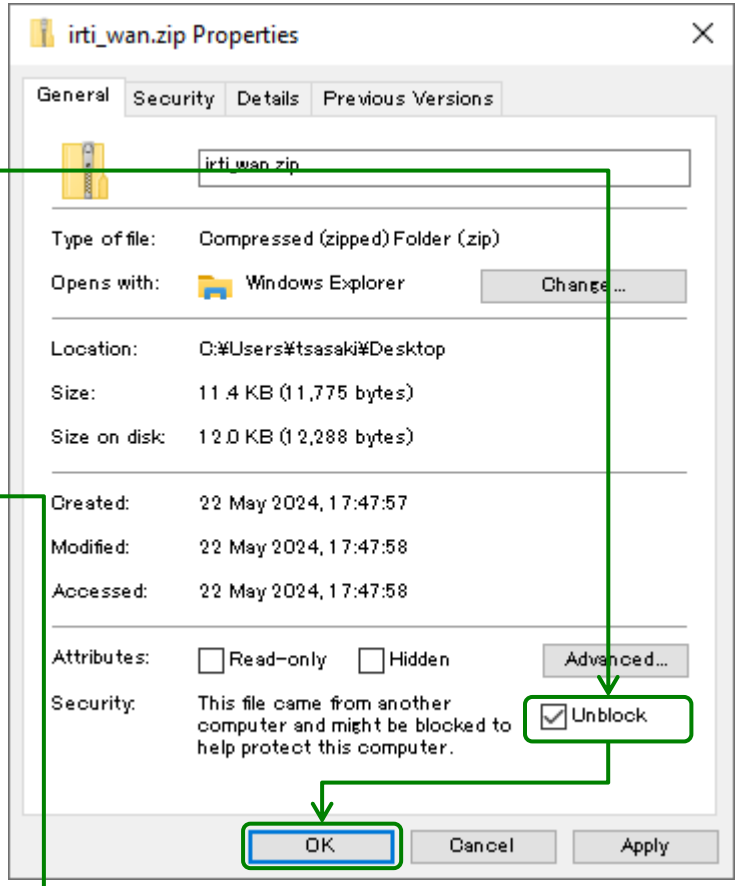
Ir-Ti thermodynamic database saved on the desktop

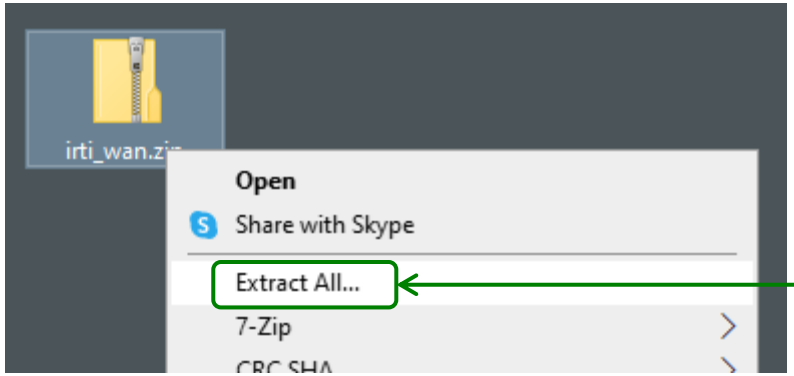
Installing the Thermodynamic Databases

1. Right-click on the downloaded zip file ⇒ properties.

2. Check “Unblock" in Security and click OK.

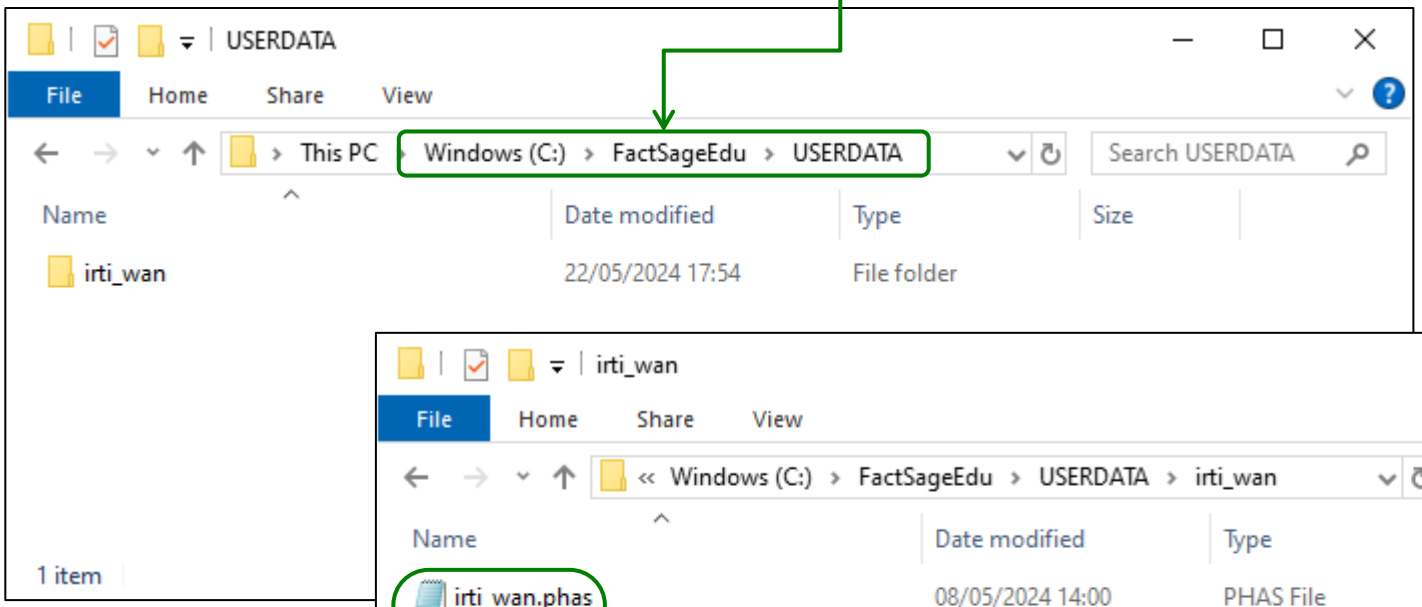
3. Right-click on the downloaded zip file ⇒ Extract All …

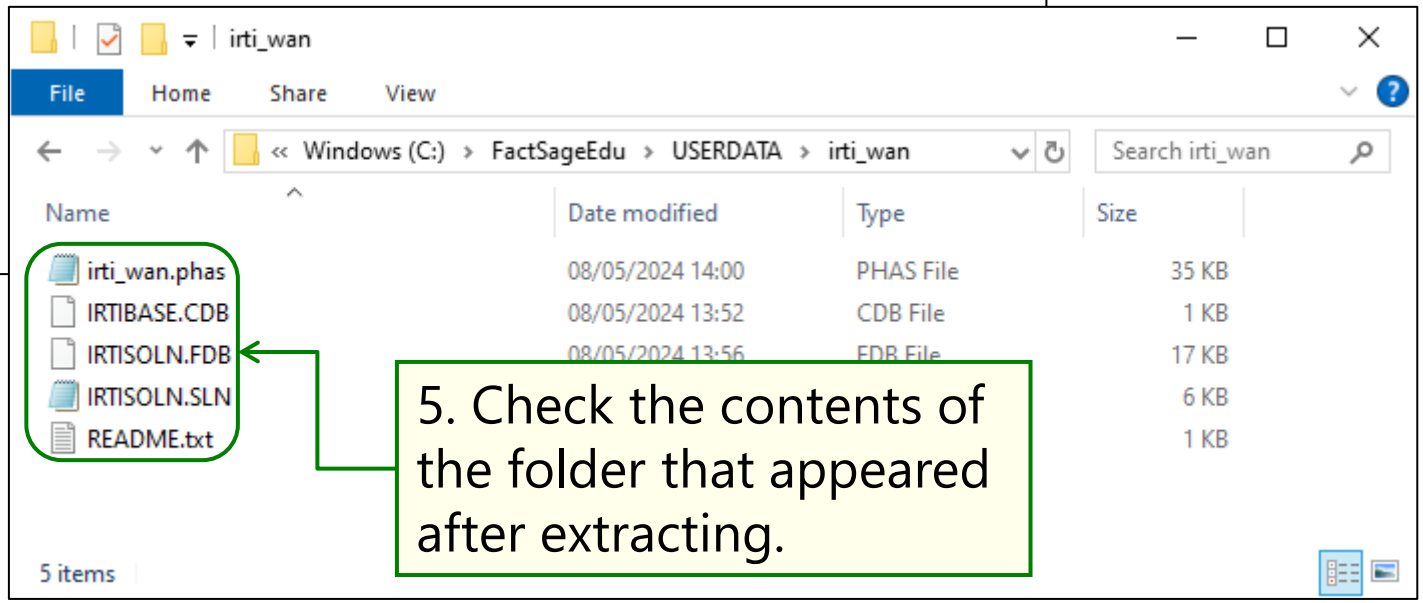




Installing the Thermodynamic Databases

4. Save the extracted folder in the FactSage or FactSage Education installation folder. You can make subfolders in the installation folder. However, the folder name must be alphanumeric (*i.e.*, not include any Japanese characters). In the example below, a new subfolder named USERDATA is created and saved.

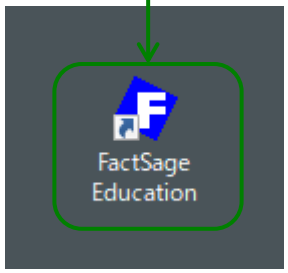




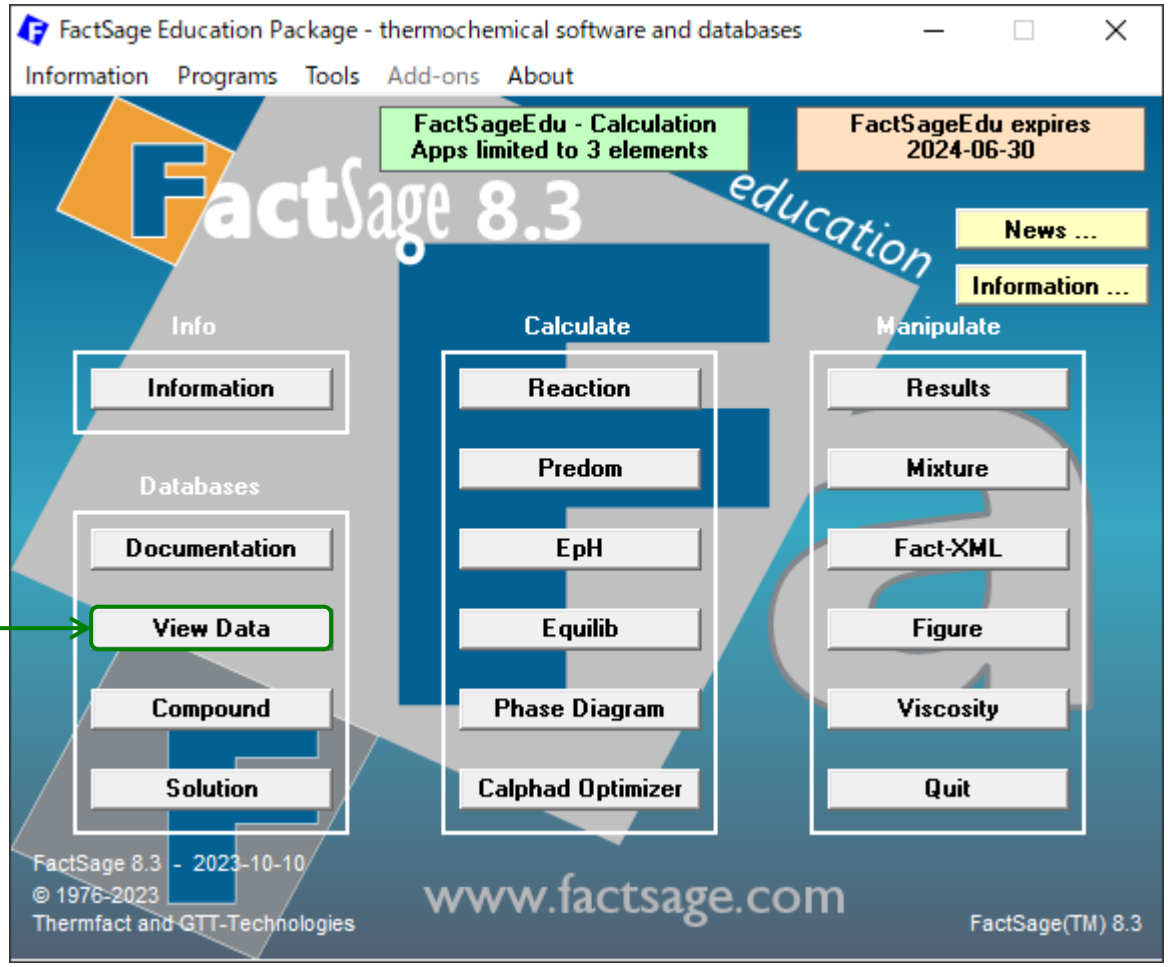
5. Check the contents of the folder that appeared after extracting.

Installing the Thermodynamic Databases

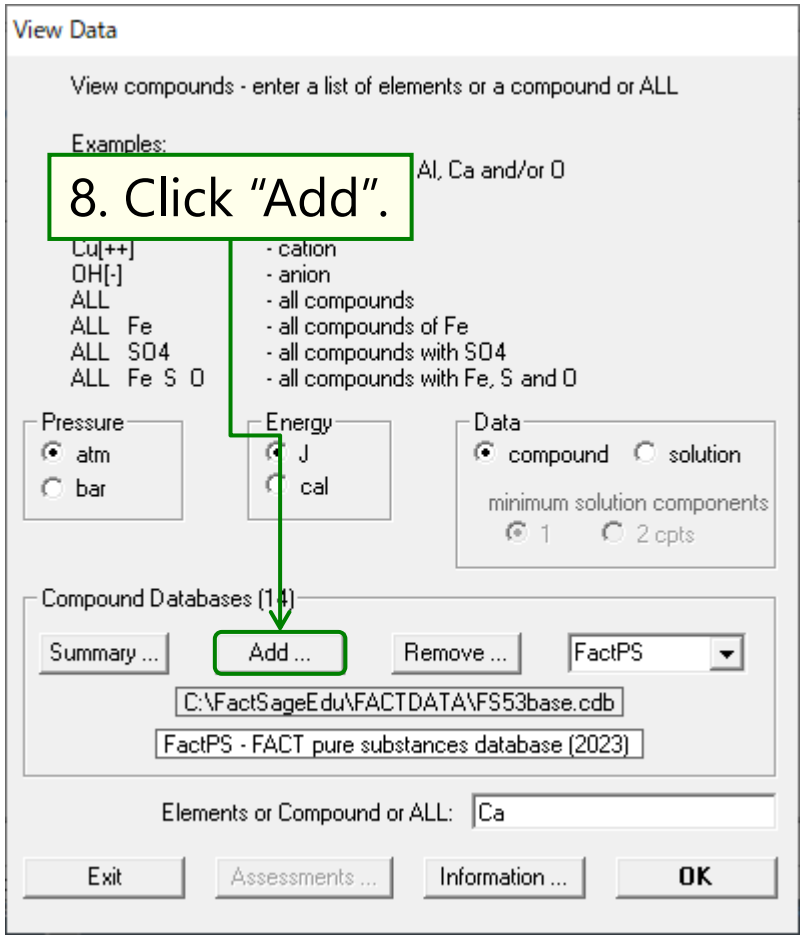
6. Launch FactSage Education.



7. Start View Data.

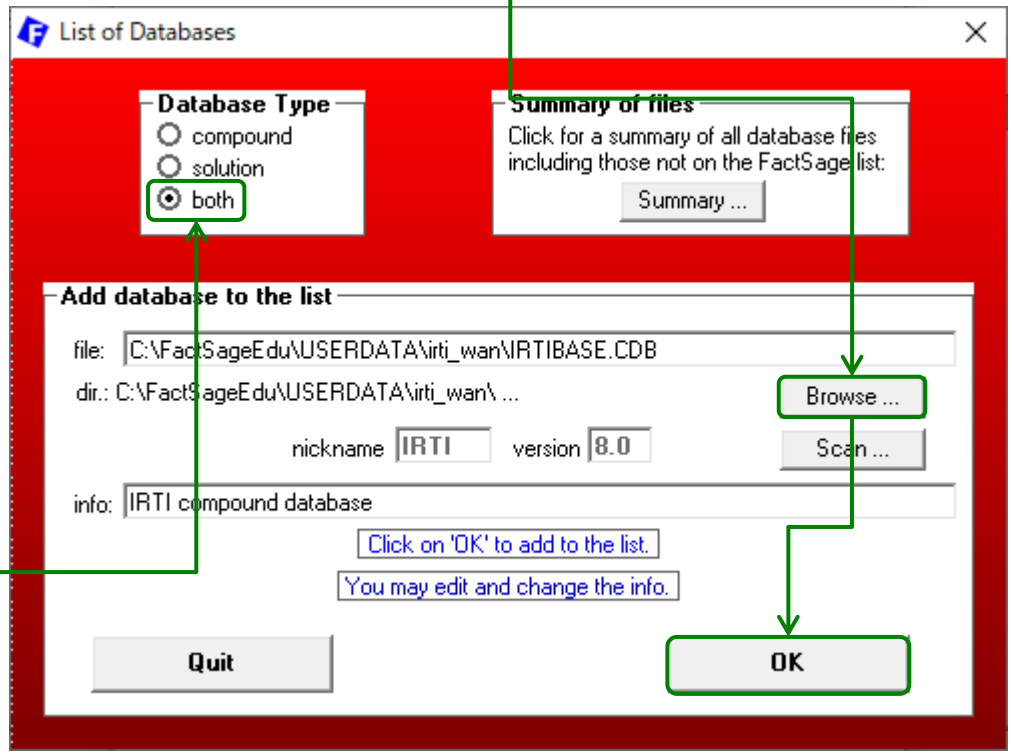


Installing the Thermodynamic Databases



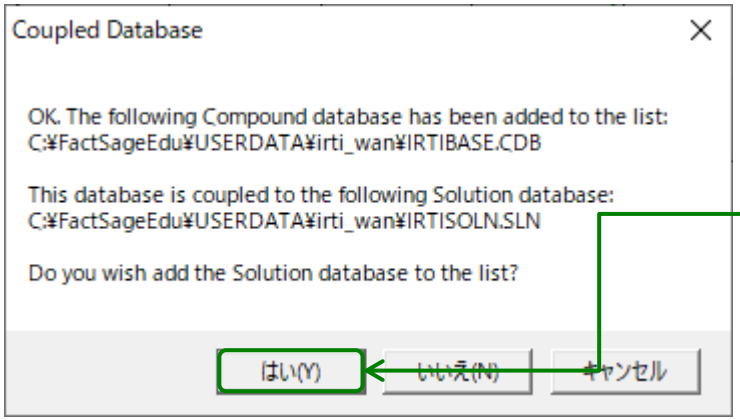
8. Click "Add".

10. Click "Browse" ⇒ Select the database file (IRTIBASE.CDB) and click "OK". You can also select IRTISOLN.SLN instead. Either one is fine.



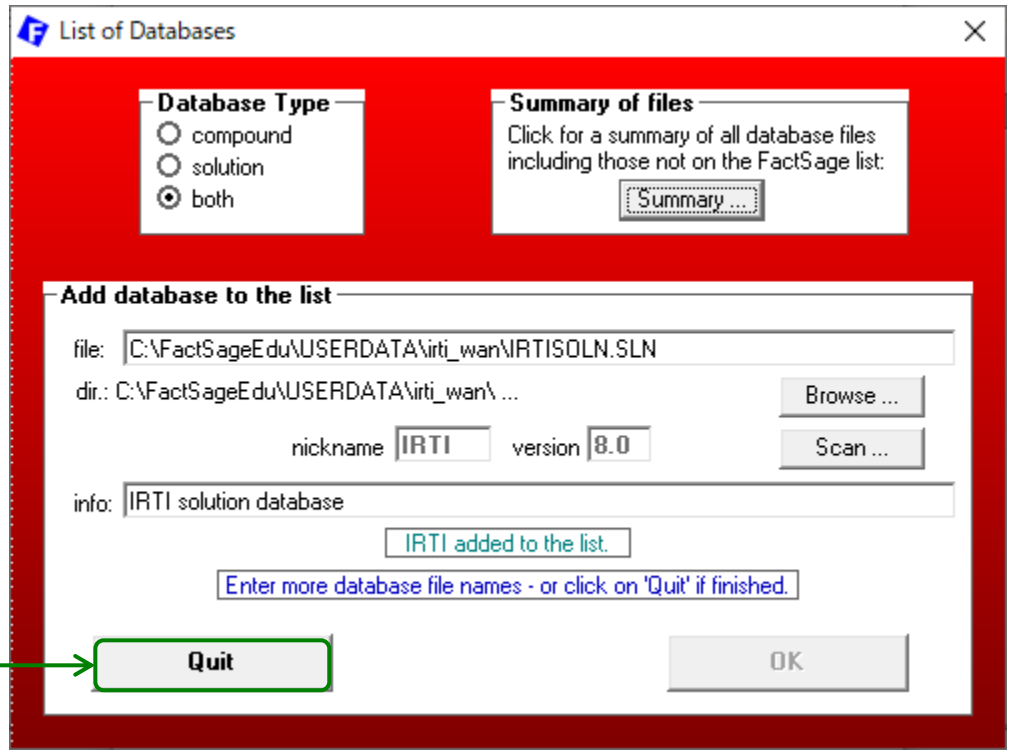
9. Select "both".

Installing the Thermodynamic Databases



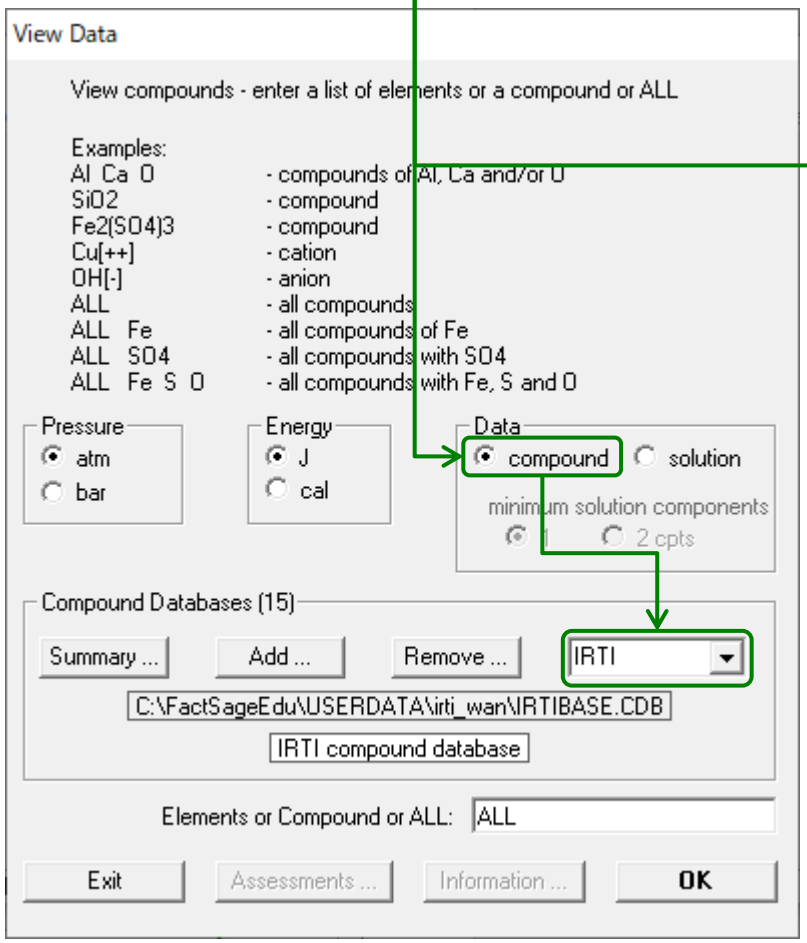
11. Click "Yes" to add both of compound and solution databases at the same time. It will take a few seconds.

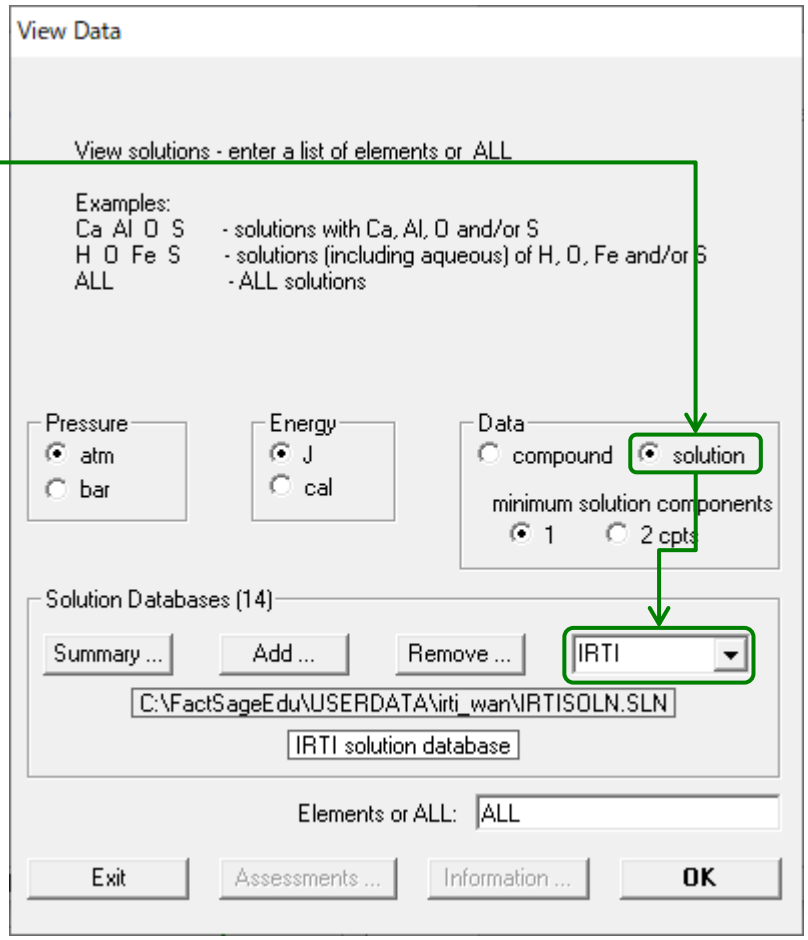
12. Click “Quit”.



Installing the Thermodynamic Databases

13. Verify that IRTI database is added.





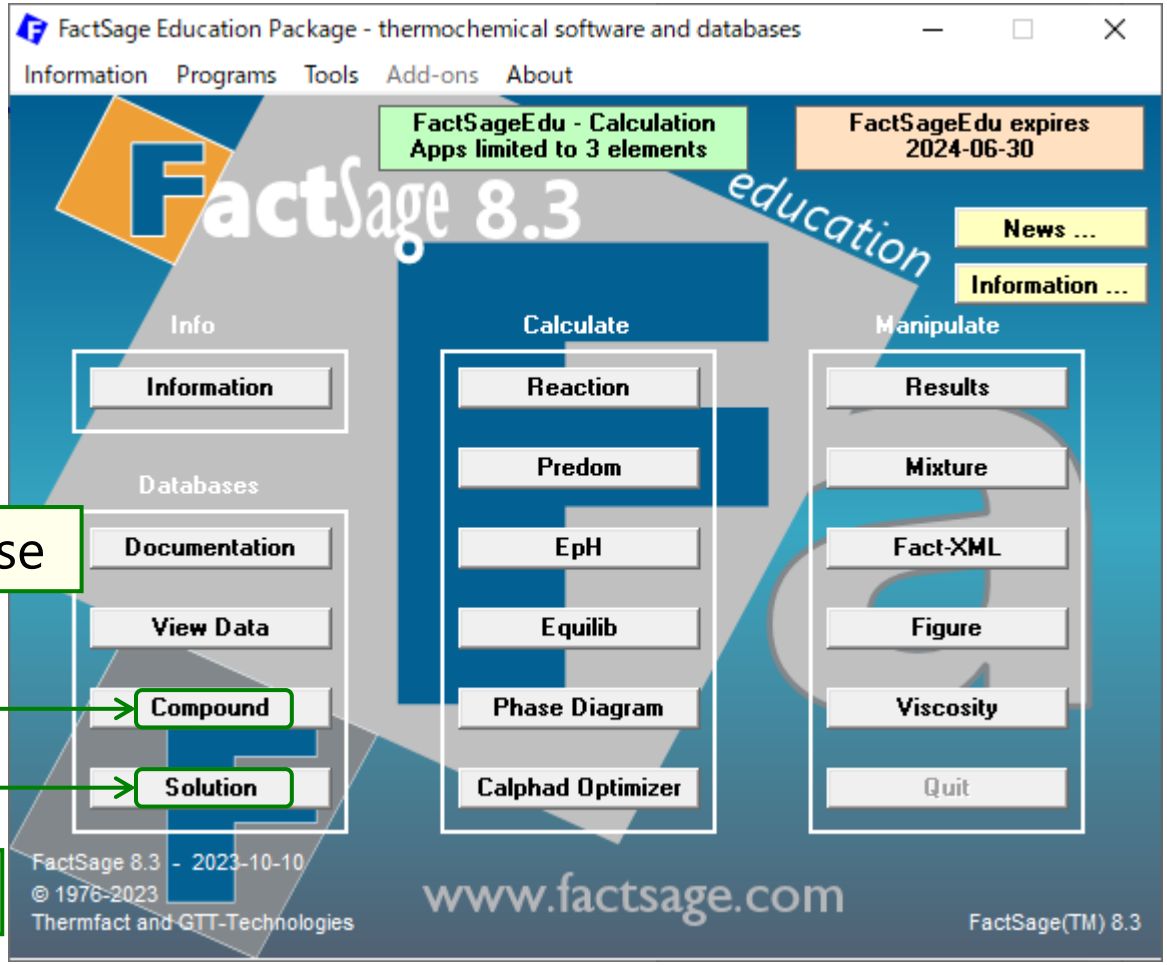
Installing the Thermodynamic Databases

You can edit thermodynamic databases by Compound and Solution apps. Here, we look at the contents of the database (details on how to use the apps are omitted).

Note: IRTI database consists only of solution phases, hence IRTI compound database is empty.

Editing compound database

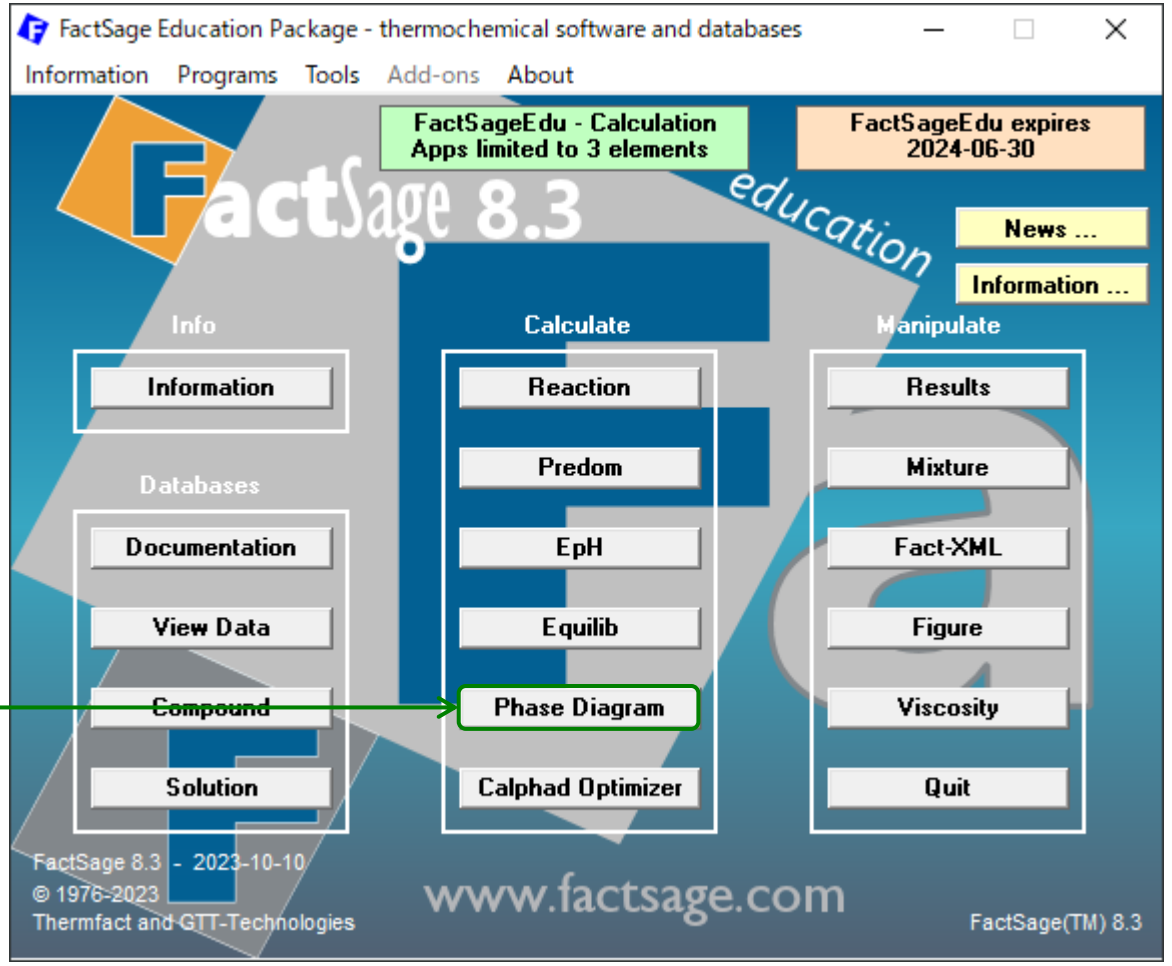
Editing solution database



2. Phase Diagram
（Using configuration files）

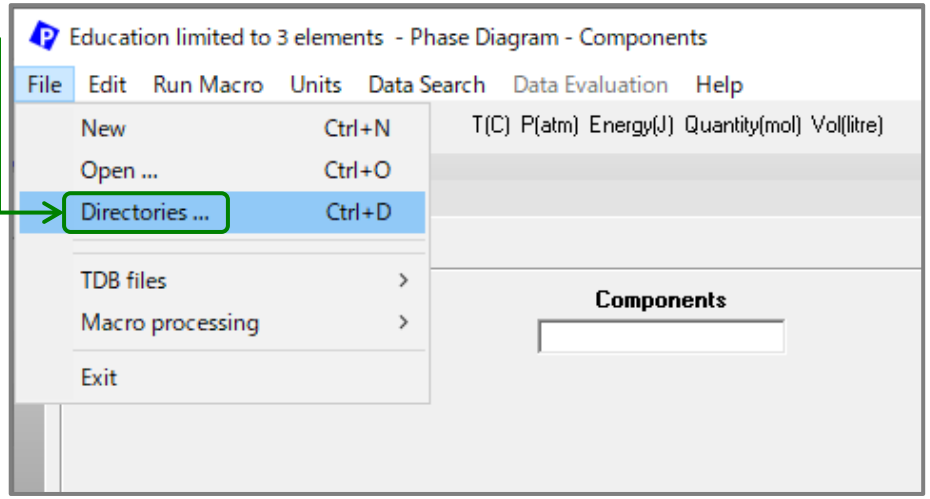
Phase Diagram（Using configuration files）

1. Launch “Phase Diagram”.

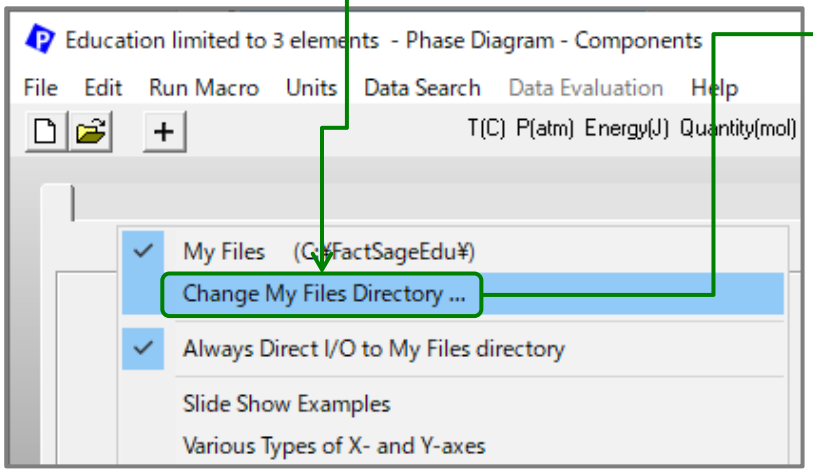


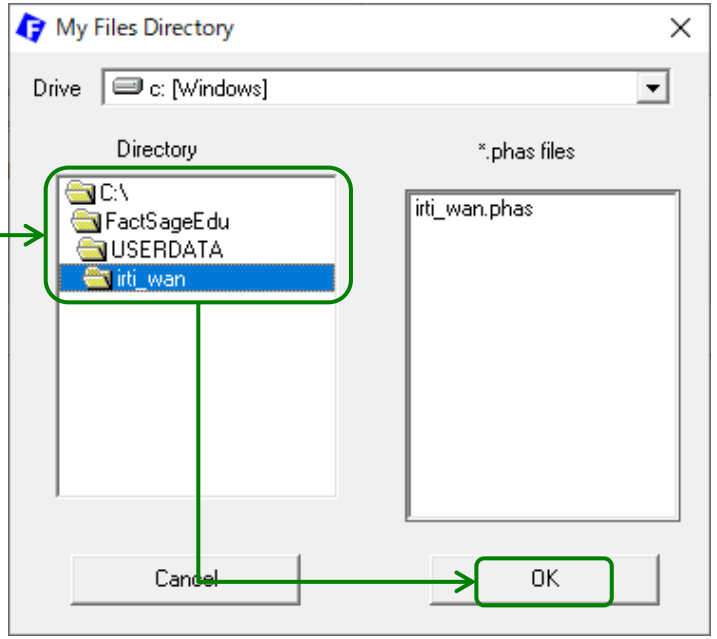
Phase Diagram（Using configuration files）

2. Click “File ⇒ Directories”.



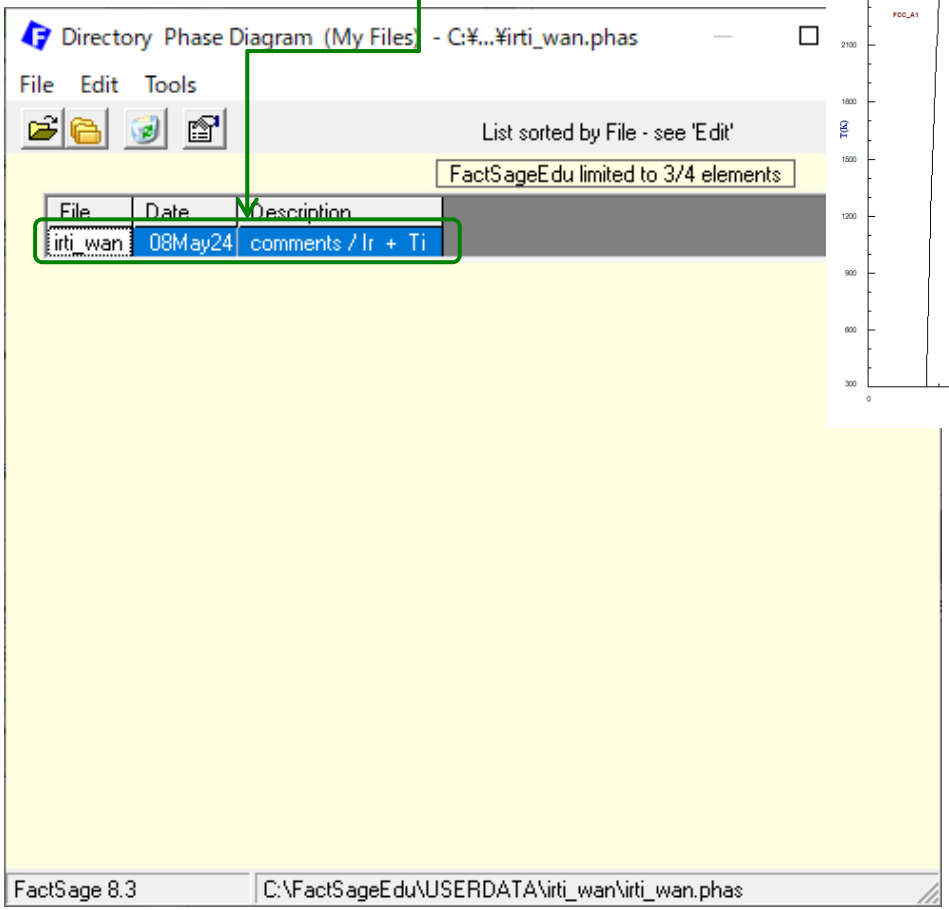
3. Click “Change My Files Directory ...”. Find and double-click the folder in which IRTI database is saved. Then click “OK”.

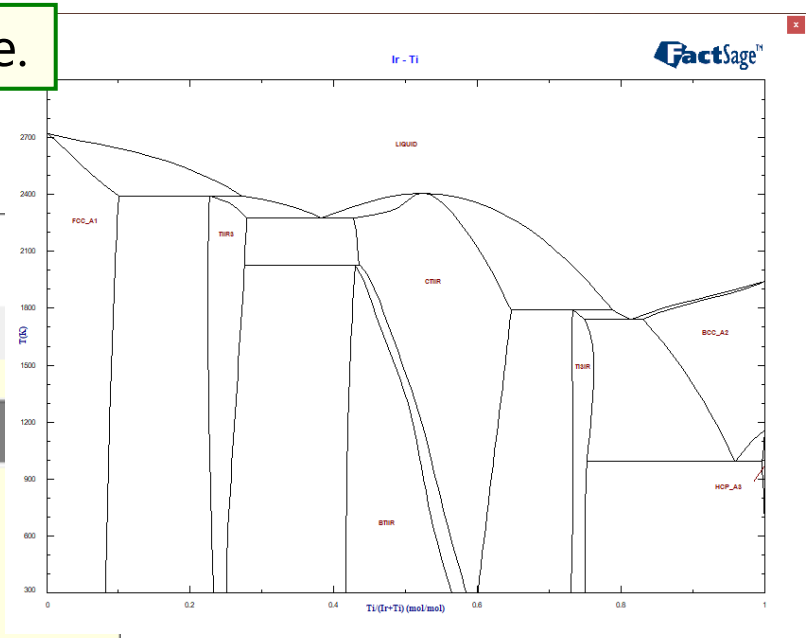


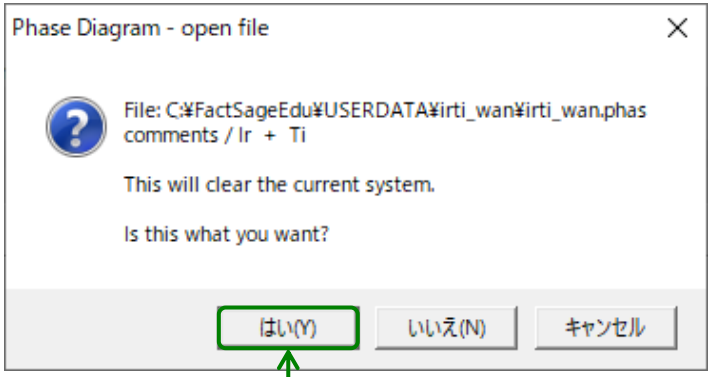


Phase Diagram（Using configuration files）

4. Double-click the configuration file.





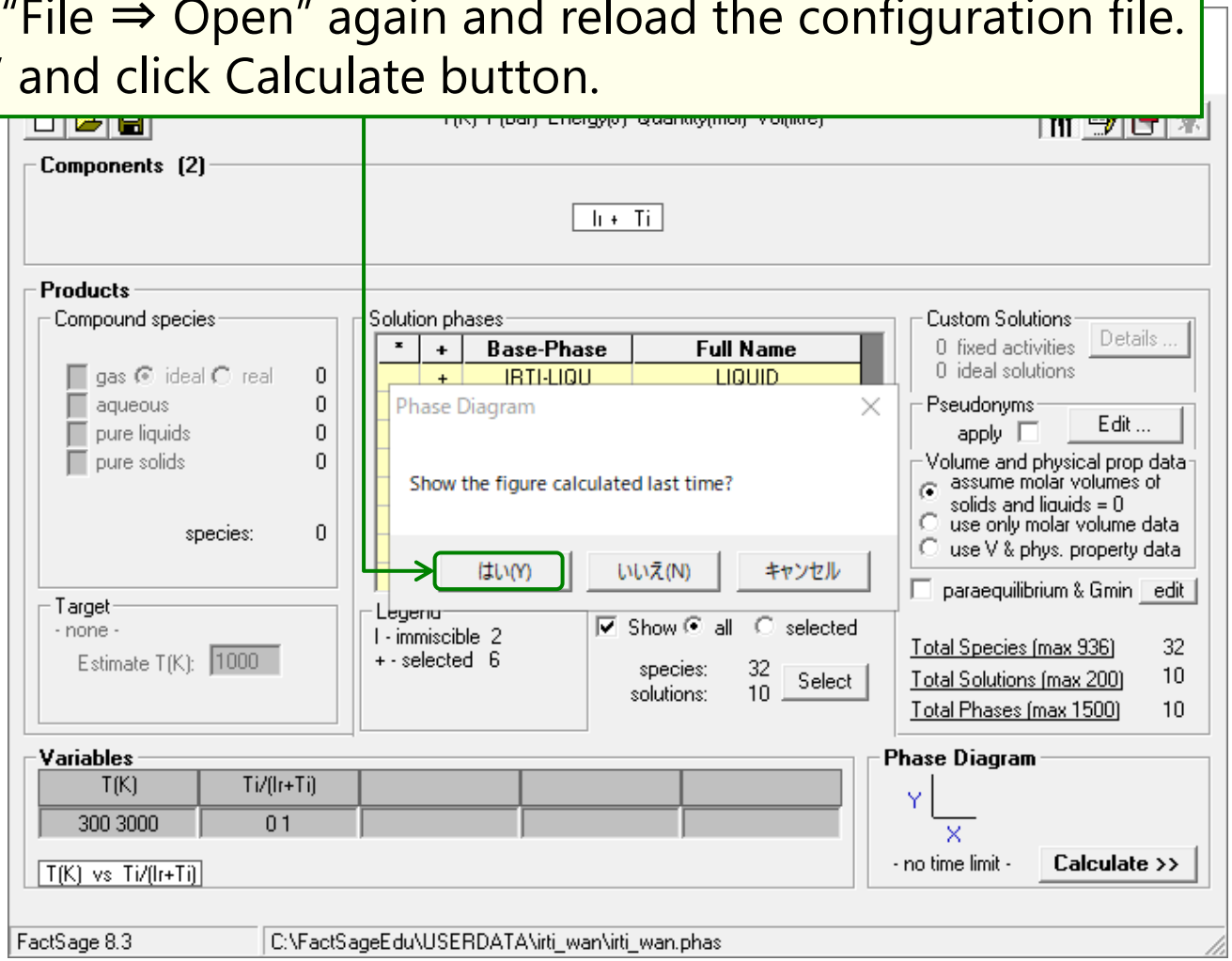


5. Click “Yes” to clear the current setting for the calculation.

Phase Diagram（Using configuration files）

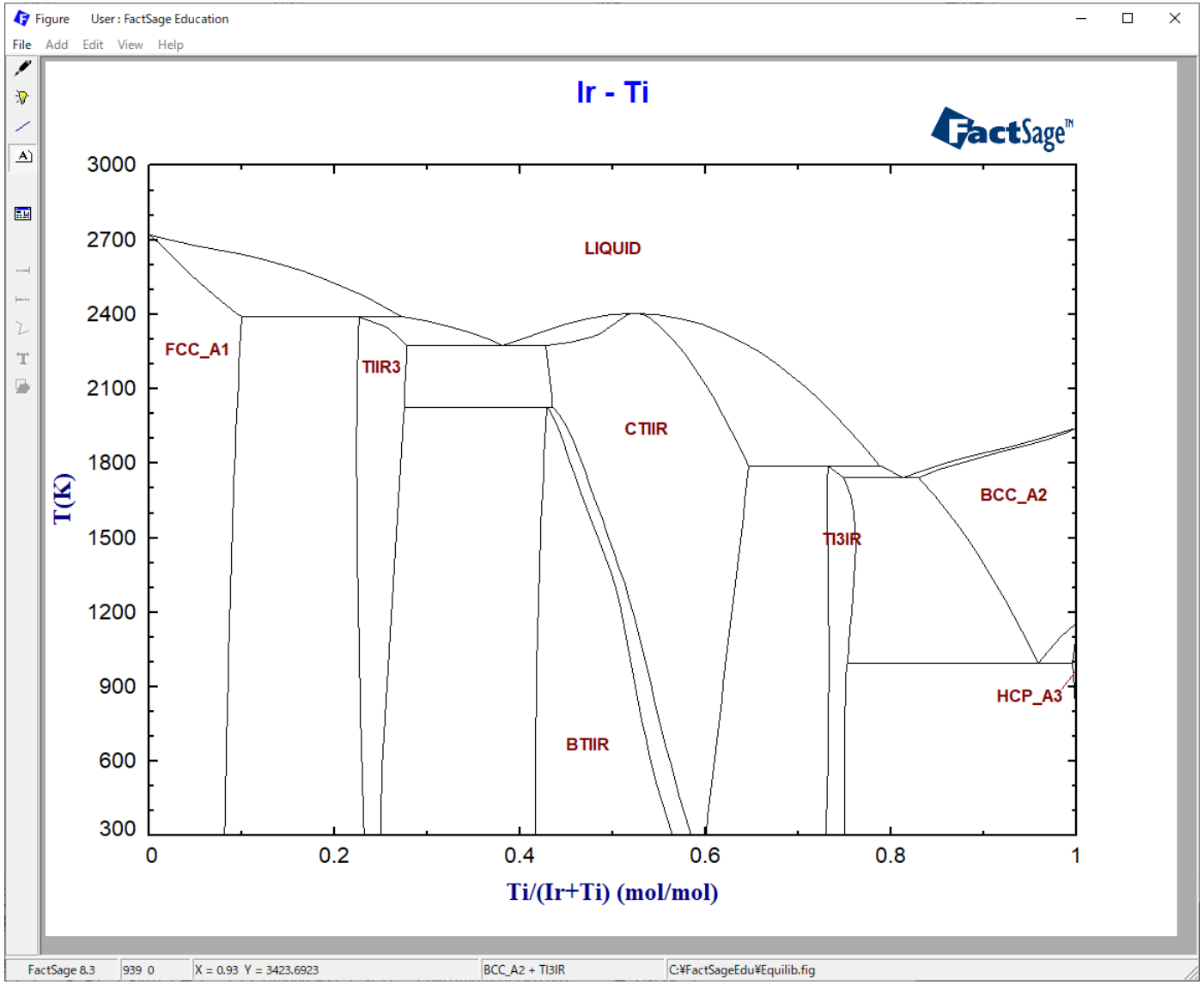
6. Click “Yes” to show the phase diagram stored in the *.phas file.

If the message “- no product species selected” was shown and any figure did not appear, click “File ⇒ Open” again and reload the configuration file. Otherwise, click “No” and click Calculate button.



Phase Diagram（Using configuration files）

Displayed phase diagram



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