CaTCalcXE

<u>C</u>hemical <u>a</u>nd <u>T</u>hermodynamic Equilibrium <u>Calc</u>ulator

Expert Edition

User's Manual

Ver. 2.9

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I. Overview

This software solves the equilibrium problem in chemical thermodynamics using the Gibbs Energy Minimization Method. A number of similar software programs have already been developed, but there still remain many problems to be aware of, especially in the case of ceramic systems. It is very easy to make mistakes unless the user is well versed in the software. This software has been developed mainly to improve this problem, with emphasis on reliability, quality and ease of use, which is necessary for a software tool used in various researches.

- The software can automatically and correctly calculate not only metals, but also ceramics and intermetallic compounds. It is not necessary to select stable phases prior to the calculation. Phase separation and global minimization problem is automatically handled.
- 2. A highly reliable algorithm that considers the problems in numerical computations, such as rounding errors, loss of trailing digits, etc., is successfully developed. The algorithm is also strong in calculation in which trace elements are important.
- 3. Various standard thermodynamic solution models are supported.
- 4. Uniformity of operation.
- Various calculation functions such as target calculation and solidification simulation, as well as the creation of phase diagrams, potential diagrams, and liquidus univariant-line projections of multicomponent systems.
- 6. Thermodynamic data assessment module is incorporated which is easy to use even for non-expert users.

Limitations of the Demo version

The number of elements that can be handled is limited to three.

II. Installation

【Requirements】

- 1. Windows 10 or later. 64bit version only.
- 2. Display resolution is 1280*728 or higher. <u>There may be a problem when a custom scale</u> <u>factor is set for Display setting in Windows. In such a case, please set it to 100%.</u>
- 3. Required HD space: about 100M bytes or more.
- 4. Memory: 1G bytes or more, the more the better.
- 5. Spreadsheet software such as Excel, LibreOffice-Calc, etc.

【Installation procedure】

- 1. Use the installer.
- 2. A CaTCalcXE folder will be created in the Documents folder of the user folder. In this folder, folders are created for storing thermodynamic data, calculation results, etc., which may or may not include the following:

Data: The default folder where thermodynamic data files are stored. However, data from any other folder can also be used.

Material: Files that define materials (mixtures) are stored

Macro: Storing Macro Files

Manual: Storing Database Manuals

Results: A standard folder for storing calculation results. However, it is recommended to create a dedicated folder for each subjects.

- 3. Shortcuts are registered to the desktop and start menu.
- 4. Software Activation: You need the license.dat file in the same folder as the program. Also, you need to install a USB-dongle.

III. Preference setting

First of all, we recommend that you set up the appearance and font setting of the software. After starting the software, the setting screen will be opened by clicking [File]-[Preference] of the main screen menu. Select Appearance in particular according to your preference.

Options	×
Output Defaults Show sublattice site-fractions Show only active (stable) phases Display-cutoff for small fractions if N>16 Use mol of atoms (gram-atoms) for all phases. Note that input is fixed to mol of formula units. Display element fractions of pure phases Use molality in aqueous system Show driving-force rather than activity Default number of digits to display values 7 Scheil Cooling Option Stop calculation if amount of the parent phase <1E-3	Miscellaneous Check Gibbs energy continuity when importing TDB files Energy shift for ordered phase (Only in PD calc) <u>5E-8</u> Special check for 4-Split-Sublattice phase model Save-mode rather than Copy-mode Save redundant phase information Logo at the top-right corner Resize chart to display legend Check for updates on start-up Set time limit in one boundary calculation (sec) <u>60</u>
Appearance and Default Font in Plot Appearance Amethyst Kamri Font Name Size Verdana 12 Font Text Editor External Text Editor C:¥Program Files¥Hidemaru¥Hidemaru.exe F	ParaEquilibrium (Partial Equilibrium) Setting Interstitial Fast Diffusing Elements C, N, O, B, H Apply/Save Cancel

This software is designed in such a way that you do not need to refer to the manual when using it. If you are unsure of how to use the software, try the pop-up menu that appears when you press the mouse right button. Many functions are available.

For more information about the operation, please refer to the sample Project calculations. When you doubleclick on the calculation result to load it, the calculation conditions will be reset.

IV. Display screen and Menu

IV-1. Main Screen

Explanation of the main screen

1	CaTCalc XE		
	File Edit Calculation Assessment Databases		
2		🔌 System 🛛 🔍 Data 🛛 🔛 Calculation 🛛 📾 Assessment 🔢 🧿 Exit	
	Project	Summary	
	4	5	
		6	

- ① Menu bar
- ② List of Project folders
- ③ Application menu
- ④ Project panel: three different tabs are displayed depending on the situation.
- (5) Viewer Panel: Three different tabs are displayed depending on the situation.
- ⑥ Note panel: displays supplementary information and notes for calculations

1 Menu bar

CaTCalc XE							
Edit Calculation Assessme	nt Databases	Help					
New Folder	•	🤌 System	Q Data	Calculation	Assessment	O Exit	
Open a Folder		Summary					
Recent Folders							
Save							
Export Plot							
Export Table							
Print							
Preference							
Exit							
EXIL							

File

New Folder : Create a new folder (project folder) to save the calculation results

Open a Folder : Open an existing folder

Recent Folders : List of recently used folders

Save : The calculation results are automatically saved. This menu is used to explicitly save the results of editing, such as adding labels afterwards, though the edited result is usually saved automatically.

Export Plot : Export plot to JPEG, PNG, etc.Export Table : Export the result table.Print : Print

Preference: Various settings (Option)

Exit : Quit CaTCalc.

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File	Edit	Calculation	Assessment	Databases	Help			
Res	Q	opy to Clipbo	bard		System	🔍 Data	Calculation	Asse
Pro	j <u>S</u> 1	wap&Copy to	o Clipboard		Summary			
-								

Edit (*Note : The Edit menu changes depending on the case of the plot view and the list view.)

Copy to Clipboard : Copy result into the clipboard. In the plot view, the diagram is copied; in List view, the list is copied.

Swap&Copy to Clipboard : In the case of list view, the rows and columns are swapped and copied into the clipboard.

CaTCalc	XE					
File Edit	Calculation	Assessment Databases Help	1		1	
Results Project	-	ynamic Data and Reaction m Calculation and Mapping		Q Data	Calculation	Asse
		Data and ReCalculate				
	Macro		+			

Calculation

Thermodynamic Data and Reaction : Same as the DATA button on the application bar.

Equilibrium Calculation and Mapping : Same as the Calculation button on the application bar.

ReLoad Data and ReCalculate : Recalculate under the same conditions. Maybe usable in database development.

Macro : Macro menu

File Edit Calculation	Assessment	atabases Help		
PD-web	Data Asses	sment and Optimization		Calculation 🛛 🙀 Assessment 🔹 🖸 Exit
Project	<u>I</u> mage Digi <u>F</u> itting Tool			
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PbO-xZrO2 #1 SiC-xTiB2 #1	ZrO2 #1 Fi <u>r</u> st Principle Data IB2 #1 Data First Structure		Þ	H <u>S</u> Cp to Phase data HS <u>C</u> p to ADB data
SrO-xTiO2 #1 Bi2O3-xSiO2 #1 MgO-xY2O3 #1	_	<u>G</u> ibbs Energy Continuity Check <u>A</u> queous Utility Programs		<u>G</u> Func to HSCp data
Mg0-xK20-ySi02 # K(MgSi)0.502-xSi02 1Cr-02 #4 1Cr-02 #3 1Cr-02 #1 1Cr-02 #1 Cr-02 #1 Cr-02 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2	2 #1			

Assessment

Data Assessment and Optimization : Same as the assessment button on the application bar.

Image Digitizer : A built-in digitizer for reading data from diagrams. Other digitizers can also be used. (See section Image Digitizer.)

Fitting Tool : A tool to make function approximation for X and Y data in the clipboard. Parameter optimization of various specific heat functions, the Redlich-Kister polynomial for excess Gibbs energy, the function for thermal expansion, and the EOS function for pressure dependence. (See section Fitting Tool.)

Convert Thermodynamic Data : Utility and inverse conversion utility to convert data of Enthalpy, Entropy, and Specific Heat polynomial parameters in the clipboard into Gibbs energy functions in the CDB format and parameter sets in the ADB format. (See section Convert Thermodynamic Data.)

First Principle Data : A utility to convert data in units of eV/atom from ab initio calculations in the clipboard to kJ/mol_atom, and a utility to estimate specific heat and Entropy assuming the Debye function.

Base Functions : A utility that refers to a file that defines the basic Gibbs energy functions of the elements by SGTE, and a file that defines the Gibbs energy functions of some basic compounds.

Gibbs Energy Continuity Check : When Gibbs energy is temperature-split, check for sufficient connection accuracy at the split point. If the difference is too large, a warning message will be displayed, so it is necessary to correct it. The connection accuracy should be at least 10 significant digits.

Aqueous Utility Programs : Displays various thermophysical properties of H2O.

File Edit Calculation Assessment	Databases	Help		
PD-web		r Datafile	. E	Assessment O Exit
Project Y2O3-xGd2O3 #1	<u>D</u> atafile <u>C</u> DB Inf	formation	-	
- 203-xLa2O3 #1 - 201 PbO-xZrO2 #2 - 201 PbO-xZrO2 #1	<u>E</u> dit CDI Re <u>b</u> uild	B File Subsystem from Activated Phases	•	
SiC-xTiB2 #1 Si-xTi-yB #1 SrO-xTiO2 #1		TDB Files		
■ Bi2O3-xSiO2 #1 ■ MgO-xY2O3 #1 ■ ▲ MgO-xK2O-ySiO2 #1	DB <u>F</u> ile-	ouncy		
- K(MgSi)0.502-xSiO2 #1 - 4 1Cr-O2 #4 - 1Cr-O2 #3 - 1Cr-O2 #2				

Databases

Register Datafile : Register a database file. Registration is required to use the database file.

Datafile List : There are sub-menus such as updating registration information.

CDB Information : Display database Information.

Edit CDB File : Database editing. Subset creation, etc.

Rebuild Subsystem with Activated Phases : A new subset of the database will be created with only the appeared/stabilized phases after calculation. Useful in the application-specific database development.

Import TDB Files : Importing files in the CALPHAD-standard TDB format.

DB File-Utility : Some utilities

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File Edit Calculation Assessment	Databases	Help			
PD-web	<u>R</u> egiste	r Datafile		ፍ Assessment 🚺 🖸 Exit	
Project	<u>D</u> atafile	: List	►	Refresh Information	1
Y2O3-xGd2O3 #1	<u>C</u> DB Inf	formation	۶.	<u>E</u> dit List	
🙀 Y2O3-xLa2O3 #1 	Edit CDB File			Re <u>b</u> uild Datafile List	
Pb0-x2r02 #2 Pb0-x2r02 #1	– Re <u>b</u> uild Subsystem from Activated Phases				
SiC-xTiB2 #1	Import	TDB Files			
	DB <u>F</u> ile-Utility				
Bi2O3-xSiO2 #1 MgO-xY2O3 #1 MgO-xK2O-ySiO2 #1 K(MgSi)0.5O2-xSiO2 #1					

Databases Datafile List:

- Refresh Information: Update the information of the registered database file.
- Edit List: Edit the database list directly.
- Rebuild Datafile List: Regenerate the registration list.

		×
File Edit Calculation Assessment	Databases Help	
Project Y2O3-xGd2O3 #1	Register Datafile Seessment Exit Datafile List CDB Information Seessment Seessment	
Y203-xLa203 #1 Pb0-xZr02 #2 Pb0-xZr02 #1 SiC-xTiB2 #1 SiC-xTiB2 #1 Sr0-xTi02 #1	Edit CDB File Current Subsystem Rebuild Subsystem from Activated Phases Current Full CDB File Import TDB Files New File DB File-Utility Import Full CDB File	
MgO-xY2O3 #1 MgO-xY2O3 #1 MgO-xX2O-ySiO2 #1 K(MgSi)0.502-xSiO2 #1 1Cr-O2 #4 1Cr-O2 #3		

Databases

Edit CDB File : Editing the Database

• Current Subsystem : Create and edit a subset file for the currently selected element only.

- Current CDB File : Edit the selected CDB file.
- New File : New Edit.

A CaTCalcNE		
File Edit Calculation Assessment	Databases Help	
PD-web	<u>R</u> egister Datafile	Assessment O Exit
Project	<u>D</u> atafile List	•
Y2O3-xGd2O3 #1	<u>C</u> DB Information	•
Y2O3-xLa2O3 #1 PbO-xZrO2 #2 PbO-xZrO2 #1 SiC-xTiB2 #1 Si-xTi-yB #1	Edit CDB File Rebuild Subsystem from Activated Phases Import TDB Files	• _
SrO-xTiO2 #1 Bi2O3-xSiO2 #1 MgO-xY2O3 #1 MgO-xX2O-ySiO2 #1 K(MgSi)0.5O2-xSiO2 #1 1Cr-O2 #4 1Cr-O2 #3 1Cr-O2 #1 Cr-O2 #1	DB Eile-Utility	Combine ADB Files Delete Duplicates Enable Select-All-Elements

Databases

DB File-Utility

- Combine ADB Files : The integration of multiple ADB format data files.
- Delete Duplicates : Removal of duplicate data.

• Enable Select-All-Elements : This is a hidden command that allows you to batch select all elements in a large database file on the data file selection screen. A button appears in the screen.

IV-2. Application menu

File Edit Calculation Assessment Databases Results Project Summary File Edit Calculation Assessment Exit Summary	

① System : Specify elements and database files to load thermodynamic data.

2 **Data** : Displays information on phases and species. If necessary, deselect each one.

③ **Calculation** : Selects, sets conditions and executes various types of calculations.

(4) Assessment : Database development.

(5) Exit : Quit CaTCalc.

Main screen

CaTCalc XE							
	Assessment Databases	Holp					
Results	•	🤌 System	🔍 Data	Calculation	Assessment	O Exit	
Project		Summary					

System screen : Select elements and database file(s) to be used.

	Co	nditi	on	Sett	ina	Util	itv											
ð		Q D	ata		d C	alcul	ate											Close
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	Specify by Files
H.																Е	He	Include Ionic Gas Species
j	Be											В	С	Ν	0	F	Ne	Include Aqueous Phase
	Mg											Al	Si	Ρ	S	Cl	Ar	Include Extra Components
ĸ	Ca			V				Co									Kr	
۱b	Sr							Rh										Include Volume (if available)
Cs -	Ba		Hf					Ir			-		РЬ	В	Ро	At	Rn	Max carbon in organics 2
Fr	Ra *	**			-			Mt Eu		-		L la	E.c.	Tree	Vb	1		OR search
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		Vam				. P		tes		Die							_	
		varre	-				140	tes										

*The "Application Menu" of the main screen is the same as the "Tab Menu" of the system screen.

CaTCalc XE File Edit Calculation Assessment Databas Results 🤌 System 📃 Data 🛛 🙀 Calculation 🛛 🙀 Assessment 🛛 🔘 Exit Project La CaTCalc XE - X File Condition Setting Utility Calculate Close 1 🔍 Data 🛛 10 1 4 5 9 11 12 13 14 15 16 17 0 2 3 6 7 8 Specify by Files Н Е He Include Ionic Gas Species Li Be BC N 0 F Ne Include Aqueous Phase Na Mg A Si Ρ S CI Ar 🔚 Include Extra Components As Se Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge Br Kr К Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Include Volume (if available) Rb Sr Te Ι Xe Cs Ba * Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn Max carbon in organics 2 Fr Ra ** Rf Db Sq Bh Hs Mt Ds Rq Ub OR search Load (4 * La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu Clear ** Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr 2) + DB Name Notes Units (K, mol) Click here to see additional imformation!

1 Periodic table

System screen

The target elements are selected here with the mouse.

2 Data file area

The thermodynamic data files containing the elements selected in the Periodic Table and their information are displayed.

3 Clear Selection

(4) Load

Load data from the selected thermodynamic data file.

la Ca	TCal	c XE																
File	Cor	nditi	on	Sett	ting	Util	lity			_	5.0							ange and the second
⊆	lose		2		d c	alcul	ate]										Close
0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	Specify by Files
Н																Е	He	
Li	Be											В	С	Ν	0	F	Ne	Include Ionic Gas Species
Na	Mg											AI	Si	Ρ	s	CI	Ar	Include Aqueous Phase
к	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	📄 Include Extra Components
Rh	Sr	v	7r	Nb	Mo	TC	Ru	Rh	Dd	An	Cd	In	Sn	Sh	То	T	Ye	Include Volume (if available)

File:

Close : Close the System screen.

Ca	TCal	c XE																9
File	Co	nditi	on	Sett	ting	Util	ity											
	9	Copy	1		Ct	rl+C	1)										Close
0	1	Past	e		Ct	rl+v		8	9	10	11	12	13	14	15	16	17	Specify by Files
Н	1	Resu	ime				- 1									Е	He	
Li		Rese	st.				- 1					В	С	N	0	F	Ne	Include Ionic Gas Species
Na	1704	1200		_	_	_	_					AI	Si	Р	s	CI	Ar	Include Aqueous Phase
к	Ca	Sc	Ti	v	Cr	Mn	Fe	Со	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	📄 Include Extra Components
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Condition:

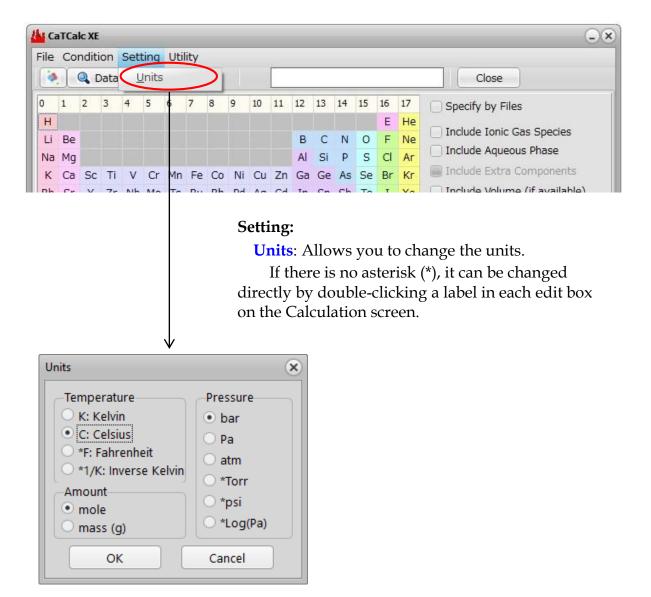
Copy : The calculation conditions are saved into the clipboard, so you can save them in Excel and so on.

Paste: You can paste and reset the calculation conditions in the clipboard.

Resume : Set the previous calculation conditions. (Useful when recalculating after changing the database.)

Reset : Reset to default settings

Unit setting



C	aTCa	alc																	×
	File	Со	ndit	ion	Se	tting	j U	tility	/										
	۵,		Q D	ata		🖌 Ca	alc		-			t Sys	stem	ı					Close
	0	1	2	3	4	5	6	L	ist P	has	es						16	17	<u>la</u>
	н							L	<u>i</u> st S	pec	ies					•	<u>O</u> r	nly N	Names
		Be						I	-Ra	nge	Che	eck					Or	<u>ı</u> ly G	G values as Species
	Na	Mg						_	_	_	_	_	Al	Si	Р		<u>G</u> ,	н, 9	S, V, Cp Js Phase
	к	Ca	Sc	Ti	v	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As		<u>H</u> 0), SC	0 and Cp components
	Rb	Sr	Y	Zr	Nb	Мо	Тс	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те	Ι	Xe	Include Volume (if available)
	Cs	Ba	*	Hf	Та	w	Re	Os	Ir	Pt	Au	Hg	тΙ	Pb	Bi	Po	At	Rn	✓ Max carbon in organics 2
	Fr	Ra	**	Rf	Dh	Sa	Rh	He	Mt	Ne	Ro	Hh							

Utility:

View Current System : Displays the thermodynamic database for the "current system" consisting of the currently loaded and selected phases.

List Phases : Displays information of the (selected) phases.

List Species : Calculates and displays information of the (selected) species of (selected) phases.

T-Range Check: For the current calculation conditions, select only the data that are within the guaranteed temperature range for each data in the database. (Use this only to identify which data may be problematic, if necessary.)

② Data screen

rCalc XE		_ ×)		
Condition Setting Utility				
🔍 Data 🔛 Calculate	La CaTCalc XE			
1 2 3 4 5 6 7 8 9	File Edit Calculation Assessment D	oatabases Help		
	Results	🝷 🄌 System 🛛 🍳 Data	Calculation 😹 Assessment 🚺 🧿 Exit	it
Be	Project	Summary		
Mg Ca Sc Ti V Cr Mn Fe Co	Ni			
Sr V Zr Nh Mo To Ru Rh				
V		V		
🕌 CaTCalc XE			- *	
File Condition Setting	Utility			
	Calculate	1	Close	
			Close	
+ Phases	DataBase Num	+ Species	T1(K) T2(K)	
			\bigcirc	
	(1)		(2)	
	J		-	
Double click Phase/	Species to calculate properties ir	ndividually.		
(3)	Calculation			
Keaction	Calculation			
		20 C		
Units (K, mol) Click her	e to see additional imformation!		li.	

Phases list: Display phases. The solid and liquid phases of pure substances are displayed together as PureSol and PureLiq.

Species list: Lists the species that make up each phase. However, pure substances indicate a phase.

Reaction Calculation: This is a reaction calculation that uses individual chemical reaction schemes. Note that calculation that takes all possible reactions into account is performed by the equilibrium calculation in the Calculate screen.

C	aTCalc							
		tion Setting Utility						
-	<u>)</u>	Data Calculation			Close			
	+ Phases	DataBase	e Num	+ Spec	es		T1(K)	T2(K)
ľ								
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						_		
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U	Inits (C, mol) Click here to see add	ditional imformation!					
	aTCalc							
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	<u>)</u>	Data 🛛 🙀 Calculation	e Num	+ Spec			T1(K)	T2(K)
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	<u>)</u>	Data 🛛 🙀 Calculation	e Num	+ Spec			T1(K)	T2(K)
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* See [<u>Reaction Calculation]</u> for details of the settings.

③ Calculation screen

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🔌 🔍 Data 📓 Cal	culation	Close
Feed/Activity Conditions		Default Unit: mol (formula)
Phase	Species	Unit Value
Phase	Species	Unit Value
1 2 Set Elements 7		Set Default Values Temperature (C) 1000 Pressure (bar)
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1 2 Set Elements 7 • Equilibrium Calc • Phase Diagram • Liquidus Projection	Add Feed Clear Feed	Set Default Values Temperature (C) 1000 Pressure (bar)
1 2 Set Elements 7 • Equilibrium Calc • Phase Diagram	Add Feed Clear Feed	Set Default Values Temperature (C) 1000 Pressure (bar) 1.01325 Transition Calc
1 2 Set Elements 7 • Equilibrium Calc • Phase Diagram • Liquidus Projection	Add Feed Clear Feed	Set Default Values Temperature (C) 1000 Pressure (bar) 1.01325 Transition Calc dGHSV Calc
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1 Set Elements • Equilibrium Calc • Phase Diagram • Liquidus Projection • Solidification Simul	Add Feed Clear Feed	Set Default Values Temperature (C) 1000 Pressure (bar) 1.01325 Transition Calc GHSV Calc

① **Set Elements** : This button is used to set the element as a Feed (Reactant). It is useful for creating a normal phase diagram of metals.

② **Add Feed** : It is used for general equilibrium calculations and phase diagram calculations for ceramics and metal systems.

③ Clear Feed : Clear all the setting.

④ Set Default Values : Typical conditions for each type of calculation are set automatically. It is used after setting up Feed conditions and calculation type.
 ⑤ Calculate: The button to start the calculation.

③ Calculation screen

CaTCalc XE					×
File Condition Setting Uti		Cr C			
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Set Elements	Add Feed	Set	: Default Values	5	Temperature (C)
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					GHSV Calc
Individual Phase Ener	gies				-
			Calculate		Fix Volume(Gas)
Extra Conditions					
				L	
Units (C, mol)			_		li.

General procedure

- ① Set the Feed (reactant), select "unit" and enter "value".
- ② Select the type of calculation.
- ③ Set parameter values, temperature, pressure and other calculation conditions.

■ Save/Reset Conditions

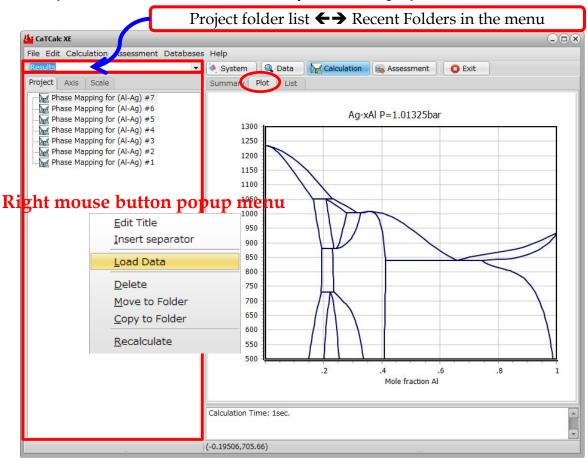
Condition Setting Utility Copy Ctrl+C				Close
Paste Ctrl+V				
<u>r</u> asce curry			Def. Unit (r	nol)
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Set Elements	Add Feed		t Setting for Mappi	

The calculation conditions can be copied into the clipboard by clicking the **[Condition]–[Copy]** menu. You may paste them in Excel or else to save. It is also possible to reset the calculation conditions by the **[Paste]** menu . **[Resume]** is to reset the calculation conditions of the previous calculation, which is useful when you try just the same calculation using different data file. Please make sure that the settings are correct.

IV-3. Viewing Projects and Calculations

① Project / Axis / Scale

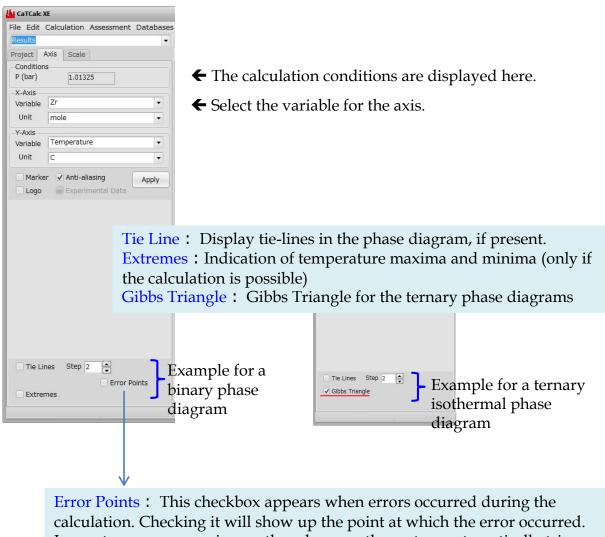
◆ Project : The results are automatically saved as a project



- For each calculation result displayed in the Project panel, you can use the pop-up menu displayed by pressing the right mouse button.
- When you click [Load Data], the calculation result is automatically loaded and displayed in the right viewer panel. Note that when the Plot tab appears to display a plot, the List tab also appears at the same time. In addition, the Axis and Scale tabs appear in the left Project panel.
- When the Plot tab does not appear, as in a single point calculation, only the List tab appears in the Viewer panel. In such a case, the Axis and Scale tabs of the Project panel will not appear.
- You can also reload the calculation results by double-clicking on the list of projects. Currently, the project list cannot be rearranged.
- The Project folder list corresponds to the Recent Folders list in the menu. To remove a folder from the list, use the right button pop-up menu in the Project folder list.

① Project / Axis / Scale



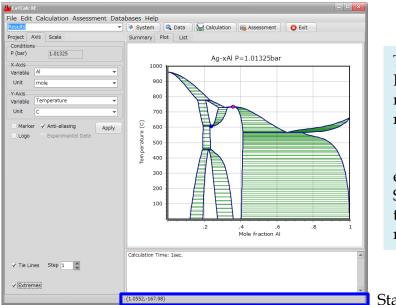


In most cases, you can ignore them because the system automatically tries recalculation if an error occurs. If the phase boundary calculation apparently failed, try a manual scan (see page 71).

① Project / Axis / Scale

♦ Axis

Tie-Lines and Extremes



The red and blue points for the Extremes indicate temperature maxima and minima, respectively.

* Detailed information about each point will be shown in the Status bar when you hold down the Shift key and move the mouse cursor near the point.

Status bar

◆ Scale : Setting the Display Scale of the Diagram

roject Axis Scale X_Axis Setting	oject Axis Scale <pre>K_Axis Setting xis_Title Mole fraction Al wis_Title Mole fraction Al wis_Del_Size 10 in 1E-05 ix 0.99999 iv 0 utoScale Yes <pre>Y_Axis Setting xis_Title Temperature (K) wis_Del_Size 10 in 500 iax 1300 iv 0 utoScale Yes</pre></pre>	esults	culation Assessment Databas
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Press the Detail button to display the detailed setting menu, if necessary.

Detailed settings

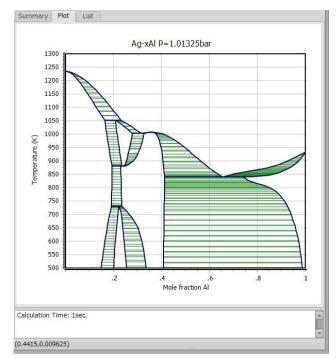
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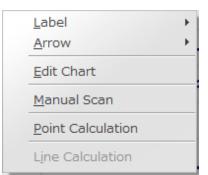
• Summary : The database and calculation conditions used for the calculation are displayed in one view.

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Results	🔹 🙋 System 🛛 🍳	Data Calculation	Assessment	O Exit	
roject	Summary Plot	List			
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	Feed/Activity				
	Phase	Species	Unit	Value	
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	Calculation Time:	Isan			
	Calculation Time:	ISEC.			

② Summary / Plot / List view

◆ Plot panel: plot the results





(Right click popup menu)

Right click on the plot area to bring up a pop-up menu. You can edit the details.

Labeling phase name : [Ctrl] + left mouse button click Enlarge the graph: Left click and drag from top left to bottom right Move the graph: [Ctrl] + right-click and drag Return to the original graph: left-click and drag from bottom right to top left

<u>L</u> abel	Add Label	<u>L</u> abel	
<u>A</u> rrow	<u>C</u> lear Labels	Arrow	Add Arrow
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<u>M</u> anual Scan	Add <u>T</u> -Label	<u>M</u> anual Scan	
Point Calculation	Add T <u>e</u> xt	Point Calculation	

For example, eutectic temperature can be labeled as follows:

1. Move the mouse cursor to the vicinity of the eutectic point with pressing the [Shift] key and display the eutectic point information on the status bar.

2. Press the right mouse button and select [Add T-Label] from the menu. The position of the Label corresponds to the axis, and it automatically follows the scaling and movement of the figure. Therefore, the Label can only be placed within the plot area.

3. Use [Add Text] to place a label outside the axis frame.

• List panel: numerical values are listed.

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All calculation results are basically displayed.

Type of data to be displayed can be selected in "Select List" of "Edit Menu".

You can use other graphing software to create graphs as well, by copying data via the clipboard using the Edit menu.

V. Various calculation methods

- V-1. Single-point and series equilibrium calculation
- V-2. Phase diagram calculation
- V-3. Liquidus Projection calculation
- V-4. Solidification Simulation
- V-5. Adiabatic calculation
- V-6. Calculation of Individual Phase Energy
- V-7. Calculation of aqueous systems

V-1. Single-point and series equilibrium calculation

The general procedure for the calculation is as follows:

1) Specification of the elements of the system and selection of the thermodynamic data file to be used.

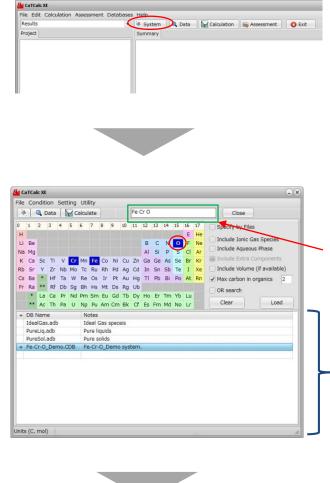
- 2) Select Phase and Species, if necessary.
- 3) Setting up the calculation conditions.
- 4) Calculation execution.
- 5) Display results as a plot and a list.

Examples are described in detail below.

1) Equilibrium Calculation



By double-clicking the shortcut key, CaTCalc is launched.





1. Press the System button.

The screen for selecting elements will appear.

2. Click directly on the element.Alternatively, you can fill in the elements list directly and press enter. (separated by a space)

• Thermodynamic data files, that contain the elements, will be displayed in the data file area. The registered data files will be displayed. By default, the files stored in the CaTCalc/Data folder are registered automatically. (Files in other locations or newly added files must be registered manually).

Next Page

1 Equilibrium Calculation

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3. Select the data file.

Check the cell next to the DB Name. Then "+" is displayed and selected.

If you need gas, select also "IdealGas.ADB" in addition.

4. Click the [Load] button.

Reads the data in the selected data file.

You will see the information about the database file in the "Summary tab".

[Data screen]

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*By clicking the [Data] button, the loaded data will be displayed in the "Phase List" and "Species List".

For pure stoichiometric phases, the Phase list shows solid and liquid phases as a group and the individual phases are listed in the Species list.

*The pure liquid phases are not selected by default because the liquid phase usually forms single solution phase.

Next page

① Equilibrium Calculation





🞙 🛛 🤍 Data 🗍 🥻	Calculate			
eed/Activity Condit	ions		Def. U	nit (mol)
hase	Species	Unit	Value	K 0.1
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D(Gas)	0	mol	У	(2)
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Equilibrium C Phase Diagrai Liquidus Proje	m 6 sction		Set Default Va	9 Pressure (bar) 1.01325



Next page

- 5. Press the "Calculation" button. • The "Calculations" screen appears.
- 6. Click the [Set Elements] button.• Each element is entered automatically.

7. Select "Equilibrium Calc".

* At this point, the typical calculation conditions are set by clicking the [Set Default Values] button, and it is convenient to set the conditions by modifying them.

8. Enter the [Value] value.

• In general, Values can be entered as numeric values, parameters, a linear function of them, (e.g., 1+2x), or a special parameter, b. In the present case, it is set up as shown in the left figure.

* There are 5 parameters available, "x", "y", "z", "w", and "a" (uppercase letters are also OK). b stands for balance, and is a dependent parameter that is automatically calculated so that the total amount of Feed is set to 1 (use "b100" if you want to calculate it as a percentage).

* After entering any of these parameters, the corresponding edit box will appear in the "Parameter Area" and you can specify their numerical values.

• Select [**Unit**] from the drop-down list that appears if you click the cell. You can also specify the activity in this list.

9. Set the values of "Temperature" and "Pressure".

10. Use the [Calculate] button to start calculation.

1) Equilibrium Calculation

e Edit Option Calculation As		System		Calculation	Assessment O Exit	
oject			list			
Fe-xCr-yO #4	•			O mol fraction	0.1	
Fe-xCr-yO #3				Cr mol fraction	0.1	
Fe-xCr-yO #2				P (bar)	1.01325	
- Fe-xCr-yC #4		Phase	DataBase	T (C)	1000	
Def Mn-xFe #2						
Mn-xFe #1		Corundum	FeCrO-Demo	mol (atom)	0.1670519	
AIN-xAI2O3 #1				Activity	1	
- Al-xMg-yZn #7 - Mar 1Ca(OH)2-CO2 #3			Element	Fe	2.984323E-06	
- A Fe-xCr-vC #3			Element	Cr	0.4013809	
Fe-xCr-02 #1			Element	0	0.5986161	
A Fe-xCr-yC #2		500.14			0.8329481	
- 🛕 C-xCr-yFe #6		FCC_A1	FeCrO-Demo		0.8329481	
- A Fe-xCr-yC #1				Activity	1	
- A C-xCr-yFe #5 - A C-xCr-yFe #4			Element	Fe	0.9604435	
A C-xCr-yFe #3			Element	Cr	0.03955654	
A C-xCr-yFe #2			Element	0	1.330511E-08	
Fe-0.1Cr-O2 #1				-		
🖬 C-xCr-yFe #1			-			
Cr-xFe-yO #1 C-xFe #2		C_Potential	Fe	kJ/mol	-62.73028	
		C_Potential	Cr	kJ/mol	-79.73136	
1Ca(OH)2-CO2 #2		C_Potential	0	kJ/mol	-392.0942	
Def CO2-1CaCO3 #1						
Al-xMg-yZn #6		Gibbs Energy	G	kl	-97,36677	
Fe-C-0.1Cr #2				ki	-2.170895	
- Cr-xNi-yO #3 - Mb-xCr-Si #2		Enthalpy	н	ĸ	-2.1/0895	
Cr-xNi-yO #2	- 1		ISERS#SHOBU		CATCALC#DATA¥IdealGas.adb CATCALCXE¥DATA¥FeCr0-Demo.CD	в
NIO-xCr2O3 #2	-					-

ile XE				
dit C	Option C	Calculation Assessment Databases Help		
`	_	/ Only Active Phases / Element Fraction for Pure Phases	Calculation	assessment 🕞
qui	<u>M</u> ass		O mol fraction	0.1
qui has	_	attice	Fe mol fraction	0.1
has	Sh <u>o</u> w	/ Molar Phase Energies	P (bar)	1.01325

The result of the calculation is automatically displayed as shown on the left.

You find the display options under [Option] in the menu.

Calculation conditions

Amount of the phase Activity of the phase Element fractions

Chemical potential of each element

The Gibbs energy of the entire system, etc. However, the volume and density are only for the gas phase if the database does not contain volume data for the solid or liquid phase.

			O mol fraction	0.1
			Cr mol fraction	0.1
			P (bar)	1.01325
	Phase	DataBase	T (C)	1000
	Corundum	FeCrO-Demo	mol (atom)	0.1670519
	7		Activity	1
01		Element	Fe	2.984323E-06
Phase		Element	Cr	0.4013809
		Element	0	0.5986161
	FCC_A1	FeCrO-Demo	mol (atom)	0.8329481
			Activity	1
		Element	Fe	0.9604435
		Element	Cr	0.03955654
		Element	0	1.330511E-08
	C_Potential	Fe	kJ/mol	-62.73028
	C_Potential	Cr	kJ/mol	-79.73136
	C_Potential	0	kJ/mol	-392.0942
	Gibbs Energy	G	kJ	-97.36677
	Enthalpy	н	kJ	-2.170895
	Entropy	S	J/K	74.77193
	Heat Capacity	С	J/K	33.58647
	Volume	V	L	0
	density	r	g/cm3	0
	ErrorCode			0
	Loop			33

(Note) mol amount

When displaying the amount of a phase in moles, it is important to note what the moles are of.

- For gases, water, etc.: Mole of molecules are natural as the molecules are real entities and important.
 - Examples: H2, O2, H2O, etc.
- For metals, moles of atoms are usually used since they are atomic units.
 - Example: BCC phase, etc.
- For pure inorganic compounds, moles of formula units are used.
 - Example: SiC, SiO2, etc.
- For solid solutions and melts, because amounts depend on the definition of the solution when moles of formula units are employed, moles of atoms are exclusively used in CaTCalc.
 - Example: SiO2-Al2O3 solid solution, mullite, etc.

Accordingly, mol of atoms is usually used in computational thermodynamics for metallic systems, though mol of formula units is usually used in chemical reaction calculations.

In the list display of the result in CaTCalc, the definition of the mole is clearly indicated, but in the graph plot, it is unclear, so care must be taken when comparing phase amounts. It is better to compare the amount of phases by mol of atoms or mass.

* The mol definition can be set in the menu [File]-[Preference]-[Output Defaults]. Note that the input of reactants (feed) is fixed to the mol of formula units.

ptions			×
Show only	ts attice site-fractions active (stable) phase toff for small fraction		Miscellaneous Check Gibbs energy continuity when importing TDB files Energy shift for ordered phase (Only in PD calc) <u>5E-8</u>
	f atoms (gram-atoms is fixed to mol of forr) for all phases. Note nula units.	Special check for 4-Split-Sublattice phase model Save-mode rather than Copy-mode
 ✓ Use molali Show drivi ✓ Default nu Scheil Cooling ✓ Stop calcu 	lation if amount of th	activity play values 7 e parent phase <1E-3	 Save redundant phase information Logo at the top-right corner Resize chart to display legend Check for updates on start-up Set time limit in one boundary calculation (sec) 30
Appearance a Appearance Font Name Arial	nd Default Font in Plo Aqua Light Slate	size	ParaEquilibrium (Partial Equilibrium) Setting Interstitial Fast Diffusing Elements C, N, O, B, H
Text Editor External Text C:\Program I	Editor Files\Hidemaru\Hiden	haru.exe	Apply/Save Cancel

② Series calculation with varying temperature

🍳 🔍 Data 🛛 🔛 C					
eed/Activity Conditions	5			Def. Unit (r	mol)
Phase	Species	U	Init	Value	X 0.1
Fe(BCC_A2)	Fe	n	nol	b	
Cr(BCC_A2)	Cr	n	nol	x	Y 0.1
D(Gas)	0	n	nol	У	
Set Elements	Add Fe	ed	Set	t Default Values	1000
Set Elements Equilibrium Calc Phase Diagram Liquidus Projectio	•	ed	Set	t Default Values	Pressure (bar)
Equilibrium Calc Phase Diagram	on	ed	Set	t Default Values	Pressure (bar)



Set Default Values

Calculate

0 3000 25

Pressure (ba 1.01325

✓ Transition Calc

dGHSV Calc

6

Fix Volume(Gas)

Set Elements

Equilibrium Calc

Phase Diagram

Extra Conditions

Liquidus Projection

Solidification Simulation

Individual Phase Energies

nits (C, mol) Set units from the pop-up mer

Add Feed

1. Set the calculation mode.

"Equilibrium Calc" should be checked. Make sure "Transition Calc" is checked to find transition points.

2. Set the [Value] value.

[Unit] can be switched individually from the list. You can also double click on the **Def. Unit** label to switch them all at once.

3. Set the value of "X", "Y".

4. Set the value of "Temperature".

Enter the initial value (start), the end value (end), and the interval value (step) in that order. Delimiter is a space or a comma.

You can switch between units by doubleclicking on a unit label. Uncommon units can be chosen only in the unit selection dialog.

5. Set the value of "Pressure".

You can switch units by double-clicking on the unit. However, units such as Log(P) can only be set in the unit selection dialog.

6. Press the [Calculate] button to start calculation.



② Series calculation with varying temperature

CaTCalc XE		
le Edit Calculation Asses	sment Databases	Help
tesults		System Q Data Det Calculation Assessment O Exit
roject Axis Scale		Summary Plot List
It = Reacting 0 #5 Fextbody 0 #5 Fextbody 0 #1 Code		Fe-xCr-yO P=1.01325bar, X=0.1, Y=0.1
- CO2-1CaCO3 #1 - Al-xMg-yZn #6		Calculation Time: 20sec. Datafilie: CUVEREXFINABUNDOCUMENTSVCATCALCWDATAVIdealGas.adb DataFilie: C:VUSERSVSHOBUVDOCUMENTSVCATCALCXEVDATAVFeCr0-Demo.CDB
Fe-C-0.1Cr #2	•	DataFile: C:¥USERS¥SHOBU¥DOCUMENTS¥CATCALCXE¥DATA¥FeCr0-Demo.CDB
		(-350.43.1.271)

The result of the equilibrium calculation is displayed as a graph.

<Fix Volume(Gas)>

e Condition Setting	g Utility Calculate	Fe Cr O		Close
eed/Activity Condition			Def. Unit (
hase	Species	Unit	Value	X 0.1
e(BCC_A2)	Fe	mol	b	
Cr(BCC_A2)	Cr	mol	x	Y 0.1
O(Gas)	0	mol	У	
Set Elements	Add Feed		Set Default Value	5 Temperature (C) 0 3000 25
Set Elements Equilibrium Calc Phase Diagram Liquidus Project			Set Default Value:	remperature (C)
Equilibrium Calc Phase Diagram	tion		Set Default Value	0 3000 25

The Pressure field changes to Volume. Note that currently only the volume of the gas is considered. If this field is gray, the gas phase is absent. Go back to the system setting and load the data for the gas phase.

③ Target calculation

Two kinds of target calculation are supported.

- Formation target
 - This determines the temperature or composition at which the target phase appears.
 - Calculations can also be made specifying the amount of the phase.
- Precipitation Target
 - This determines the temperature or composition at which other phases precipitate from the target phase.

In both cases, the Data screen is used to specify the phase of the Target, and the settings are also displayed on the Calculation screen.

[Data screen]

as FeCrO-Demo 13 QUID FeCrO-Demo 13 SF4. FeCrO-Demo 1 mant Phase Tormation Target Phase R3SI FeCrO-Demo 1 Clear FeCrO-Demo 1 FeCrO-Demo 2 FecrO-Demo 2 FecrO-Demo 2 FeCrO-Demo 1 FeCrO-Demo 1 FeCrO-Demo 1 FeCrO-Demo 1 FeCrO-Demo 1	as FeCro-Demo 1 QUID FeCro-Demo 5 STA mant Phase GINNDUM FeCro-Demo 1 Fer3va 298.15 3000 Fer3va 298.15 3000 Fer3va 298.15 6000 Fer3va 298.15 6000 Fer3va 298.15 6000 Fer3va 298.15 6000 Fer3va 298.15 6000 Clear Clear Clear Fer3va 298.15 6000 Fer3va 298	as FeCro-Demo 1 QUID FeCro-Demo 1 Ferro-Demo 1 Ferro-Demo 1 Ferro-Demo 1 Ferro-Demo 1 Ferro-Demo 1 Ferro-Demo 1 Ferro-Demo 1 Ferro-Demo 1 Ferro-Demo 1 Classi Ferro-Demo 1 Ecc, at Fecro-Demo 1 Ecc, at Fecro-	as Fe(CrO-Demo 13 UDUD FE(CrO-Demo 5 LSFE4 FE(CrO-Demo 1 CrT3Va 298.15 3000 + Fer3Va 298.15 6000 + CrT3Va 298.15 6000 + CrT3Va 298.15 6000 + Fer3Va 298.15 6000 + Fer3Va 298.15 6000 - CrT3Va	as Fe(CrO-Demo 13 UDD Fe(CrO-Demo 5 LSFE4 Fe(CrO-Demo 1 Crr3Va 298.15 3000 + Fe'3O 298.15 3000 + Fe'3O 298.15 3000 + Fe'3Va 298.15 6000 + Fe'3Va 298.15 6000 + Fe'3Va 298.15 6000 - Fe'3Va 29	🔍 Data 🛛 🚂 Ca	alculation 🔤 🔩 Cell	Reactor	Fe Cr (·	Close		
UQUID F6CO-Demo 5 F6CO-Demo 1 F6CO-Demo 1	UQUID FeCr0-Demo 5 ALSFE4 FeCr0-Demo 4 FeCr0-Demo 4 FeCr0-Demo 4 FeCr0-Demo 4 FeCr0-Demo 4 FeCr0-Demo 4 FeCr0-Demo 4 FeCr0-Demo 4 FeCr0-Demo 4 FeCr0-Demo 1 FeCr0-Demo 1 FeC	URUID FCCO-Demo 5 ALSFE4 FCO-Demo 1 CORUMDUM FCCO4 CORUMDUM FCCO4 CORUMDUM FCCO4 FCCO-Demo 4 FCCO4 CORUMDUM FCCO4 FCCO-DEmo 1 FCCO4 CORUMDUM FCCO4 FCCO-DEmo 1 FCCO4 CCCA1 FCCO-DEmo 1 FCCO-DEmo 1 FCCO4 FCCO-DEmo 1 FCCO4 FCCO-DEmo 1 FCCO4 FCCO-DEmo 1 FCCO4 FCCO-DEmo 1 FCCO4 FCCO4 FCCO-DEmo 1 FCCO4 FCCO-DEmo 1 FCCO4 FCCO-DEmo 1 FCCO4 FCC	UQUID PECCO-Demo 5 ALSFE4 PECO-Demo 4 Criget Phase CORUNDUM FECO-DE CORUNDUM FECO-DE CORUNDUM FECO-DE CORUNDUM FECO-DE CORUNDUM FECO-DE CORUNDUM FECO-DE CORUNDUM FECO-DE UB A13 FECO-DE CORUNDUM FECO-DE CORUNDUM FECO-DE UB A13 FECO-DE CORUNDUM FECO-DE CORUNDUM FECO-DE UB A13 FECO-DE CORUNDUM FECO-DE UB A13 FECO-DE CORUNDUM FECO-DE DIAMOND FECA FECO-DE CORUNDUM FECO-DE CORUNDUM FECO-DE CORUNDUM FECO-DE CORUNDUM FECO-DE CORUNDUM FECO-DE CORUNDUM FECO-DE CORUNDUM FECO-DE FECO-DE FECO-DE CORUNDUM FECO-DE FECO-	UQUID PECCO-Demo 5 ALSFE4 PECO-Demo 4 Criget Phase CORUNDUM PECCO-Demo 1 Formation Target Phase CORUNDUM FECCO- CORISI FECCO-Demo 1 FECCO-DEmo 1 FEC	Phases	DataBase	Num		+	Species	T1(K)	T2(K)
ALSE4 FeCrO-Demo 1 man tPhase formation Target Phase CORUNDUM FeCrO-Demo 1 FeCrO-C CUB A13 FeCrO-C Grass FeCrO-C CUB A14 FeCrO-Demo 1	ALSFE4 FeCrO-Demo 1 + Cr3Va 298.15 6000 FeCroal Demo 2 + Cr3Va 29	ALSFE4 FeCO-Demo 1 + Fe ² Va 298.15 6000 Mant Phase 0 2 298.15 6000 298.15 6000 CORUNDUM FeCO-0 Clear Clear 298.15 6000 CR35 FeCO-0 Clear Clear Clear Clear FeCO-0	ALSFE4 FeCO-Demo 1 + r°3Va 298.15 6000 Immatt Phase pon 4 + r°3Va 298.15 6000 CORUNDUM FeCro-Q Clear Clear 200.15 6000 CORUNDUM FeCro-Q Clear Clear Clear Clear FeCro-Q FeCro-Q Clear FeCro-Q	ALSFE4 FeCO-Demo 1 + Fr3Va 298.15 6000 Immatt Phase pon 2 pon 2 28.15 6000 CORUNDUM FeCro-d Clear Date Period 2 2 6000 CR35 FeCro-d Clear Clear Clear E	Gas	FeCrO-Demo	13	4	+	Cr*30	298.15	3000
mant Phase mo 4 + Fer3Va 298.15 600 CORUNDUM FeCro-C Parent Phase Parent Phase <t< th=""><td>mant Phase mod 4 er3va 298.15 6000 riget Phase </td><td>Transmit Phase Transmit Phase Transmi</td><td>Topological Topological <thtopological< th=""> <thtopological< th=""></thtopological<></thtopological<></td><td>Transmit Phase Pool 4 #* #*3va 238.15 6000 CORUNDUM Fecro-Q Eormation Target Phase Eormatio</td><td>LIQUID</td><td>FeCrO-Demo</td><td>5</td><td></td><td>+</td><td>Fe*3O</td><td>298.15</td><td>3000</td></t<>	mant Phase mod 4 er3va 298.15 6000 riget Phase	Transmit Phase Transmi	Topological Topological <thtopological< th=""> <thtopological< th=""></thtopological<></thtopological<>	Transmit Phase Pool 4 #* #*3va 238.15 6000 CORUNDUM Fecro-Q Eormation Target Phase Eormatio	LIQUID	FeCrO-Demo	5		+	Fe*3O	298.15	3000
Image Phase Image Phase CORUNDUM FeCro-C CRSI FeCro-C Clear Clear DUMOND_FCC_A4 FeCro-D	Image: Phase 2 CORUNDUM Fecro-c CORUNDUM Fecro-c CRSI Fecro-c Clear Clear DIMANDAPCC,M Fecro-c Clear Clear DIMANDAPCC,M Fecro-d Clear Clear DIMANDAPCC,M Fecro-Demo FEZR2 Fecro-Demo FEZR3 Fecro-Demo HUITE Fecro-Demo	CRUNDUM Fector CORUNDUM Fector CUBAI3 Fector CUBAI3 Fector CUBAI3 Fector CLAS Fector CLAS Fector CLAS Fector Fecto	CRUNDUM Fecro-C CRS Fecro-C CUB_AT3 Fecro-C CUB_AT3 Fecro-C CUB_AT3 Fecro-C CUB_AT3 Fecro-C CUB_AT3 Fecro-C CUB_AT3 Fecro-C CUB_AT3 Fecro-Demo 1 FEZR3 Fecro-Demo 1 HAUTE FECRO-	CRUNDUM Fecro-C CRS Fecro-C CUB_AT3 Fecro-C CUB_AT3 Fecro-C CUB_AT3 Fecro-C CUB_AT3 Fecro-C CUB_AT3 Fecro-C CUB_AT3 Fecro-C CUB_AT3 Fecro-Demo 1 FEZR3 Fecro-Demo 1 HAUTE FECRO-	AL5FE4		1		+	Cr*3Va	298.15	6000
CORUNDUM Fecro-c Earnet Thase CASI Fecro-c Clear DUMOND_FCC_A4 Fecro-c Clear	Image: Phase Formation Target Phase CORUNDUM Fecro-Q CR351 Fecro-Q DIMAKOND,FCC,AI Fecro-Q Clear Clear FEZR3 Fecro-Q FEZR3 Fecro-Q FEZR3 Fecro-Q FEZR3 Fecro-Q Fecro-Q 1 FEZR3 Fecro-Q Fecro-Q 1 FEZR3 Fecro-Q Fecro-Q 1	Orget Phase Dama CORUNDUM Fecro-Q CRSI Fecro-Q Clear Clear DUMOND/FCC,AI Fecro-Q CLA Fecro-Q CLA Fecro-Q CLA Fecro-Q ER283 Fecro-Q FE278 Fecro-Q FE278 Fecro-Q FE278 Fecro-Q FE278 Fecro-Q FE278 Fecro-Q FE278 Fecro-Q FE279 Fecro-Q VID-12 Fecro-Q	Image: Phase Image: Construction Target Phase CORUNDUM Fecro-o CRSIS Fecro-o Clear Clear DUMOND/FCC,A4 Fecro-o CCAL Fecro-o Clear Clear FEZR3 Fecro-o FEZR3 Fecro-O-Demo HALITE Fecro-O-Demo HALITE Fecro-O-Demo	Image Image <th< td=""><td></td><td>mo pmo</td><td></td><td></td><td>+</td><td>Fe*3Va</td><td>298.15</td><td>6000</td></th<>		mo pmo			+	Fe*3Va	298.15	6000
CORUNDUM FeCro-c Parent Phase CR3Si FeCro-c Clear DUMOND_FCC_A4 FeCro-Demo 1	CORUNDUM Fecro-c Parent Phase CR35 Fecro-c Clear DUMOND/FCC,A4 Fecro-c Clear FEZR2 Fecro-c Fecro-c FEZR2 Fecro-c Fecro-c FEZR3 FeCro-Demo 1 FEZR3 FeCro-Demo 1 FEZR3 FeCro-Demo 1	CORUNDUM Fecro-c Parent Phase CR31 Fecro-c Clear UBA13 Fecro-c Clear DIMOND/FCC,M Fecro-Demo 1 FE2R3 Fecro-Demo 1 FE2R3 Fecro-Demo 1 HAUTE Fecro-Demo 1	CORUNDUM Fecro-c Darent Phase CRSI Fecro-c Clear ULBA13 Fecro-c Clear DUMOND/JCC,A Fecro-Demo 1 FEZR3 Fecro-Demo 1 FEZR3 Fecro-Demo 1 HAUTE Fecro-Demo 1 HAUTE Fecro-Demo 1	CORUNDUM Fecro-c Darent Phase CRSI Fecro-c Clear DUMOND/FCC,A Fecro-Demo 1 FEZR3 Fecro-Demo 1 FEZR3 Fecro-Demo 1 HAUTE Fecro-Demo 1		imo		T 10				
CR3si FeCro- CUB_A13 FeCro-2 DUMOND_CC_A4 FeCro-Demo 1	CR3D Fecro d Clear C08_A13 Fecro d Clear DMAOND_FCC_A Fecro demo 1 FC_A1 Fecro demo 1 FER2 Fecro demo 1 FER3 Fecro demo 1 FER4 Fecro demo 1	CRS1 FECO-0 Clear CUB_A13 FECO-0 Clear DUMOND_FCC_A4 FECO-0 1 FC_A1 FECO-0 1 FEZR2 FECO-0 1 FEZR3 FECO-0 1 HALTE FECO-0 1	CCRS1 FECO-0 Clear CUB_A13 FECO-0 Clear DUMOND_FCC_A4 FECO-0 1 FCC_A1 FECO-0 1 FEZR2 FECO-0 1 FEZR3 FECO-0 1 HALTE FECO-0 1	CCBS1 FECO-0					nase			
CUB_A13 FeCrO-Dlear DIAMOND_FCC_A4 FeCrO-Demo 1	CUB_A13 FeCro-D Lear DUMAOD_FCC,A FeCro-Demo 1 FECA FeCro-Demo 4 FEZR2 FeCro-Demo 1 FEZR3 FeCro-Demo 1 FeCro-Demo 1 FeCro-Demo HUITE FeCro-Demo 4	CUB_A13 FeCro_CEear DMMOND_FCC_A4 FeCro_Demo 1 FeCro_TER25 FeCro_Demo 4 FEZR2 FeCro_Demo 1 HALITE FeCro_Demo 4 HALITE FeCro_Demo 4	CUB_A13 FeCrO-Demo 1 FeCrO-Demo 1 FEZR2 FeCrO-Demo 1 FEZR3 FeCrO-Demo 1 HALITE FeCrO-Demo 4 VER.12 FeCrO-Demo 4	CUB_A13 FeCrO_Demo 1 FeCrO_Demo 1 FEZR3 FeCrO_Demo 1 FEZR3 FeCrO_Demo 1 HALITE FeCrO_Demo 4 VER_33 FeCrO_Demo 4		recio d =	ent Pha	se				
CUB_A13 FeCrO-D DIAMOND_FCC_A4 FeCrO-Demo 1	CUB_A13 FeCrO-Dimo DUMOND_FCC_A4 FeCrO-Demo 1 FCC_A1 FeCrO-Demo 4 FEZR2 FeCrO-Demo 1 FEZR3 FeCrO-Demo 1 FEZR3 FeCrO-Demo 1 FeLTD FeCrO-Demo 1	CUB_A13 FeCrO-Demo 1 FCC_A1 FeCrO-Demo 1 FCC_A1 FeCrO-Demo 1 FCC_A1 FeCrO-Demo 1 FEZR2 FeCrO-Demo 1 HALITE FeCrO-Demo 4 URD 12 FeCrO-Demo 4	CUB_A13 FeCrO-DEmo 1 FCC_A1 FeCrO-Demo 1 FCC_A1 FeCrO-Demo 1 FEZR2 FeCrO-Demo 1 FEZR3 FeCrO-Demo 1 HALITE FeCrO-Demo 4 URD 12 FeCrO-Demo 4	CUB_A13 FeCrO-D=mo 1 FCC_A1 FeCrO-Demo 1 FCC_A1 FeCrO-Demo 1 FEZR2 FeCrO-Demo 1 FEZR3 FeCrO-Demo 1 HALITE FeCrO-Demo 4 UTP 12 FeCrO-Demo 4		Cle	ar					
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	FEZR3 FeCrO-Demo 1 HALITE FeCrO-Demo 4	FEZR3 FeCrO-Demo 1 HALITE FeCrO-Demo 4	FEZR3 FeCr0-Demo 1 HALITE FeCr0-Demo 4	FEZR3 FeCr0-Demo 1 HALITE FeCr0-Demo 4								
	HALITE FeCrO-Demo 4	HAUTE FECO-Demo 4	HAUTE FCCO-Demo 4	HAUTE FECTO-Demo 4		FeCrO-Demo	1					
FEZR3 FeCrO-Demo 1			1/// 23 Fridd Dune / •									
	UCD 13 5000 Dume 14 12					FeCrO-Demo	1					
		Reaction Calculation	Reaction Calculation	Reaction Calculation	FEZR3 HALITE	FeCrO-Demo						
Reaction Calculation					FEZR3 HALITE	FeCrO-Demo	4		ulatio	n		

[Calculation screen]

📃 🔍 Data 📓 🤇	Calculation				
		🖧 Cell Reactor	Fe Cr O		Close
ed/Activity Condition	s			Default (Jnit: mol (formula)
lase	Spe	cies	Unit	Value	x 0.1
C_A2	Forr	nation Target	mol	0.03	× 0.1
	Fe		mol	b	
	Cr20	03	mol	x	
 Equilibrium Calc Phase Diagram Liquidus Projecti Solidification Sin 		Clear Feed		Set Default Va	alues Temperature (C) 1000 Pressure (bar) 1.01325 ✓ Transition Calc dGHSV Calc

(1) Right-click on the phase row to open the menu shown in the left figure, and specify the target phase.

The "Parent Phase" specifies the phase of the precipitation target.

(The Dormant phase is a phase that is not included in the calculation but whose stability is evaluated.)

"F" or "P" will appear in the left column of the phase name.

Then, back to the Calculation screen to set conditions.

1. Target calculation is performed in the equilibrium calculation mode.

2. The variable for the Target calculation is the quantity whose edit box is yellow. The variable can be changed by mouse-clicking on the label (upper right corner).

The phase amount can be specified, but since phase amounts often change discontinuously, we recommend that you first obtain an approximate value by series calculation and then refine it by Target calculation using that as the initial value.

④ Extended functions

[Data] panel

Condition Se	tting Utility		_				_
🕨 🔍 Data	Calculate	Fe Cr O			Close		
Phases	DataBase	Num	+	Species		T1(K)	T2(K)
Gas	IdealGas	9	+	CrO3		298.15	4000
BCC_A2	FeCrO-Demo	4	+	FeO3		298.15	4000
Corundum	FeCrO-Demo	6	+	Cr		298.15	4000
FCC_A1	FeCrO-Demo	4	+	Fe		298.15	4000
Halite	eCrO-Demo	4					
SIGMA	FeCrO-Demo	2					
Spinel	FeCrO-Demo	32					
Liquid	FeCrO-Demo	5					
Double click Ph	ase/Species to calculate	properties ir	ndividu	ally.			
Read	tion Calculation						

BCC_A2					CEM
SubLattice	Size	Constituent	Site Fraction	T (C)	0
0	1	Cr	b	D (here)	1.01325
		Fe	x	P (bar)	1.01325
1	3	0	b	×	0.5
		Va	x		
No SplitCh	eck con	straint for ORIGINA	AL PHASE!		
		straint for ORIGINA			Close
✓ Exe	ec Split	Check Set Initial			Close
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1) Double-click the Phase name.

The Property Calculation window appears.

In the Property Calculation window, the molar Gibbs Energy calculation and minimization calculation under for a set of specified chemical potentials can be performed. If you do not specify the [Exec Split Check] option, the initial value of Site Fraction is used as the initial value for the minimization calculation, and if you do, it will automatically try some of the initial values to find multiple minima of the Gibbs energy.

To calculate the Gibbs Energy of multiple phases at once, use the Individual phase energy calculation function in the [Calculation] panel.

④ Extended functions

📋 🔍 Data 🛛	ting Utility Calculate	Fe Cr O		Close	
Phases	DataBase	Num	+ Species	T1(K)	T2(K)
Gas	IdealGas	9	+ Cr	200	20000
BCC_A2	FeCrO-Demo	4	+ CrO	200	20000
Corundum	FeCrO-Demo	6	+ CrO2	200	6000
FCC_A1	FeCrO-Demo	4	+ CrO3	200	6000
Halite	FeCrO-Demo	4	+ Fe	200	20000
SIGMA	FeCrO-Demo	2	+ FeO	200	6000
Spinel	FeCrO-Demo	32	+ 0	200	20000
Liquid	FeCrO-Demo	5	+ 02	200	20000
			+ 03	200	6000
	ise/Species to calculate	properties in	ndividually.		

2) Double-click the Species name.

The <Properties> calculation dialog for the species appears.



roperty Calculatio	n	(
Cr		Chromium
DataFile	IdealGas.adb	т (с) 0
Code	М	5 (I.) I 01225
Reference	G 7/97	P (bar) 1.01325
Molar Weight	51.9961	
density	0	



3) Set the conditions and click the "Calculation" button.

You can calculate the individual G, H, etc. for each Species.

The [Utility]-[List Species] menu in the menu is useful when you want to calculate multiple species in a batch.

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Project		Summary	Lis	t						
Fe-xCr-yO #5		Cr		IdealGas.ad	ib					
Fe-xCr-yO #4		T (C)		P (bar)		G (kJ/mol)	H (kJ/mol)	S (J/molK)	V (L/mol)	Cp (J
Fe-xCr-yO #3 Fe-xCr-yO #2			0	1.013	325	349.8738	396,9603	172,3836	22.41396	20
Fe-xCr-yO #1			×.	11011		01010700	0,0,000	1, 1,0000	22112070	
-bat Fe-xCr-vC #4										
Mn-xFe #2										
Mn-xFe #1										
- 🙀 AlN-xAl2O3 #1										
🛕 Al-xMg-yZn #7										
- 🙀 1Ca(OH)2-CO2 #3										
🛕 Fe-xCr-yC #3										
A Fe-xCr-yC #2										
🛕 C-xCr-yFe #6										
A Fe-xCr-yC #1										
A C-xCr-yFe #5										
🛕 C-xCr-yFe #4 🛕 C-xCr-yFe #3										
🛦 C-xCr-yFe #2										
- A C-xCr-yFe #2 - M Fe-0.1Cr-O2 #1										
- 🛦 C-xCr-yFe #2 - 🕁 Fe-0.1Cr-02 #1 - 🕁 C-xCr-yFe #1	Ш									
←▲ C-xCr-yFe #2 →₩ Fe-0.1Cr-02 #1 →₩ C-xCr-yFe #1 → Cr-xFe-yO #1	l									
← ▲ C-xCr-yFe #2 ← Fe-0.1Cr-02 #1 ← ← C-xCr-yFe #1 ← C-xFe-yO #1 ← C-xFe #2	l									
	l				_					
← C-XCr-yFe #2 ← E-0.1Cr-O2 #1 ← C-XCr-yFe #1 ← C-XCr-yFe #1 ← C-XCr+Fe #2 ← 1Ca(CH)2-CO2 #2 ← 1Ca(CH)2-CO2 #1	l									
		Calculation '								
	•	Calculation DataFile: C:	¥US	ERS¥SHOBL			TCALC¥DATA¥Ide TCALCXE¥DATA¥I		в	

Display of calculation results

(5) Notes on calculation conditions

Selection of phases and species to be included in calculations

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Calculation Assessment Database	es Help						
		A Data	Calculation	Assessment O Ex	it)		
	Summary Plot	List					
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ep Calc for (Cr-Fe-O) #5	Database-Info:	Fe-Cr-	O_Demo system. !				
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Reaction Calculation

nits (C, mol)

1. Click the [Data] button.

The Data panel will be displayed.

For example, if you select "Gas" in the <Phases> list and uncheck the "Fe" in the <Species> list, the calculation does not take "Fe" in the Gas phase into account.

2. After setting, click [Calculation].

Go to the "Calculation" panel.

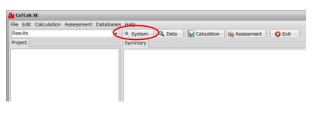
V-2. Phase diagram calculation

①Procedure to calculate phase diagrams

The calculation procedure is the same for both binary and ternary systems. The following is a detailed example of a ternary phase diagram calculation.



By double-clicking the shortcut key, CaTCalc is launched.





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Na	Mg											A	si	Р	S	CI	Ar	
К	Ca	Sc	Ti	٧	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	Include Extra Components
Rb	Sr	Υ	Zr	Nb	Мо	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	Ι	Xe	Include Volume (if available)
Cs	Ba	*	Hf				Os					TI	Pb	Bi	Po	At	Rn	Max carbon in organics 2
Fr	Ra	**					Hs											OR search
	*						Sm											
	**	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		Clear Load
+	DB	Nam	e			N	otes											
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		ELiq.					ire li											
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1. Press 💽 System button.

The "Element Selection" screen will appear.

2. Click elements.

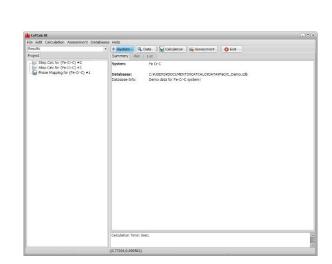
The thermodynamic data files containing the element will be listed in the data file area.



Next page

① Phase diagram calculation procedure

						Util					-							
1		۹ ۵	Pata	10	d c	alcul	ate				Fe (Cr C						Close
K Rb Cs	Sr Ba		Zr Hf	Nb Ta	Mo W	6 Mn Tc Re Bh	Ru Os	Co Rh Ir	Pd Pt	Ag Au	Cd Hg	B Al Ga In	C Si Ge Sn	N P As Sb	Те	E F Cl Br I	Xe	Specify by Files Include Ionic Gas Species Include Aqueous Phase Include Extra Components Include Volume (if available) Max carbon in organics 2 OR search 2
~	FeC Idea	Ac Nam rC_D	Th e emo	Pa	U	De	Pu otes emo eal (Am data Gas s	Cm for	Bk Fe-(cf	Es	Fm					Clear
		Eliq.a					ire li ire s											(4





3. Select the data file.

Check the cell next to the DB Name to set "+".

4. Click [Load] button.

You will see the information of the DB you selected in the "Summary" tab of the main screen.

Detailed information on the database will be displayed by clicking the [Data] button.

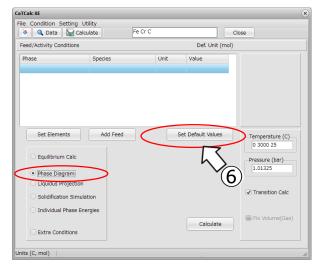
[Data] screen

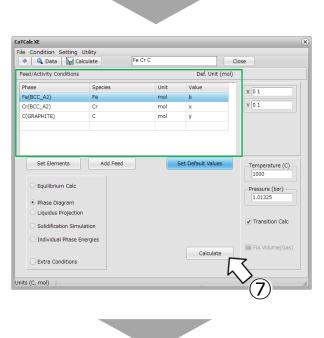
Name Database Num + Species TL(K) T2(K) T2(K) <tht2(k)< th=""> T2(K) T2(K)</tht2(k)<>	in I con I hi	tting Utility	Fe Cr C			Close		
Ligaid FPGCC_Demis 3 C 2015.15 4000 FCC_A1 FPGC_Demis 4 HCPLA3 FPGC_Demis 4 HCPLA3 FPGC_Demis 4 SolVA FPGC_Demis 4 SolVA FPGC_Demis 2 Graphite FPGC_Demis 2 HCG3 FPGC_Demis 2 HCG4 Double click Phase/Species to calculate properties individually.				-		Close		
ECC_A2 FeCC_Demo 4 • Or 298.15 6000 FCC_A1 FeOC_Demo 4 • Fe 298.15 6000 + KPC_A3 FeOC_Demo 4 • Fe 298.15 6000 + KSTAA FeOC_Demo 2 • Graphte FeOC_Demo 2 • Graphte FeOC_Demo 2 • M32G3 FeOC_Demo 2 + M325 FeOC_Demo 2 • M31C2 FeOC_Demo 2 M31C2 FeOC_Demo 1 • M31C2 FeOC_Demo 2	+ Phases			+				
				Jacob State				
+ ICP_A3 FeoC_Demo 4 > GOMA FeoC_Demo 2 + Graphite FeoC_Demo 1 + Constrite FeoC_Demo 2 + N205 FeoC_Demo 2 + N205 FeoC_Demo 2 + N202 FeoC_Demo 2 > NUC2 FeoC_Demo 1	+ BCC_A2			+	Cr		298.15	
\$1074. FPGC_Dem 2 Graphite FPGC_Dem 1 Cimentitie FPGC_Dem 2 H226 FPGC_Dem 4 MC3 FPGC_Dem 2 MC2 FPGC_Dem 1 Double click Phase_Species to calculate properties individually.				+	Fe		298.15	6000
Graphite FPGCC_Dema 1 FPGCC_Dema 2 H32G5 FPGCC_Dema 4 H32G5 FPGCC_Dema 2 H32G2 FPGCC_Dema 1 Double click Phase/Species to calculate properties individually.	+ HCP_A3	FeCrC_Demo	4					
Commente FeCT_Demo 2 HV3C6 FeCT_Demo 4 HV1C3 FeCT_Demo 2 HUC2 FeCT_Demo 1 Double clok Phase/Species to calculate properties individually.	+ SIGMA	FeCrC_Demo	2					
HV3C5 FPGC_Dems 4 HV5 FPGC_Dems 2 HV5 FPGC_Dems 1 Double click Phase/Species to calculate properties individually.	+ Graphite	FeCrC_Demo	1					
HTC3 PEOC_Demo 2 HC2 PEOC_Demo 1 Double click Phase/Species to calculate properties individually.								
H3C2 PECC_Demo 1 Double click Phase/Species to calculate properties individually.	+ M23C6	FeCrC_Demo	4					
Double click Phase/Species to calculate properties individually.	+ M7C3	FeCrC_Demo	2					
	+ M3C2	FeCrC_Demo	1					
			e properties	indiv	idually.			

① Phase diagram calculation procedure



5. Click the [Calculation] button.





The Calculation screen is displayed.

The following shows how to use [Set **Default Values**] to set conditions. If you want to use [Set Elements] / [Add Feed], please refer to page 48 and 49.

Check that "Phase Diagram" is selected as the calculation type.

6. Click the [Set Default Values] button.

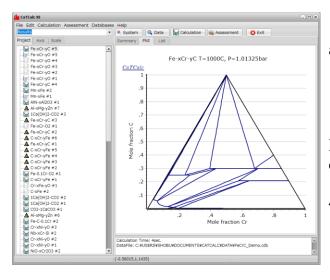
Typical values are set for the Feed/Activity Condition. For a ternary system, an isothermal phase diagram calculation is selected.

7. Press the [Calculate] button.

The phase diagram calculation starts.

Next page

① Phase diagram calculation procedure



The results will be displayed automatically.

From the next page, following items will be explained:

Changing the calculation conditions (p. 48)

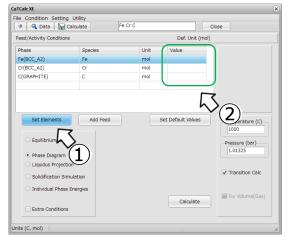
- ◆ Edit the results (P.51)
- ◆ Use the [Data] screen (P.53)

② Changing the conditions for Feed

- ◆ There are three ways to set up the Feed.
- 1. Use the [Set Elements] button
- 2. Use the [Add Feed] button
- 3. Specify in the Data screen

CaTCalc XE

1. Use the [Set Elements] button



① Click the [Set Elements] button.

The elements in the standard state will be set in [Feed / Activity Conditions].

(2) The Value value can be entered manually, or by pressing [Set Default Values] button. In this case, you can also use b,x,y.

2. Use the [Add Feed] button. Feed can be of any composition.

File Condition Setting Uti		Fe Cr C			Clos	2 0
Feed/Activity Conditions				Def. Unit		
Phase	Species	U	nit	Value		
Set Elements Equilibrium Cale Phase Diagram Liquidus Projection Solidification Simulati Individual Phase Ener		ح 1	Set	Default Value		Temperature (C) 1000 Pressure (bar) 1.01325 Transition Calc Fix Volume(Gas)
Units (C, mol)						
File Condition Setting Ut		5.0.0			1	
🍳 🔍 Data 🛛 🙀 Calcu		Fe Cr C	_	Def Uni	Ck	
	Species	U	Jnit nol Set	Def. Unit Value	es	
Calcul Calcul	Species	U	nol	Value	es	Temperature (C) 100 Pressure (bar) 1.01325 Transition Calc

1 Click the [Add Feed] button.

A single blank row will be inserted in the [Feed / Activity Conditions] list and if you leave Phase name as "---", you can manually enter a desired composition in the Species column.

② If you click the [Phase] cell, you can choose from the list.
*Note: "Material" of mixed compositions is described in page 67.

🤌 🔍 Data	Calculate	Fe Cr C		Close
+ Phases	DataBase	Num	+ Species	T1(K) T2(K)
+ Liquid	FeCrC_Demo	3	+ Cr	298.15 6000
+ BCC_A2	FeCrC_Demo	4	+ Fe	298.15 6000
+ FCC_A1	FeCrC_Der	7 4	+ C3Cr	298.15 6000
+ HCP_A3	FeCrC_Der	4	+ C3Fe	208 15 6000
+ SIGMA	FeCrC_Demo	0	Eeed Species	s (Reactants)
+ Graphite	FeCrC_Demo	(1)		
+ Cementite	FeCrC_Demo	Ŀ	'	
+ M23C6	FeCrC_Demo	4		
+ M7C3	FeCrC_Demo	2		
+ M3C2	FeCrC_Demo	1		
	hase/Species to calculate	properties	individually.	

3. Set Feed in the [Data] screen.

(1) On the Data screen, select a Phase that includes a Species that you want to use as a feed, then select the Species from the list of Species and set it as a Feed Species in the pop-up menu that appears by right-clicking the mouse. Only species or pure stoichiometric phases can be set for Feed.

le Condition Set		_			-		
🤌 🔍 Data 🛛	Calculate	Fe Cr C			Close		
+ Phases	DataBase	Num	+	Species		T1(K)	T2(K)
+ Liquid	FeCrC_Demo	3	+	CFe3		298.15	6000
+ BCC_A2	FeCrC_Demo	4	+	CCr3		298.15	6000
+ FCC_A1	FeCrC_Demo	4					
+ HCP_A3	FeCrC_Demo	4					
+ SIGMA	FeCrC_Demo	2					
+ Graphite	FeCrC_Demo	1					
+ Cementite	FeCrC_Demo	2					
+ M23C6	FeCrC_Demo	4					
+ M7C3	FeCrC_Demo	2					
+ M3C2	FeCrC_Demo	1					
Double click Pha	ase/Species to calculate	properties	indivi	idually.	Feed Specie C3Fe in BC CFe3 in Ce	C_A2	culation

🧎 🔍 Dara 🛛 🖥	Calculate			Close
ed/Activity Condition	ions		Def. Un	it (mol)
hase	Species	Unit	Value	
ICC_A2	FeC3	mol		
ementite	Fe3C	mol		
Set Elements	Add Feed		Set Default Valu	JesTemperature (C)
 Equilibrium C Phase Diagram Liquidus Proje Solidification 	m			1000 Pressure (bar) 1.01325 ✓ Transition Calc

(2) The selected Feeds will be set in the Feed/Activity field of the Calculation screen, and will be displayed in a list as shown in the left figure, which can also be viewed on the Data screen (deletion from this list is not possible, so it will be done on the Calculation screen).

③ When you go to the Calculation screen, the Feed is set. This method is most useful for calculations of enthalpy changes associated with the reaction.

Recommendations

1. General reaction calculation: Use of the [Data] screen

2. Phase diagram calculation of metallic systems: [Set Elements]

3. Calculation of ceramics systems: [Add Feed] or the [Data] screen

Of course, combinations are possible.

Removing Feed settings

e Condition Settin	Calculate C Cr Fe		Close	
eed/Activity Conditions	5		Default Unit:	mol (formula)
Phase	Species	Unit	Value	× 0 1
C(GRAPHITE)	С	mol	b	
Cr(BCC_A2)	Cr	Delete		Y 01
Fe(BCC_A2)	Fe	Clear All		
Set Elements	Add Feed Clear	Feed	Set Default Values	Temperature (C)
Set Elements Equilibrium Calc Phase Diagram Liquidus Projecti		Feed	Set Default Values	Temperature (C)- 1000 Pressure (bar)- 1.01325 V Transition Calc
Equilibrium Calc Phase Diagram	pn	Feed	Set Default Values	Pressure (bar) 1.01325
Equilibrium Calc Phase Diagram Liquidus Projecti	on	Feed	Set Default Values	Pressure (bar) 1.01325

① Press the [Clear] button to clear everything.

(2) You can delete the target line of the list by [Ctrl] + left mouse click. Alternatively, as shown in the left figure, you can use the pop-up menu with the right button (depending on where you click, the pop-up may not appear. Try a different position).

Notes on the formula of Feed

There are restrictions on the format that can be set for Feed, as shown in the following example:

OK
OK
Not OK
Not OK
OK
OK

In general, when the last character of a chemical formula that ends with a right parenthesis, the part enclosed by the parenthesis is not recognized as a part of the formula, but as ancillary information. Ancillary information includes, for example, information that distinguishes the isomers of an organic substance.

Also note that **mol of Feed is always mole of formula units, and not mole of atoms**. You can set the mole of atoms as the standard output type in Preferences. If you want to set the mole of atoms in Feed, you should always use the "Elements" to specify Feeds.

② Changing the conditions for Feed (gas pressure)

◆You can also specify the chemical potential or gas partial pressure as a feed. Since calculations using the oxygen partial pressure (0.21 bar) as the atmospheric pressure at 1 atm are often performed, we have registered the condition in the dropdown menu so that it can be set easily. The default value is log(0.21)=-0.6777807 from the partial pressure of oxygen in the atmosphere, but it can be changed to any oxygen partial pressure.

eed/Activity Conditi	one			Default Unit: r	mol (formula)
					i (i or mula)
Phase	Specie	s	Unit	Value	x 0 1
	Fe2O3		mol	b	
	Cr2O3		mol	x	
	-		mol		
 Material	<u> </u>				
Cr(BCC_A2) Fe(BCC_A2) O(1/2_O2_Gas) Set Elements	-				
Set Elements Equilibrium C Phase Diagra Liquidus Proje	m	Clear Feed		Set Default Values	Temperature (C) 0 3000 Pressure (bar) 1.01325
 Equilibrium C Phase Diagra 	alc m ection Simulation	Clear Feed		Set Default Values	Pressure (bar)

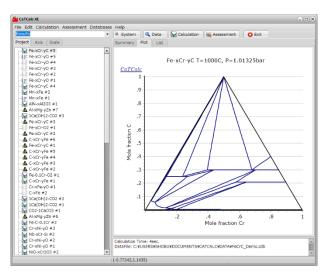
When controlling P(O2), the so-called buffered gas mixture method is sometimes used to control gas pressure ratios such as CO2-CO and H2O-H2. In this case, P(O2) varies depending on temperature, and Virtual_Gas is provided to perform calculations under such conditions. For example, by controlling P(CO2)/P(CO) ratio, P(O2) can be controlled as shown in the figure below. For now, the ratio is limited to less than 1. Choose log10(P) as the Unit and give the logarithm of the P(CO2)/P(CO) ratio in Value. Note that although only the P(O2) is considered in this method, in reality the chemical potential of carbon is also determined, so carburization, etc., may occur, and particular attention should be paid.

🝳 📔 🔍 Data 🛛 🕍 Cal	culation O Fe Cr		Close	
eed/Activity Conditions			Default Uni	t: mol (formula)
Phase	Species	Unit	Value	x 0 1
	Fe2O3	mol	b	
	Cr2O3	mol	×	
Virtual Gas CO2/CO	• 0	mol		
P(O2)_in_atmosphere	^			
Fe(BCC_A2) O(1/2_O2_Gas)	=			
Virtual Gas H2O/H2	dd Feed Clear Fee	ed	Set Default Value	es Temperature (C)
Equilibrium Calc		ed.	Set Default Value	-Temperature (C)-
Virtual_Gas_H2O/H2 Set Elements	dd Feed Clear Fee	ed.	Set Default Value	Pressure (bar)
Virtual Gas_H2O/H2 Set Elements A Equilibrium Calc Phase Diagram Liquidus Projection	add Feed Clear Fee	ed	Set Default Value	0 3000 Pressure (bar) 1.01325

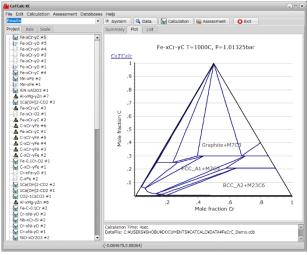
If you want to specify the partial pressure of other gases or the activity of other species, use the method of using the aforementioned data screen to select the component of the relevant phase as the Feed, and then click on the Unit column of Feed/Activity Conditions to select and set the activity specification.

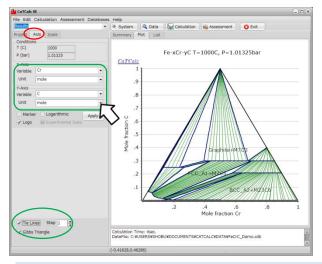
CaTCalc				
File Condition Setting Uti	lity			
🔄 🔍 Data 🔤 Calcula	ition 🛛 🔩 Cell Reactor	C O Ca		Close
Feed/Activity Conditions			Default Unit: mo	l (formula)
Phase	Species	Unit	Value	x -30 0
	CaCO3	mol	1	× 30 0
Gas	CO2	log10(P)	×	
		mol g log10(P) RTin(P)		
Set Elements Add Equilibrium Calc Phase Diagram Liquidus Projection	Feed Clear Feed		Set Default Values	Temperature (C) 0 3000 Pressure (bar) 1.01325
 Solidification Simulatio Individual Phase Energy 				Transition Calc
Extra Conditions			Calculate	Fix Volume(Gas)
Units (C, mol) Set units from	n the pop-up menu.			

③ Edit the diagram



If the shape of the resultant figure is out of the equilateral triangle, please adjust the whole frame of CaTCalc. In addition, you can move the boundary between Plot area and Note area.





To add a label (phase name) to a phase region

Put your mouse over the area you want to name and click [Ctrl] + left mouse button. Then the phase name of the area will be displayed.

If you want to show the Tie Lines:

Select the [Axis] tab in the left pane. If you check the "**Tie Lines**" box, they will appear in green, as shown in the figure.

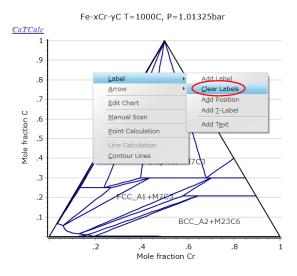
If you want to change the elements of X and Y:

Change the variables of "X-Axis" or "Y-Axis" and click the [Apply] button.

Tie-Line: a line connecting the points that indicate the compositions of two coexisting phases.

③ Edit the diagram

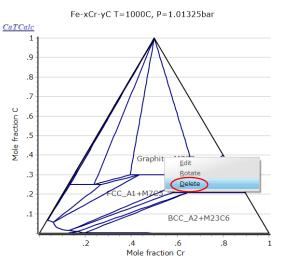
Remove all



To remove the label (phase name) of a phase region

Remove all: Right-click on the graph to display the pop-up menu. Delete all labels by [Label]-[Clear Labels].

Remove each label



Remove a label: Select the phase label you want to delete by moving mouse cursor to the center of the label, and right click on the phase label and select [Delete] in the pop up menu.

You can use the [Edit Chart] pop-up menu, which appears when you rightclick on the chart, to edit the chart in more detail.

For detailed editing of each line, please use the edit box that appears when left-double-clicking the line. You can also double-click each label to open the edit box.

④ Overlaying the experimental points

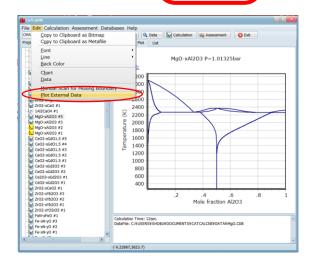
F	ם יר י ה			
ファ	イル ホ-	-ム 挿入	ペー	ジレイアウト 数式 データ れ
E7	Ŧ	: ×	$\sqrt{-f_3}$	=B7-273.15
	А	в	С	F
1	X(Al2O3)	т(к)		X(Al2O3) T(C)
2	0.028853	2633.31		0.028853 2360.16
3	0.053753	2389.27		0.053753 2116.12
4	0.08	2249		0.08 1975.85
5				
6	0.06579	2227.92		0.06579 1954.77
7	2.82E-02	2128.83		0.0282 1855.68
8	0.015038	1971.74		0.015038 1698.59
9	0.003759	1777.43		0.003759 1504.28
10				
11	0.06015	2972.31		0.06015 2699.16
12	0.140977	2727.99		0.140977 2454.84
13	0.317669	2249		0.317669 1975.85
14	0.317669	2249		0.317669 1975.85
15	0.370301	2317.64		0.370301 2044.49
16	0.5	2378		0.5 2104.85

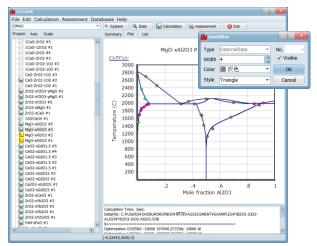
This section shows how to add experimental data to the calculation results.

Copy the experimental data to the clipboard as X-Y data with the titles. Pay attention to scales, such as temperature units.

Group the data by empty rows. Marker colors are automatically set for each group.

Click [Edit]-[Plot External Data] in the menu to plot the data.





Edit Marker: Double-click on a marker and an edit box will appear.

Delete: select the marker and use the [Delete-Series] in the right mouse button pop-up menu.

🤌 🔍 Data	Calculate	Fe Cr C		Close	
+ Phases	DataBase	Num	+ Species	T1(K)	T2(K)
+ Liquid	FeCrC_Demo	3	+ C	298.15	6000
+ BCC_A2	FeCrC_Demo	4	+ Cr	298.15	6000
+ FCC_A1	FeCrC_Demo	4	+ Fe	298.15	6000
HCP_A3	FeCrC_Demo	4			
⊢ SIGMA	FeCrC_Demo	2			
+ Graphite	FeCrC_Demo	1			
+ Cementite	FeCrC_Demo	2			
+ M23C6	FeCrC_Demo	4			
+ M7C3	FeCrC_Demo	2			
+ M3C2	FeCrC_Demo	1			
Double click Ph	ase/Species to calculate	properties	individually.		
	tion Calculation				

Details of the data selected on the System screen are displayed.

Phase: list of phases

Species: The list of species that comprise the selected phase

Reaction Calculation: Open a panel to calculate chemical reactions

④ Extended functions (Reaction Calculation)

DataBase FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo	Num 3 4 4 2 1 2 1 2 4 2	++	Species C Cr Fe	T1(K) 298.15 298.15 298.15	T2(K 6000 6000 6000
FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo	4 4 2 1 2 4 2	+	Cr	298.15	6000
FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo	4 4 2 1 2 4 2				
FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo	4 2 1 2 4 2	+	Fe	298.15	6000
FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo	2 1 2 4 2				
FeCrC_Demo FeCrC_Demo FeCrC_Demo FeCrC_Demo	1 2 4 2				
FeCrC_Demo FeCrC_Demo FeCrC_Demo	2 4 2				
FeCrC_Demo FeCrC_Demo	4 2				
FeCrC_Demo	2				
FeCrC_Demo					
	1				
e/Species to calculate		indiv	ridually.		
				z/Species to calculate properties individually.	

[Reaction Calculation]

It performs individual chemical reaction calculations specifying reactants and products. The overall reaction, which takes into account all reactions, is calculated in the equilibrium calculation of the Calculation screen.

ا 🔍 🚺	Data 📔 🙀 C	alculate		Fe Cr C				Close	2	
Phases		DataBase		Num	+	Spec	cies		T1(K)	T2(K)
Liquid		FeCrC_Den	no	3	+	Cr22	Fe8		298.15	6000
BCC_A2		FeCrC_Der	no	4	+	Cr4F	e26		298.15	6000
FCC_A1		FeCrC_Den	no	4				reactant I		
HCP_A3		FeCrC_Den	no	4			Add to	product lis	st	
SIGMA		FeCrC_Den	no	2						
Graphite	2	FeCrC_Den	no	1						
Cement	ite	FeCrC_Den	no	2						
M23C6		FeCrC_Den	no	4						
M7C3		FeCrC_Den	no	2						
- M3C2		FeCrC_Der	no	1						
	1							-		
	Phase		Speci	es			mole	Ba	lance Re	action
eactants	BCC_A2		Cr				1			
	BCC_A2		Fe				13/2		mperatur	
									2000 10	
roducts	SIGMA		Cr4Ee	26			1/4		essure (b .01325	ar)
			0.410							
								Calcul	ate	Close

Conception of the second of th

Reactants and products can be set up in the pop-up menu of the Species list after pressing the [Reaction Calculation] button, and opening Reactants and Products sheets.

You can automatically balance the reaction scheme by pressing the [Balance Reaction] button.

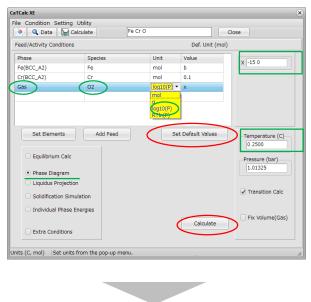
Set the temperature and pressure, and press [Calculate] button to start the reaction calculation.

The result will be displayed as a plot for the continuous calculation, or as a List for the one-point calculation. Note that the result of the reaction calculation is not saved automatically. If you want to save it, please use [Edit] in the menu and save it manually.

⁽⁵⁾ Potential diagram

Potential diagrams can be calculated in the same way as phase diagrams.

ile																		
	Cor	nditi	on	Set	ting	Util	lity											
		Q, C	ata		Чc	alcul	ate				Fe (Cr O						Close
0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	Specify by Files
н																E	He	Include Ionic Gas Species
Li Na	Be											B	C Si	N P	0 S	F	Ne Ar	Include Aqueous Phase
K	Ca	Sc	Ti	v	Cr	Mn	Fo	Co	NI	0	Zn				-		Kr	Include Extra Components
Rb	Sr	Y	Zr		_	Тс	_									I	Xe	Include Volume (if available)
Cs	Ba	*	_	Та						-	Hg							Max carbon in organics 2
Fr	Ra	**	Rf	Db	Sg	Bh					-							OR search
	*	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	ть	Dy	Но	Er	Tm	Yb	Lu		
	**	Ac	Тh	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		Clear Load
3	DB	Nam	e				No	tes										
		10-D			В							en f	rom	R. L	uom	a, P	hD Tl	hesis, Helsinki Uni., 2002, ISBN 951-6
		lGas)				eal G			eis							
		Liq.a						re lio re so										
	Pure	:501.4	aub				Pu	re su	mus									
nits	(C,	mol)																



1. Select Fe, Cr, O on the System screen. *Select FeCrO_Demo.cdb and IdealGas.adb here.

2. Click the [Load] button.

• Reads the thermodynamic data.

• Set the calculation conditions on the Calculation screen.

3. The type of calculation is "Phase Diagram"

4. Click on [Set Default Values].

• Change the default value as follows: Click on the "Phase" O (Gas) with your mouse to bring up the pull-down list and select "Gas". Do the same for "Species" and select "O2". Finally, change "Unit" to "log10(P)" (partial pressure).

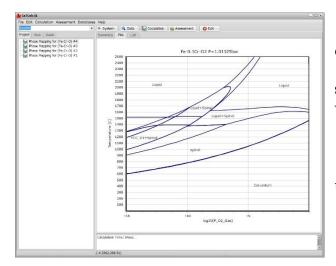
• Set the Value of Fe and Cr to b and 0.1, respectively, and the Value of O2 to x.

• Specify the temperature and x-value as shown in the figure.

5. Click "Calculate".

Next page

(5) Potential diagram



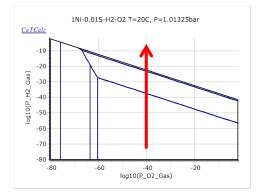
• The result of the calculation will be displayed.

Depending on the conditions, it may take some time to calculate, but please wait for a while.

* In the left figure, [Cntl] + left click is used to label the phase names.

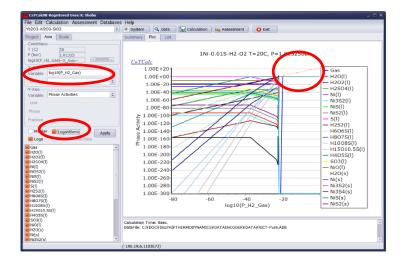
* Note: In this case, b = 1 - y. That is, the O2 amount, which is determined as a result of the activity specification calculation, is not included in the total amount: b.

* Unstable Regions in Potential diagrams



• Sometimes labeling may show area that is labeled "Unstable" or "Error". If this happens, use the equilibrium calculation to check the cause.

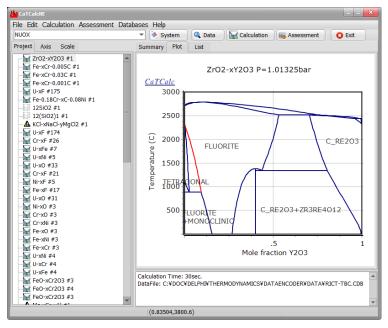
• The left figure shows the results of the equilibrium calculation along the red line as an example. If you display the phase activity, you will see that there are phases with activity greater than 1. Namely, the equilibrium state cannot be achieved under the condition.

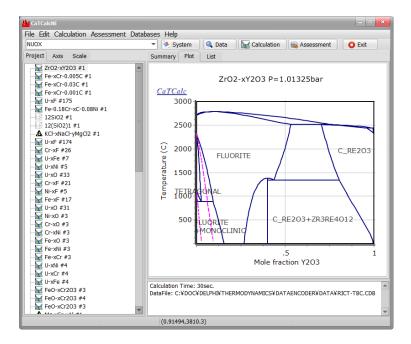


• You can find out the phase name by doubleclicking the line to display the Editor.

⁽⁶⁾ T0-Line calculation

T0-temperature is the temperature at which two phases of the same composition have the same Gibbs energy. The T0-temperature is important in diffusionless transformations such as martensitic transformations.





• Here is an example of a T0 line calculation for martensitic transformation in the system ZrO2-Y2O3.

• In this system, the martensitic transformation from the cubic Fluorite phase to the tetragonal phase occurs.

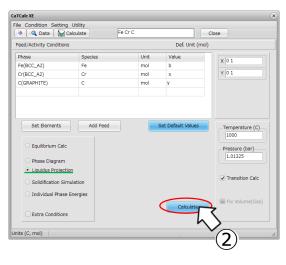
• Select the phase boundary line shown in red, and press [**T0-line Scan**] of the right button menu to automatically calculate the T0 temperature line.

• The T0 line from Tetragonal to Monoclinic phase is also calculated, and the results are shown in the left figure.

V-3. Liquidus projection

① Liquidus projection calculation

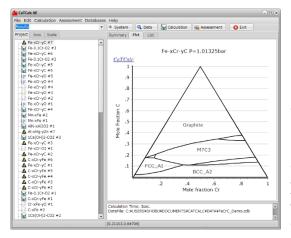
The liquidus projection diagram is represented by Univariant Line and Isotherms (temperature contours). Calculate the Univariant Line first. Usually, the Univariant Line calculation is two dimensional (2D) in a 3-component system, but in a general case of multi-component system, the Univariant Line can be calculated from 1D to 6D.



1. Use FeCrC_Demo.cdb to read the data of the Fe-Cr-C system.

2. Select "Liquidus Projection" as the type of calculation and click [Set Default Values].

- 3. Click the [Calculate] button.
 - The calculation starts.



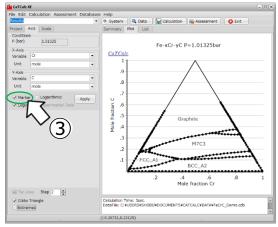
• The liquidus projection diagram will be displayed. Labeling is done as needed.

* The phase label in the liquidus projection diagram is the phase name of the primary phase (the solid phase that first crystallizes out of the liquid phase as the temperature decreases).

*Note: The upper limit of liquidus temperature is set to 4000K.

① Liquidus projection calculation

Marker

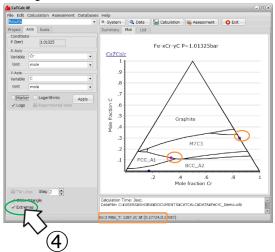


3. Check the "Marker" checkbox in the [Axis] tab.

• Marker indicates a calculation point. You can see the calculation point on the axis.

* Note: The liquidus temperature calculation is made to an upper limit of 4000K.

Temperature extremes



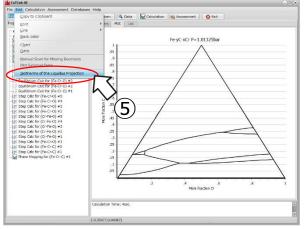
4. Check "Extremes" in the [Axis] tab.

* "Extremes" display temperature maxima (red) and minima (blue), e.g. on a Univeriant Line.

• If you hold down the Shift key and move the mouse over these extreme points, the information will be briefly displayed in the Status bar at the bottom of the screen.

① Liquidus projection calculation

X



Calculation of isotherms

Isothermal Curve

Highest Temperature : 3726.85 C Lowest Temperature : 1150.665 C Optimal setting: 1200 3700 100

Number of Isothermal Planes: 26

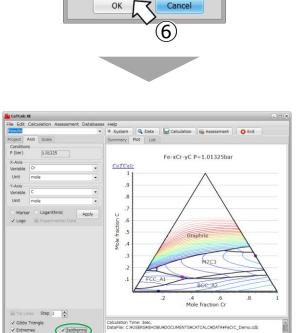
OK

Isothermal Scanning 1200 3700 100

5. Select "Isotherms of the Liquids Projection" from the menu, or select "Isothermal Curve" of the pop-up menu in the Plot screen.

• The <Isothermal Curve> screen will be displayed, which will automatically calculate and display the best setting based on the information obtained from the Liquidus Projection calculation. You can change the settings (Start value, End value, and Step value) as necessary.

- 6. Click the OK button.
 - Isothermal curve calculation starts.



-0.11009.-0.14844

* In the [Axis] tab, an "Isothermal" checkbox appears. The display of isotherms can be turned off or on here.

* [Edit Chart] in the pop-up menu allows you to make more detailed settings.

* The upper temperature limit for liquid phase line detection is internally set to 4000 K, and isotherms above this limit will not be calculated.

Taking the above 2D case as an example, the algorithm for a three-component liquidus projection calculation is as follows:

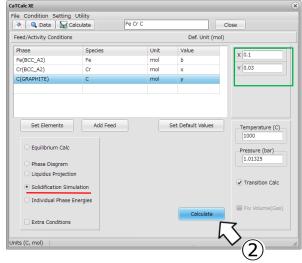
- (1) The liquidus point is detected at each end-member composition of (X,Y) = (0,0), (0,1), and (1,0).
- (2) Define the liquidus univariant lines of the three two-component systems with these liquidus points as the initial endpoints. Then the endpoints of the liquidus univariant lines of the three-component system are determined, and
- (3) Finally, the Univariant-line of the three-component system is traced from these endpoints.

Therefore, in the case of three-component systems, detection of liquidus univariant lines would be perfect in most cases.

However, in a multi-component system of four-components and more, the procedure is simplified. That is, according to the order of the parameters (X,Y,Z,W,A), firstly, the liquidus point is detected with a single point composition (component for the balance) with all the other parameters as zero, then the liquidus univariant line of 2D for B-X, then the line of 3D for (B,X,Y), then the line of 4D for (B,X,Y,Z) and so on... to define the Univariant line of the multi-dimensional system. Therefore, it is necessary to calculate the ND univariant line by swapping the parameters. Note that the ND Extreme is only on the liquidus lines. The other phase than the liquid phase can be selected as the parent phase by specifying the target phase in the phase list (see VII).

V-4. Solidification simulation

In the solidification simulation, all the calculation conditions are set to single fixed values.



1. Load thermodynamic data from the FeCrC_demo.CDB. Then, select "Solidification Simulation" as the calculation type, press "Set Default Values", and modify the settings as shown in the left figure.

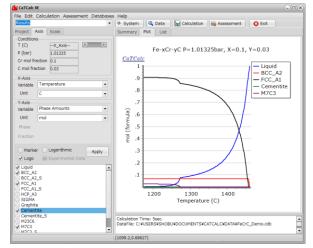
2. Click the [Calculate] button.

Cooling Simulation Scheil-Gulliver Equilibrium Back Diffusion C T-Step -1 OK Cancel 3

3. "Cooling Simulation" dialog appears.

• Click the [OK] button without checking the box for "Back Diffusion" in the present case.

* The simulation that takes into account the diffusion of C is called a para-equilibrium calculation.



• After the calculation, the graph is automatically displayed. For more information on solidification simulation and the meaning of the results, please refer to books and/or literature.

V-5. Adiabatic calculation

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+ Pur + Pur								quids	3								2

e Condition Setting Uti				Clo	se
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Phase	Species (3)	Unit	Value		
C(GRAPHITE)	c U	mol	1		
SI(DIAMOND_A4)	Si	mol	1		
Set Elements	Add Feed	5	Set Default Val	Jes	Temperature (C)
Equilibrium sale Phase Diagram Liquidus Projection	4 • H-S Targe • dH • dB • S • Fix Feed	et Condition	Set Default Val	Jes	Temperature (C) 0 3000 Pressure (bar) 1.01325 ✓ Transition Calc
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1. In the System screen, specify Si and C and select IdealGas.adb, PureLiq.adb and PureSol.adb.

- 2. Click the [Load] button.
 - Load data from the selected DBs.

3. Click the [Calculate] button.

- 4. Click the [Set Elements] button.
 - Set the value of Value to "1" for each.
 - · Check "Equilibrium Calc".

• Check the "Extra Conditions" and "H-S Target" boxes, and then select the "Fix Feed Condition". Set the temperature to 1400°C. This is because the reaction starts rapidly at this temperature.

The color of the "Temperature" edit box changes to yellow to indicate that the temperature is the target variable to be calculated.

5. Click [**Calculate**] to perform the calculation.

• The result of the calculation will be displayed.

* The adiabatic reaction temperature is close to 2800 °C, and the solid phase SiC is produced. This means that the temperature increased due to the heat of reaction between Si and C.

V-6. Individual Phase Energy

The energy calculations for individual phases are useful when comparing the behavior of the Gibbs energy of each phase at a time. It can also calculate the enthalpy and entropy of mixing of each phase, the change in phase composition, as well as the Curie temperature of a magnetic phase.

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+ Liquid	FeCrC_Demo	3		Cr		298.15	6000
+ BCC_A2	FeCrC_Demo	4	_	Fe		298.15	6000
+ FCC_A1	FeCrC_Demo	4	-	C3Cr		298.15	6000
+ HCP_A3	FeCrC_Demo	4		C3Fe		298.15	6000
+ SIGMA	FeCrC_Demo	2	-				
+ Graphite	FeCrC_Demo	1					
+ Cementite	FeCrC_Demo	2					
+ M23C6	FeCrC_Demo	4					
+ M7C3	FeCrC_Demo	2					
+ M3C2	FeCrC_Demo	1					
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Cr(BCC_A2)	Cr		mo			Y 0.1	
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Calculate

1. Select the target phases on the Data screen.

2. Set the calculation conditions on the Calculation screen.

- Check "Individual Phase Energy".
- Click the [Set Default Values] button.

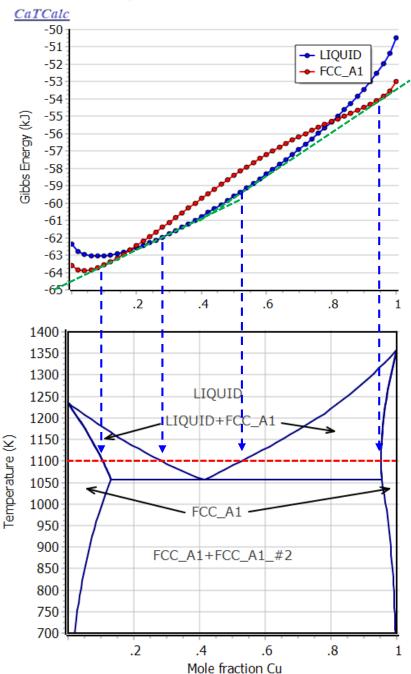
3. Click the [Calculate] button.

The result of the calculation is displayed. * An error message will appear if the calculation includes pure substance phases of stoichiometric composition that cannot be calculated under the specified conditions. Ignore the message in such cases.



(1) Relationship between Gibbs energy of phases and phase diagram

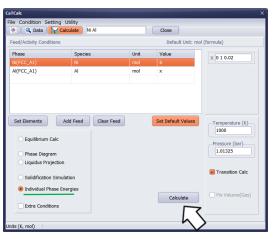
The figure below shows the relationship between Gibbs energy of LIQUID phase and FCC_A1 phase of Ag-Cu system at 1100K and phase diagram. The phase or combination of phases that gives the lowest Gibbs energy of the whole system appears as the stable phase set.



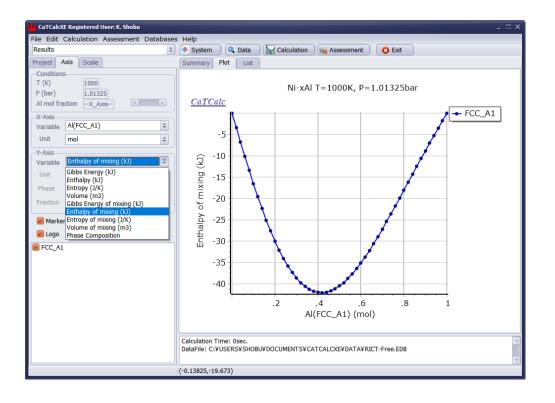
Ag-xCu T=1100K, P=1.01325bar

② Enthalpy of mixing, entropy of mixing and composition of phase

The calculation of enthalpy and entropy of mixing, and phase composition is shown using the FCC_A1 phase of the Ni-Al system as an example.



- 1. Load Ni-Al data from RICT-Free.EDB in the [System] screen. (Not shown.)
- 2. Select only FCC_A1 phase in the [Data] screen. (Not shown.)
- 3. In the [Calculation] screen, select "Individual Phase Energies" and click [Set Default Values].
- 4. Set the temperature, and click the [Calculate] button.
- 5. Select "Enthalpy of mixing" as the Variable for Y-Axis to see the result as shown in the figure below. You can also display the entropy of mixing and the composition of the phase.



③ Bohr magnetron and Curie temperature

The Inden-Hillert-Jarl model is used as a standard for magnetism, and the calculation method of the Bohr magneton and Curie temperature is shown using the Fe-Co FCC_A1 phase as an example.

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	Calculate	Fe Co		Close	
Feed/Activity Condition				Default Unit: m	iol (formula)
Phase	Spec	es	Unit	Value	
Fe(BCC_A2)	Fe		mol	b	X 0 1 0.02
Co(HCP_A3)	Co		mol	x	
Set Elements Equilibrium Cal Phase Diagram Liquidus Project	1	Clear Feed		Set Default Values	-Temperature (C) 1000 -Pressure (bar) 1.01325
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Equilibrium Cal Phase Diagram Liquidus Projec Solidification Si Individual Phas	lc tion imulation <u>ie Energie</u> s	Clear Feed		Set Default Values	Pressure (bar) 1.01325
Equilibrium Cal Phase Diagram Liquidus Projec Solidification Si	lc tion imulation <u>ie Energie</u> s	Clear Feed		5	Itoo Pressure (bar) Itotazz ✓ Transition Calc

1. Load the data of the Fe-Co system using RICT-Free.EDB (not shown).

2. Select only FCC_A1 phase in the [Data] screen (not shown)

3. In the [Calculation] screen, select "Individual Phase Energies" and click [Set Default Values] as shown in the left figure, and click the [Calculate] button. (You can use any value for the calculation temperature.)

4. The result will be displayed in the list only. For a magnetic phase, the Bohr magneton and Curie temperature (or Néel temperature, if negative) are displayed in the bottom line. For graphing, use [User-defined Function] to draw them.

File Edit Option Calculation Database	es Heln									
Results	 Syst 	em 🔍	Data 🛛 🙀 Ca	alculation	O E	kit 🗍				
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Fe-xCo #5			P (bar)	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.0132
Fe-xCo #4			T (C)	1000	1000	1000	1000	1000	1000	100
Fe-xCo #2	Phase	DataBase	Co mol fraction	1E-10	0.02	0.04	0.06	0.08	0.1	0.:
Fe-xCo #1	FCC_A1	RICT-Free	mol (atom)	1	1	1	1	1	1	
Projection Calc for (Nb-Cr-Si) #1			Activity	1	1	1	1	1	1	
Phase Mapping for (Nb-Cr-Si) #1		Element	Fe	1	0.98	0.96	0.94	0.92	0.9	0.8
Phase Mapping for (Zr-Al-O) #1		Element	Co	1E-10	0.02	0.04	0.06	0.08	0.1	0.
Phase Mapping for (Fe-Al) #3 Projection Calc for (Al-Mg-Zn) #2		Total values	G (kJ)	-62.29883	-63.50307	-64.40485	-65.18672	-65.88731	-66.5249	-67.110
Phase Mapping for (Fe-Cr) #1 Phase Mapping for (Fe-C) #1			H (kJ)	37.61999	37,43552	37,26055	37.09497	36,93865	36,7915	36.653
Projection Calc for (Fe-Al-C) #2			S (J/K)	78,48158	79.28256	79.85344	80.3375	80,765	81.15021	81,501
Projection Calc for (Fe-Al-C) #1			V (m3)	0	0	0	0	0	0	
Phase Mapping for (AI-N-O) #2		Magnetic	BMag		-0 591313	-0.4879236	-0 3897193	-0 2965876	-0 208416	-0 1250
Phase Mapping for (Al-N-O) #1		- agricele	TC (K)			-52,43537		-35.58483		
G-Energy Calc for (Nb-Cr-Si) #1				-07	-00.01749	-32.43337		-55.30405	-20.3/20/	-10.0/3-
Projection Calc for (ALMg-Zn) #1										
Phase Mapping for (Fe-Cr-C) #2 Phase Mapping for (Fe-Cr-C) #1										

V-7. Aqueous system

CaTCalc XE

① Phase diagram calculation

An aqueous solution phase can also be considered in combination with other phases.

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	alc) dit 100 Fe-3 AlN Fe-3 AlN AlN AlN Al-3	Calo DH2C DH2C DH2C CH CAL CAL CAL CAL CAL CAL CAL CAL CAL CAL	Scz I-H(+ I-xCa I 03 # 03 # 03 # 03 # 03 # 03 # 03 #	ale 1)-E- Ο-γΟ 4 3 2 1 #1 2	zFe i	#1	t Da		•	Sumi	aten nary	Ph alc .2 18	ot [List	0-x	CaC)-yC	02 T=25	5C, P	-1.01	O Exit
	alc 3 dit 100 Fe-1 AlN Fe-2 AlN AlN Al-2 Fe-1 AlN Fe-1 Fe-2 Fe-2 Fe-2 Fe-2 Fe-2 Fe-2 Fe-2 Fe-2	Calci cxis DH2C DH2C DH2C CAI = :xAI2 :XAI2	Scz -H(+ -xCa 1 03 # 1 1 03 # 1 1 03 # 1 1 03 # 2 1 2 7 2 7 2 7 2 7 2 7 7 7 7 7 7 7 7 7 7 7 7 7	sle 1)-E- 0-yO 4 3 2 1 4 1 2 1 1	zFe i	#1	t Da		•	Sumr	nstern mary	Ph alc .2 18 16	ot [List DH2	0-x	CaC)-yC	02 T=25	5C, P	-1.01	O Exit
	alc 3 dit 100 100 Fe-: AlN Fe-: Fe-: AlN Al-x Al-x Fe-i Fe-:	Calci oxis DH2C DH2C DH2C CH2 CAL CAL CAL CAL CAL CAL CAL CAL CAL CAL	Sct -H(+ -xCa 1 03 # 1 03 # 03 # 03 # 03 # 03 # 03 # 2n # Zn #	sle 1)-E- 0-yO 4 3 2 1 1 1	zFe i	#1	t Da		•	Sumr	nstern mary	Ph alc .2 18 16 14 a 12	ot [List DH2	0-x	CaC)-yC	02 T=25	5C, P	-1.01	O Exit
	alc 3 dit 100 100 Fe-3 AlN Fe-3 Fe-3 AlN Al-x Al-x Fe-1 100 100	Calci cols DH20 DH20 DH20 DH20 CAL = xAl2 xAl	Scz -H(+ -xCa 1 03 # 1 03 # 1 03 # 03 # 03 # 1 27 # 27 # -zFe -zFe	sle 1)-E- O-yO 4 3 2 1 #1 2 1 1 #2 #1	zFe 1	*1			•	Sumr	art C	Pi alc .2 18 16 14 a 12 .1	ot [List DH2	0-x	CaC)-yC	02 T=25	5C, P	-1.01	O Exit
	alc 3 dit 100 Fe-3 AIN Fe-3 AIN AIN AIN AIN AIN AIN AIN AIN AIN AIN	Calci 0H20 0H20 0H20 0H20 cAl # xxAl2 cCr # xxAl2 xXAl2 xxAl	Scz -H(+ -xCa 1 03 # 1 03 # 1 03 # 1 03 # 2n # 2n # Cr # -zFe appin appin	sle 1)-E- Ο-γΟ 4 3 2 1 #1 2 1 4 #1 2 1 4 #1 2 1 g for g for	zFe + 02 # (AI-Y (NI-C		2		•	Sumi	TTC	Pi alc .2 18 16 14 a 12 .1 08	ot [List DH2	0-x	Ga:)-yC	02 T=25	Gaco	-1.01	O Exit
	alc) dit 100 100 Fe-: AlN Al-x Al-x Fe- 100 100 Pha Pha Pha	Calci 0H20 0H20 0H20 0H20 cCr # cCr	Scz -H(+ -xCa 1 03 # 1 03 # 1 03 # 1 03 # 1 03 # 1 03 # 1 03 # 1 1 1 1 1 1 1 1 1 1 1 1 1	sle 1)-E- Ο-γΟ 4 3 2 1 #1 2 1 1 4 #1 2 1 1 1 g for g for g for g for g for	2Fe + 02 # (AI-Y (NI-C (Nb-(*1 1 1 (r-Si) (r-Si)	2		•	Sumr	TTC	Pi alc .2 18 16 14 a 12 .1	ot [List DH2	0-x	Ga:)-yC	02 T=25	Gaco	-1.01	O Exit
	alc) dit 100 100 Fe-: AlN Al-x Fe- 100 100 Pha Pha Ste	Calci 0420 0420 0420 0420 44 # 	Scz -H(+ -xCa 1 03 # 1 03 # 1 03 # 1 03 # 1 03 # 1 27 # 27 # 27 # 1 -zFe appin appin appin c for	sle 1)-E- Ο-γΟ 4 3 2 1 #1 2 1 1 4 #1 2 #1 g for g for g for (Si-C-	(AI-Y (NI-C (Nb-((Nb-((Nb-(*1 1) *1 Cr-Si) *2	2 #4		•	Sumr	TTC	Pi alc .2 18 16 14 a 12 .1 08	ot 0000	List DH2	0-x	Ga:)-yC	02 T=25	Gaco	-1.01	O Exit
	alc) dit 100 100 Fe-: AIN Fe-: AIN AIN AIN AIN AIN AIN AIN AIN AIN AIN	Calci 0H20 0H20 0H20 0H20 0H20 0H20 0H20 0H2	Scc 1-H(+ 1-xCa 1 03 # 1 1 03 # 1 1 03 # 1 1 03 # 1 1 03 # 1 1 1 03 # 2 1 2 7 # 1 -zFe -zFe -sppin appin appin -sppi	sie 1)-E- 0-yC 4 #1 2 1 #1 2 1 #1 g for g for	(AI-Y (NI-C (NI-C (NI-C)) # (SI-C (Zr-A	O) =)) = 1 Cr-Si) -2 O) =	2 #4 #3		•	Sumr	TTC	Pi alc .2 18 16 14 4 3 12 .1 .1 08 08	ot 0000	List DH2	0-x	Ga:)-yC	02 T=25	3(s)	=1.01	Det
	alc) dit 100 100 Fe-: AIN Fe-: AIN AIN AIN AIN AIN AIN AIN AIN AIN AIN	Calci 0H20 0H20 0H20 0H20 0H20 0H20 0H20 0H2	Scc 1-H(+ 1-xCa 1 03 # 1 1 03 # 1 1 03 # 1 1 03 # 1 1 03 # 1 1 1 03 # 2 1 2 7 # 1 -zFe -zFe -sppin appin appin -sppi	sie 1)-E- 0-yC 4 #1 2 1 #1 2 1 #1 g for g for	(AI-Y (NI-C (NI-C (NI-C)) # (SI-C (Zr-A	*1 1) *1 Cr-Si) *2 :-O) *	2 #4 #3		•	Sumr	TTC	Pi alc .2 18 16 14 a 12 .1 08 06 04	ot 0000	List DH2	0-x	Ga:)-yC	02 T=25	3(s)	=1.01	O Exit
	alc) dit 100 100 Fe-: AIN Fe-: AIN AIN AIN AIN AIN AIN AIN AIN AIN AIN	Calci 0H20 0H20 0H20 0H20 0H20 0H20 0H20 0H2	Scc 1-H(+ 1-xCa 1 03 # 1 1 03 # 1 1 03 # 1 1 03 # 1 1 03 # 1 1 1 03 # 2 1 2 7 # 1 -zFe -zFe -sppin appin appin -sppi	sie 1)-E- 0-yC 4 #1 2 1 #1 2 1 #1 g for g for	(AI-Y (NI-C (NI-C (NI-C)) # (SI-C (Zr-A	O) =)) = 1 Cr-Si) -2 O) =	2 #4 #3		•	Sumr	TTC	Pi alc .2 18 16 14 a 12 .1 08 06 04	ot 0000	List DH2	0-x	Ga:)-yC	02 T=25	3(s)	=1.01 3(s) (OH)22	Det
	alc) dit 100 100 Fe-: AIN Fe-: AIN AIN AIN AIN AIN AIN AIN AIN AIN AIN	Calci 0H20 0H20 0H20 0H20 0H20 0H20 0H20 0H2	Scc 1-H(+ 1-xCa 1 03 # 1 1 03 # 1 1 03 # 1 1 03 # 1 1 03 # 1 1 1 03 # 2 1 2 7 # 1 -zFe -zFe -sppin appin appin -sppi	sie 1)-E- 0-yC 4 #1 2 1 #1 2 1 #1 g for g for	(AI-Y (NI-C (NI-C (NI-C)) # (SI-C (Zr-A	O) =)) = 1 Cr-Si) -2 O) =	2 #4 #3		•	Sumr	TTC	Pi alc .2 18 16 14 a 12 .1 08 06 04	ot 0000	List DH2	0-x	Ga:)-yC	02 T=2! ueous+C us+CaCO Aqueou	5C, P CaCO 3(s) s+Ca	=1.01 3(s) (OH)22	• bx

IU¥DOCUMENTS¥CATCALCXE¥DATA¥DiluteAq.adb IU¥DOCUMENTS¥CATCALCXE¥DATA¥IdealGas.adb 1. In the System screen, check [Include Aqueous Phase], specify the elements as shown in the left figure, then select DiluteAq.adb, IdealGas.adb, and PureSol.adb to read the data. DiluteAq is a database of dilute aqueous solutions.

2. Set the calculation conditions on the Calculation screen.

- Check the "Phase Diagram"
- Click the [Set Default Values] button.

• Modify the second and third lines as shown on the left.

3.Click the [Calculate] button.

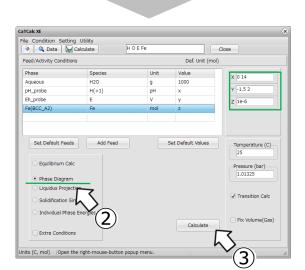
• The result will be displayed.

2 Pourbaix Diagram

Since charge is required in the Pourbaix Diagram (E-pH diagram) calculation, we also select E as an element. The following is an example for Fe.

CaTCalc XE																			
File Condition Setting Utility																			
🔌 🔍 Data 🛛 🙀 Calculate 🛛 🕹 H O E Fe														Close					
0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15		17	Specify by Files	
H Li	Be											в	с	N	0	F	He Ne	Include Ionic Gas Species	
Na	Mg											Al	Si	Ρ	s	Cl	Ar	Include Aqueous Phase	
к	Ca	Sc	Ti	٧	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	Include Extra Components	
Rb	Sr	Y	Zr	Nb	Мо	Тс	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те	Ι	Xe	 Include Volume (if available) 	
Cs	Ba	*	Hf	та	W	Re	Os	Ir	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn	✓ Max carbon in organics 2	
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Ub							OR search	
	*	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	ть	Dy	Но	Er	Tm	Yb	Lu			
	**	Ac	Тh	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		Clear Load	
DB Name Notes																			
+	Dilut	eAq	.adb				Ide	Ideal Aqueous speceis											
	IdealGas.adb Ideal Gas specels																		
	PureLiq.adb Pure liquids																		
+	+ PureSol.adb Pure solids																		
Units	(C,	mol])	Oper	n the	righ	it-m	ouse	-but	ton	popu	p m	enu.				_		

1. On the System screen, check [Include Aqueous Phase], specify elements as shown in the left figure, select DiluteAq.adb, IdealGas.adb, and PureSol.adb to read the data.



 We cancer but
 Image: Second Secon

2. Set the calculation conditions on the Calculation screen.

- Select the "Phase Diagram"
- Click the [Set Default Values] button.

* If E is included, pH and Eh are set at the same time by default. If you do not need, just delete it or both.

• Modify the parameter values as shown in the left figure

3. Click the [Calculate] button

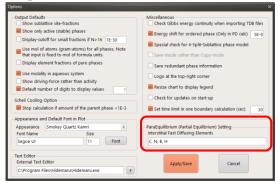
• The result of the calculation will be displayed.

(*Important note)

It is possible to include E explicitly in the usual calculation of aqueous systems under neutral conditions. In a multi-component system, calculation may be more stable.

V-8. Para-equilibrium calculation

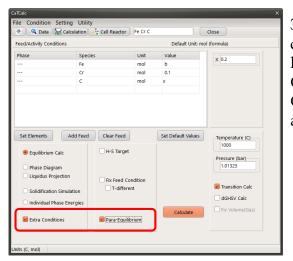
For example, in the case of solid solution of carbon in Fe-BCC phases, carbon is small and enter the interstitial site and diffuse very rapidly at high temperatures, so that equilibrium is quickly achieved. On the other hand, elements in substitutional solid solution with Fe may not diffuse well and remain in non-equilibrium state. Such a state is called para-equilibrium, and the calculation method is shown below.



1. Elements of fast diffusion are set by [Files]-[Preference] in the menu.

lalc					
Condition Se	tting Utility d Calculation	Reactor	Fe Cr C	Close	
Phases	DataBase	Num	+ Species	T1(K)	T2(K)
		3	+ C		6000
BCC_A2	FeCrC_Demo	4	+ Cr	298.15	6000
FCC_A1	FeCrC_Demo	4	+ Fe	298.15	6000
HCP_A3	FeCrC_Demo	4			
SIGMA	FeCrC_Demo	2			
Graphite	FeCrC_Demo	1			
Cementite	FeCrC_Demo	2			
M23C6	FeCrC_Demo	4			
M7C3	FeCrC_Demo	2			
M3C2	FeCrC_Demo	1			
		Reactio	n Calculation		

2. As an example, we show the paraequilibrium calculation of the Fe-Cr-C system. First, load the data of the Fe-Cr-C system from FeCrC_Demo.CDB. In paraequilibrium, the ratios of components other than C are fixed, so only phases containing all elemental components need to be considered. Also, since it will always be singular, a Gas phase is required. These settings are made on the data screen as shown in the left figure.

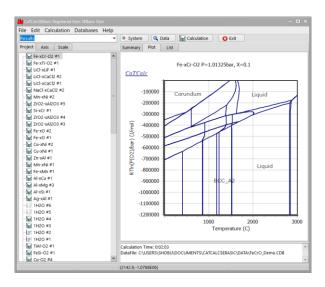


3. Next, refer to the left figure for the calculation conditions. The setting in the left figure is b=0.7, which means that the Cr/Fe ratio is 1/7, and confirm that the Cr/Fe ratio of each phase in the results is also 1/7.

V-9. Ellinghum diagram calculation

Ellingham diagrams can be calculated easily as one of the potential diagrams. However, to simplify the process of setting conditions, a dedicated calculation mode is provided. Currently limited to oxides, this mode can be easily modified to handle nitrides, sulfides, and other compounds as well. Calculations can be performed not only for pure substances but also for complex compounds and solid solutions.

H E He Include tonic Gas Species Li Be B C N P F Ja Mg Al Si P S Li Ar Include Aqueous Phase K Ca Sc Ti V C M M P Co Ni Cu Zn Ga Ge As Se Br Kr Sb Sr V Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe Include Volume (favailable) Sb 8 * HT av Re Os Ir P Au Hq Ti Pb Bi Po At Rn Max carbon in organics * La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu Clear Load * La Ce N D V Dy Npu Am Cm Bk Cf Es Fm Md No Lr Clear Load		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	Select database(s) first
Li Be B C N O F Ne Include Aqueous Phase A S P S Cl Ar S Ca Sc Ti V C Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr Separate LQ and Slag Separate LQ and Slag Include Volume (if available) CS Ba * Hf Ta W Re Os Ti P A u H qT 1P B Bi Po At Rn Ø Aac carbon in organics 2 Fr Ra ** Rf Db Sq Bh Hs Mt Ds Rq Ub O Clear U Company (if available) Clear U Clear U Company (if available) Clear U Company (if available) Clear U Clear U Company (if available) Clear U Cle	н																Е	He	
Na Mg	Li	Be											в	с	N	0	F	Ne	
K Ca St III V K Ca St III V K Ca St III V Indude Volume (if available) CS Ba * Hf Ta W Re Os Ir Pt Au Hq TI Pb Bi Po At Rn Max carbon in organics 2 Max carbon in organics 2 Fr Ra ** Rf Db Sq Bh Hs Mt Ds Rq Ub Max Carbon in organics 2 R Search R Search * La Ce Pr Nd Pm Sne UG dTb Dy Ho Er Tm Yb Lu R Search Clear Load * D8 Name Notes FeCrO_Denno.CDB FeCrO_Postem taken from R. Luoma, PhD Thesis, Helsinki Uni, 2002, ISBN 951-666-61 IdealGas.adb Ideal qas species ver 2019/10/151 RICT-Geram.EDB RICT-Geram.EDB RICT-Geram.EDB	Na	Mg											AI	Si	Ρ	s	CI	Ar	Include Aqueous Phase
CS Ba H Ta W Re Os tr Na Ta W Re Start Max carbon in organics 2 Fr Ra R Db Sg Bh Hs Mt Ds Rg Ds Gs Search Li Ce Ds Search Li Li Ar Th Pa U Np< Pu	к	Ca	Sc	Ti	v	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	Separate LIQ and Slag
Fr Ra ** Rf Db Sq Bh Hs Mt Ds Rq Ub OR Search * La Ce Pr Nd Ms Ms LG Ga Ce Pr A Th ND Dy Ho Fr Th Ub Clear Load Load + De Non Th Se Fr Se Fr Se Fr Se Fr Ce Load + De Non Che Fr Th No Lr Load + De No Lr Load + De No Lr Load + DE No Lr Load De Se Fr Cr <o< td=""> System taken from R. Luona, PhD The Load De Se Se Se Se Se Fr Cr<ord< td=""> Se Pr Se Se Se Se Se Se Se</ord<></o<>	Rb	Sr	Y	Zr	Nb	Мо	Тс	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те	1	Xe	 Include Volume (if available)
It a Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu Ok setect Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr Clear Load I DB Name Notes FeCr0_Demo.CDB FeCrC-O system taken from R. Luoma, PhD Thesis, Helsinki Uni, 2002, ISBN 951-666-61 I dealGas.adb I deal gas species ver 2019/10/15 ! RICT-Ceram.EDB RICT-Ceram EDB RICT-Pure.EDB Pure solids, liquids and gas species ver 2022/08/28 ! Pure solids, liquids and gas species ver 2022/08/28 !	Cs	Ba	*	Hf	Та	w	Re	Os	Ir	Pt	Au	Hg	TI	Pb	Bi	Ро	At	Rn	Max carbon in organics 2
** Ac Th Pa U Np Pu Am Cf Es Fm Mol Iclear Load + DB Name Notes -	Fr	Ra	**	Rf	Db	Sq	Bh	Hs	Mt	Ds	Rg	Ub							OR search
In Act in Pa O top put am Cm sic Cr Es Pm Mid No Cr Interview + DB Name Notes + DB Name Notes + FeCrO_Demo.CDB Fe-Cr-O system taken from R. Luoma, PhD Thesis, Helsinki Uni, 2002, ISBN 951-666-61 IdealGas.adb Ideal gas species ver 2019/10/15 ! RICT-Ceram.EDB RICT-Ceram ver 2.3 RICT-Pure.EDB Pure solids, liquids and gas species ver 2022/08/28 !		*																	dur land
Fe-Cr-O pemo.CD8 Fe-Cr-O system taken from R. Luoma, PhD Thesis, Helsinki Uni, 2002, ISBN 951-666-61 IdealGas.adb Ideal gas species ver 2019/10/15 ! RICT-Ceram.EDB RICT-Ceram ver2.3 RICT-Pure.EDB Pure solids, liquids and gas species ver 2022/08/28 !		**	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		Clear
IdealGas.adb Ideal gas species ver 2019/10/15 ! RICT-Ceram.EDB RICT-Ceram ver2.3 RICT-Pure.EDB Pure solids, liquids and gas species ver 2022/08/28 !	+	DB N	lam	e															
RICT-Ceram.EDB RICT-Ceram ver2.3 RICT-Pure.EDB Pure solids, liquids and gas species ver 2022/08/28 !						B											a, Ph	nD Th	hesis, Helsinki Uni., 2002, ISBN 951-666-61
RICT-Pure.EDB Pure solids, liquids and gas species ver 2022/08/28 !													er 2	019/	10/1	5!			
		RICT	-Cer	am.	EDB														
RICT-Salt.EDB RICT-Salt ver. 1.2									ure s				and	gas	spe	cies	ver	2/08/28 !	
		RICT	-Pur	e.EL	0														
					-			R	CT-	Salt v	/er. 1	.2						-0	
					-			R	CT-	Salt v	/er. 1	.2							
					-			R	ICT-:	Salt v	/er. 1	.2						2022	
					-			R	ICT-	Salt v	/er. 1	.2						2022	
					-			R	ICT-	Salt v	/er. 1	.2							
					-			R	ICT-:	Salt v	ver. 1	.2						LULL	
					-			R	ICT-	Salt v	/er. 1	.2						LULL	
					-			R	ICT-	Salt v	ver. 1	.2							
					-			R	ICT-	Salt	/er. 1	.2							
					-			R	ICT-	Salt v	/er. 1	1.2							
					-			R	ICT-	Salt v	ver. 1	1.2							



Example: Reading data from the Fe-Cr-O_Demo.CDB solution database as shown in the left figure.

*When using RICT-Ceram, it is recommended to uncheck the [Separate LIQ and Slag] checkbox on the right.

Proceed to the Calculation Screen and Set Calculation Conditions

- 1. Add Feed Materials: Begin by clicking the "[Add Feed]" button twice to add iron (Fe) and chromium (Cr) as feed materials.
- Select Calculation Mode: Choose "Ellingham Diagram" as the calculation mode.
- 3. Set Default Values: Click the "[Set Default Values]" button to establish default values for the calculation. The key point is to configure only non-oxygen-related parameters, as the oxygen potential and its range are automatically set.
- 4. Refine Calculation Parameters (Optional): If necessary, adjust other conditions, such as the x-axis variable, and initiate the calculation.
- 5. Analyze Results: The calculation outcome is an Ellingham diagram as shown in the left figure. The units of the y-axis can be switched between kJ/mol and eV using the "Axis" tab.

VI. Material(Mixture) and user-defined function

VI-1. Using Material

* Material is a mixture and is defined by its elemental composition.

* The definition file is a text file with an SMF extension and should be saved in the following folder: /User/Documents/CaTCalcXE/Materials

* Material is used to set up calculation conditions. Click [Add Feed] button and select material from the drop down list.

CaTCalc				×				
File Condition Setting Utility Image: Calculate Image: Calcu								
Feed/Activity Conditions			Def. Unit (mol)					
Phase	Species	Unit	Value	X 0 1				
P(WHITE_P)	Р	mol	b					
Material 💌	Eutectic_YAS	mol	1					
Alerial								
=								
B2_BCC								
CBCC_A12 CUB_A13								
HCP_A3								
KAPPA_E21	Add Feed	Se	t Default Values	Temperature (C)				

Next, click on the Species column and select your desired material from the dropdown list.

	File Condition Setting Utility									
Feed/Activity Condition	ns			Def. Unit ((mol)					
Phase	Species		Unit	Value	X 0 1					
P(WHITE_P)	Р		mol	b						
Material	Eutectic YAS	-	mol	1						
	NASA_CMAS NASA_CMAS2 Smialek_CMAS SolAAA Stainless_Steel SUS304 SUS316									
Set Elements	Tset	T		Set Default Value	esTemperature (C)					

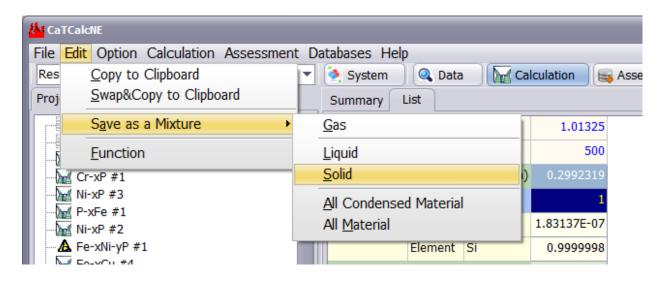
* If the thermodynamic data for the components defined in the material has not yet been loaded, a message will appear and you will be taken to the data loading screen automatically.

* After setting the Feed, click [File]-[Save as a mixture] menu to save it.

CaTCalc				×
File Condition Setting U	Itility			
Save as a mixture	ulate 🛛 🔩 Cell Reactor		Al Si	Close
Close			Def. Unit (mol)	
Phase	Species	Unit	Value	
Al(FCC_A1)	Al	mol	0.1	
Si(DIAMOND_A4)	Si	mol	0.3	

In this case, only the elemental components are set.

* After the one-point equilibrium calculation, it is possible to save the data separately for the gas phase, liquid phase and solid phase. This is done using the menu on the main screen.

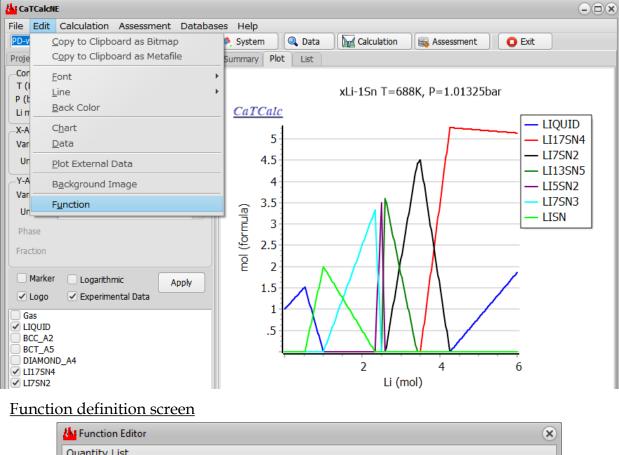


*Note

In the case of Material defined by weight percentages, the molar weight of each element used in the equilibrium calculation will be the value defined in the Elements.DBC file, which is one of the definition files of CaTCalc. The calculated values may differ slightly from those calculated using data defined in the CDB data file.

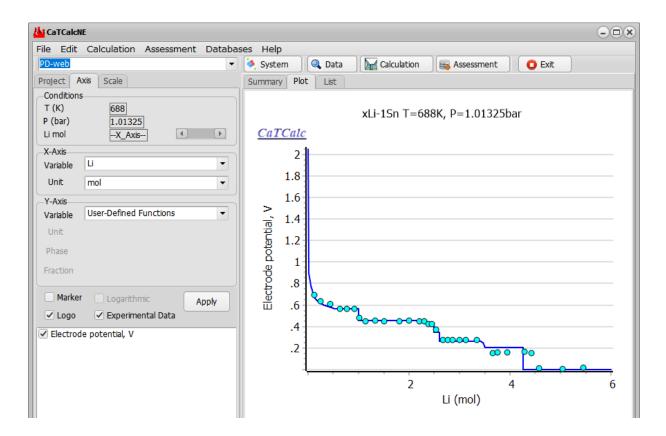
VI-3. User-defined function

*Using the results of the equilibrium calculation, the user can define and calculate arbitrary quantities. After the equilibrium calculation, click [Edit]-[Function] in the menu to open the definition screen.



Name	Definition		Value
Electrode Potential, V	-mu(LIQUID,Li)/96485		
	1		1
		Apply	Close

The function name and its definition are defined in this screen, and Name will be used as the title of the vertical axis of the graph. The standard format for displaying units is a comma followed by the unit. In Definition, you can set up formulas that include physical quantities, though multiplying or dividing multiple physical quantities is not yet supported. Please refer to the "Quantity list" in the menu (see the next page) for the available quantities. After these settings are made, the result is automatically displayed by pressing the "Apply" button. The Value in the Function Editor shows the calculated value at the first point, which can be used for a simple verification of the calculation.



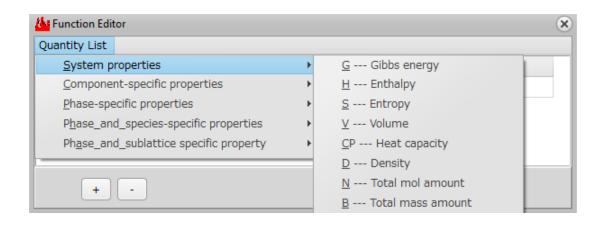
* Example of electrode potential calculation. Note that <u>the measured experimental</u> <u>data is also plotted</u>.

Reference: https://doi.org/10.1016/j.pnsc.2019.05.007

As shown above, user-defined functions are automatically set to [User-Defined Functions] in the Y-axis selection menu in the Axis Tab. In the List view, they are listed in "Functions".

Physical quantities that can be referenced by Function

*The list of physical quantities that can be referenced is categorized into those related to systems, elemental components, phases, etc., as shown in the figure below. For example, [Phase-specific properties] are quantities related to phases, and the phase must be specified in parentheses. For example, G(BCC_A2) is used to calculate the molar Gibbs energy of the BCC_A2 phase. On the other hand, G alone is the total Gibbs energy itself.



[Note]

*Phase and component names are case-sensitive. The physical quantity itself can be in either upper or lower case.

*Function definitions support linear formulas, but not arbitrary formulas such as multiplication of physical quantities. Therefore, please verify thoroughly that the desired formula is calculated correctly. It is not possible (for now) to use function to define another Function.

*The function also supports [individual phase energy] calculations, so G and H calculations are possible. However, this individual phase calculation does not calculate Cp or CTE, so if necessary, please calculate them separately using the normal equilibrium calculation.

*Cp (specific heat) is obtained by the temperature derivative of Enthalpy. Therefore, if the composition of the solution phase changes with temperature, the effect is also taken into account in the value. Namely, the specific heat may be different even if the composition is the same.

VII-1. Macro Calculator

The general procedure for macro calculations is as follows:

1. Creating and Editing Macro Files

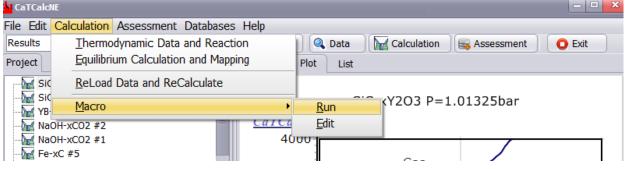
* By default, macros are stored in the Macro folder in the user's folder. /User/Documents/CaTCalcXE/Macro

* The macro is a text file with the extension CMF, so you create and edit it with an appropriate editor. [Calculation]-[Macro]-[Edit] in the menu opens the editor specified in [Preference].

* Each step of the macro is represented by a single line. The following commands are currently available; see the example in the Macro folder.

rc cf sw DatabaseName def Fe Cr C get rp GRAPHITE ip GRAPHITE lp su T=C,P=bar,A=g sc T=(100 300 10) sc x(Fe)=b100 sc w(Cr)=7 sc x=(0 0.4 0.2) st ATitle ce	 : reset all conditions, DBs and elements : clear Feed/Activity conditions : switch (set) Database : define system elements : get data from databases : exclude phases from the calculation : include phases in the calculation : list phases accounted in the calculation : set-units : set-condition of T : set mol amount of Fe to be b100 : set weight-amount of Cr to be 7(g) : set title of the calculation : calculate equilibrium, save and plot
ce map	: calculate equilibrium, save and plot
1	1 . 1

2. The saved macro file is executed by clicking [Calculation]-[Macro]-[Run] in the menu as shown below.



VII-2. Console mode

- 1. To open the console, click [File]-[Console] in the menu.
- 2. The following commands are available in addition to the ones described in the previous page

?	: list all available commands
clear	: clear the command history
save	: save the history as a macro-file
edit	: edit a macro-file
run	: run a macro-file
exit	: exit console-mode

3. Commands you enter will be automatically stored in a command history, but you can clear the command with the clear command.

4. After performing a calculation with the macro command, you can save it as a macro file with the save command.

5. In addition, you can edit a macro file by edit or run it, which is the same as the menu described on the previous page.

6. To exit console mode, use exit.

* The Calculation screen of CaTCalc can be displayed and edited in the console mode. Check conditions whenever necessary.

	🤼 Console _ 🗆 🗙
GatCalcNE File Edit Calculation	CaTCalc Expert Current path: C:\Users\xxxx\Documents\CaTCalcXE\Results
New Folder Open a Folder Recent Folders	CMD:>? The following commands are available: rc : reset all conditions, DBs and elements cf : clear Feed/Reactants condition sw DatabaseName : switch(set) Database
Save	def Fe Cr C : define system elements get : get data from databases rp GRAPHITE : exclude phases from the calculation
Export Plot Export Table	<pre>ip GRAPHITE : include phases in the calculation lp : list phases accounted in the calculation su T=C,P=bar,A=g : set-units sc T=(100 300 10),P=1 : set-condition of T and P</pre>
Print	sc x(Fe)=b100: set mol amount of Fe to be b100sc w(Fe)=7: set weight amount of Fe to be 7sc x=(0 0.4 0.2): set parameter:x
Preference	st ATitle : set Title of the calculation ce : calculate equilibrium, save and plot map : map, save and plot
Console	clear : clear the command history
Exit	save : save the history as a macro-file edit : edit a macro-file
Al-xSi #2	exit : exit console
	CMD:>sw RICT-Fe.CDB Current Database ==> C:\USERS\SHOBU\DOCUMENTS\CATCALCNE\DATA\RICT-FE.CDB CMD:>
	81

VIII-1. General errors

Thermodynamic equilibrium calculations are an optimization problem, but very small amounts of components may be critically important, or they may vary numerically discontinuously.

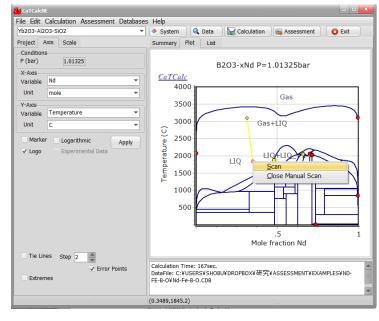
If a calculation error occurs, try adding a gas phase if one is not included. (It is usually added automatically, but not, for example, in phase name labeling calculations.) Note that it is sometimes advisable to add the gas phase even in metallic system calculations.

If multiple valences are possible, such as transition metal oxides, it is more stable to specify the oxygen partial pressure in the calculation.

Check the database for any other problems. For multi-component systems, there is a way to try recalculating the system with only the major components.

VIII-2. Phase diagram calculation

In the phase diagram calculation, the transition point is first found on the frame of the calculation area, and then the phase boundary is traced from there. It is possible that boundary tracing fails somewhere, or detection of the transition point fails due to errors in the numerical calculation. In such cases in the phase diagram calculation, try [Manual scan] of the right button menu. The function, however, is not supported in the liquidus projection calculation at present.



Using the Manual scan

Calculation of the phase boundary between LIQ and Gas+LIQ failed in the left figure. In this case, use the Manual scan mode of the right button popup menu to draw a line across the phase boundary as shown in the left figure, and then scan. Be sure to close this mode after completing the calculation.

IX. Thermodynamic data and database

IX-1. Phase model

The following phase models are supported by CaTCalc:

- Gas phase
 - Ideal gas
- Liquid phase
 - Ionic two-sublattice liquid model
 - Associate solution model
 - Modified QuasiChemical Model
- Solid phase (crystalline phase)
- Compound energy formalism (Sublattice model)
- Magnetism
 Inden-Hillert-Jarl model for magnetic contribution
- Order-disorder transition Split-sublattice model for order-disorder transition
- Pressure dependence Birch-Murnaghan EOS Grover EOS
- Aueous phase HKF Aqueous phase models Extended UNIQUAC model

We plan to develop a non-ideal gas model and other models in future.

There are two standard text formats, ADB and CDB. In both format, the Gibbs energies are expressed as functions of temperature and pressure.

1.ADB format

The former is a TAB-separated CSV format and is used for gaseous species and pure substances with stoichiometric composition, which represents Gibbs energy function, and is editable with spreadsheet software.

First Row: DB description; information displayed in the comment column of the List view.

Second row: Indicates the data storage format, where the number G represents the order: G(70), G(80), G(90), and G(99) represent sqrt(T), T*sqrt(T), ln(T), and T*ln(T), respectively. Density, thermal expansion coefficient, etc. will be supported in due course.

Third row and below: Data separated by TAB.

2.CDB format

It is a text format that conforms to SGTE's TDB format and can be edited with an appropriate editor. Please refer to the CDB Format Database Manual for details.

3.TDB files

ThermoCalc-TDB files in normal one-file format can be converted to CDB format using the Import conversion function. Select [Databases]-[Import TDB files] from the menu to open the file selection dialog.

IX-3. Databases

The following databases are available for CaTCalc.

- 1. RICT-Pure: Pure substance (solid and liquid phases) and gas phase species.
- 2. RICT-Fe: Database for iron-based alloys
- 3. RICT-Sol: General-purpose metal database
- 4. RICT-Ceram: Ceramic materials database
- 5. RICT-Cerm: Cermet and hard materials database
- 6. Various application-specific databases are available.

These are provided in encrypted form for a fee. Please contact us for more information.

X. References

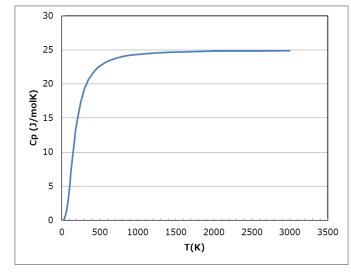
- "Development of New Equilibrium Calculation Software: CaTCalc", K. Shobu and T. Tabaru, Mater. Trans., Vol. 46, No. 6, p. 1175 (2005). https://doi.org/10.2320/matertrans.46.1175
- "CaTCalc : New thermodynamic equilibrium calculation software", Kazuhisa Shobu, CALPHAD, 33 (2009), pp 279-287. https://doi.org/10.1016/j.calphad.2008.09.015
- 3. "Challenges in determining individual chemical potentials of system elements by Gibbs energy minimization", K. Shobu, CALPHAD, 85 (2024) p102691. https://doi.org/10.1016/j.calphad.2024.102691

XI. Development of thermodynamic database

- XI-1. How to use Image Digitizer
- XI-2. Usage of Fitting Tool
- XI-3. Thermodynamic Data Conversion Methods
- XI-4. Optimization of Thermodynamic Parameters
- XI-5. How to Use First-Principles Calculation Data

XI-1. How to use Built-in Image Digitizer

The following shows how to use the Digitizer, using specific heat diagram data as an example.



📔 🚾 Calculation 🛛 😹 Assessment 📄 💽 Exit

SiO3-xMgO P=1.01325bar

Edit Calculation

Yb2O3-Al2O3-SiO2

Project Axis Scale

Adds Scale Intr-XAIN #2 TIN-XAIN #2 TIN-XAIN #1 CaSIO3-XMg0 # CaSIO3-XMg10 # CaSIO3-XMg

103Sb2 #1 Sb2O3 #1

Databases Hel Data Assessment and Optimization

Convert Thermodynamic Data

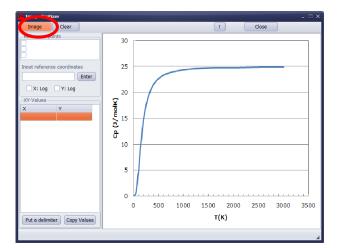
ຸຍ 1800

Eitting Tool

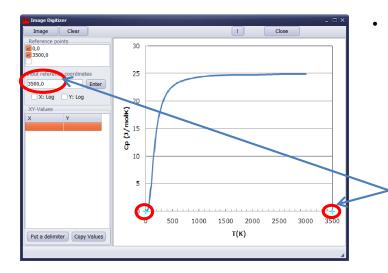
Function Fitting First Principle Data Base Functions Gibbs Energy Continuity Check Convert PV param Aqueous Utility Programs

Figure Example .

Launch the digitizer from the menu [Assessment]-[Image digitizer].

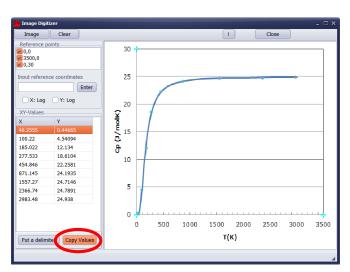


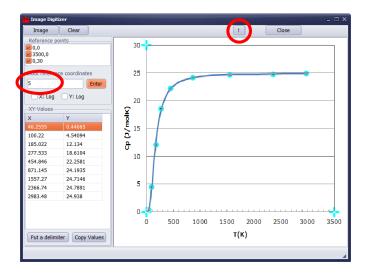
Copy the figure to the clipboard and press the Image button to load the figure. Adjust the size of the figure using the whole frame.



Set up three reference points. First, click on a suitable point as the origin and set its coordinates. In the same way, set a point on the X and Y axes. The left image shows a point on the X-axis.

Setting Coordinates





- Click a point on the curve to convert and read the data. Move the cursor to the vicinity of the point to change the shape of the cursor and select that point, so you can modify the data. You can also click the right button to delete the data.
- Click [Copy Values] button at the bottom of the screen to copy the data to the clipboard, and then paste the data into an Excel file.
- By pressing the [i] button at the top, you can change the size of the drawing point.

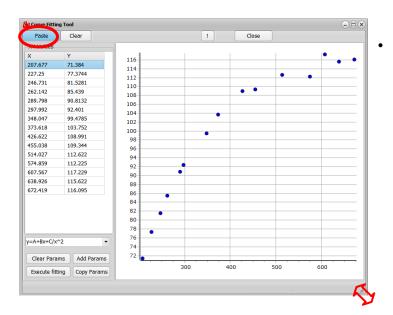
XI-2. How to use the Fitting Tool

The following shows how to use the built-in Fitting Tool, using specific heat data as an example.

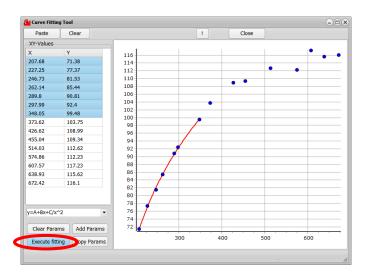
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ファ	イルホーム	ム 挿入	ページレイフ	ማት 1
B2	Ŧ	: ×	√ f _x	71.38
	А	В	С	D
1	т(к)	Cp(J/molK)		
2	207.68	71.38		
3	227.25	77.37		
4	246.73	81.53		
5	262.14	85.44		
6	289.8	90.81		
7	297.99	92.4		
8	348.05	99.48		
9	373.62	103.75		
10	426.62	108.99		
11	455.04	109.34		
12	514.03	112.62		
13	574.86	112.23		
14	607.57	117.23		
15	638.93	115.62		
16	672.42	116.1		
17				

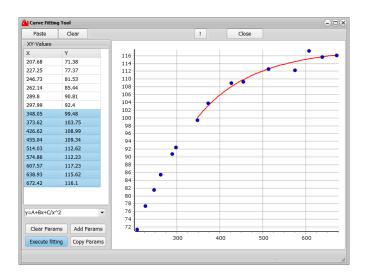
Example of specific heat data. Copy this to the clipboard. The title line is not necessary but may be included.

CaTCalcNE				
File Edit Calculation	Assessment	Databases Help		
PD-web	<u>D</u> ata Ass	essment and Optimization		C
Project Axis Scale	Image D	igitizer		
Conditions	<u>F</u> itting To	ol		
P (bar) 100	<u>C</u> onvert	Thermodynamic Data	×	
X-Axis Variable Nb205	Fi <u>r</u> st Prin	ciple Data	×	



- Launch the Fitting Tool from the menu [Assessment]-[Fitting Tool].
- Paste the data in the clipboard by pressing the Paste button. The data will be plotted automatically, but its size should be adjusted using the overall frame.





E	ਜ਼ਿ 'ਨੇ ∼ ਵੇ ∼ ਦ											
ファ	イルホ・	-ム 挿入	ページレイ	(アウト 翌	ご式 データ	校閲	表示 ^	リレプ AT	OK拡張ツー			
E23	3	• : ×	✓ f _x									
	А	в	с	D	E	F	G	н	I			
1	то	T1	C(0)	C(1)	C(-2)	C(2)	C(3)	C(-0.5)	C(-3)			
2	207.6	8 348.0	5 79.23175	0.084709	-1099875	0	0	0				
3	348.0	5 672.4	2 128.8465	-0.00855	-3127195	0	0	0				
4	1											

- In fitting, one usually tries several functions to find the best one, but here we use the default function and show how to divide the temperature range into two and approximate it. As shown in the left figure, the split point is selected at 348K, and the data from 207K to 348K is selected. Then, press [Execute fitting] to perform fitting, and the result is displayed as a red line in the plot.
- If the fitting is good, click [Add Params] to temporarily save the parameters for this temperature range.

•

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- Next, select data of the rest of the temperature range and perform the fitting in the same way. If the fitting is good, save additional parameters with [Add Params]. (Note that small difference at the junction point would give negligible effect to the Gibbs energy, as the specific heat is the second derivative of the latter.)
- Then, copy the parameters to the clipboard using the [Copy Params] button and paste them into Excel or other application.
 - The left figure shows an example of parameters, where T0 and T1 represent the lower and upper limits of the temperature range, and C(N) is the coefficient of the Nth order term of temperature in the polynomial equation of specific heat.
- See the next section, <u>"Conversion Methods for</u> <u>Thermodynamic Data</u>," for how to use this data to obtain the Gibbs energy function.

XI-3. Thermodynamic Data Conversion

Below are the methods for converting H, S, and Cp data to Gibbs energy and vice versa.

(1) Using spreadsheet software

1. Conversion from Enthalpy, Entropy, and specific heat to Gibbs energy

	А	В	С	D	Е	F	G	н	I	J	к
1	Phase	Formula	state	то	T1	H0	S0	C(0)	C(1)	C(-2)	Ref
2	MxO	MxO	S	207.68	348.05	-1086000	84.83	79.23175	0.084709	-1099875	
3	MxO	MxO	S	348.05	672.42			128.8465	-0.00855	-3127195	

4

- As shown in the figure above, create a table of temperature functions of specific heat with information on phase, formula, state, temperature range, standard Enthalpy and Entropy of formation at 298.15 K. (The function of specific heat obtained on the previous page is used as an example. Note that the Enthalpy and Entropy of formation were obtained separately from the literature.) The item name is required, and the state is s, l, or g for solid phase, liquid phase, and gas, respectively. Also, when using H and S at T0, use HT and ST instead of H0 and S0 at 298.15K in the item name.
- Copy the entire table to the clipboard, including the item names, and select [Assessment]-[Convert Thermodynamic Data]-[HSCp to GFunction] from the menu to convert the data in the clipboard to the Gibbs energy function.
- The result is saved in the clipboard and can be pasted into a data file. If you select [HSCp to Phase data], Phase information in CDB format is also added. [HSCp to ADB data] converts the data to ADB format for pure substances.

🚹 CaTCalcNE			
File Edit Calculation	Assessment Databases Help		
PD-web	Data Assessment and Optimization		Calculation Sseessment
Project	Image Digitizer		
Nd2O3-xAl2O3 #1	<u>F</u> itting Tool		
Nd203-xSiO2 #1	Convert Thermodynamic Data	Þ	HSCp to GFuncion
Nd203-xCaO #2	First Principle Data	Þ	H <u>S</u> Cp to Phase data
MoB-xCrB #1	Base Functions	•	HS <u>C</u> p to ADB data

2. Conversion from Gibbs energy to Enthalpy, Entropy, and specific heat

• As shown in the example below, copy the remaining part of the Gibbs energy function from the starting temperature to the clipboard and select [GFunc to HSCp data] from the menu. The converted result will be saved to the clipboard in the TAB-separated text format.

Function GCU20SOL 298.15 -194216.99+344.07921*T-63.5877*T*LN(T)↓ -0.00942505*T**2+289373.5*T**(-1); 6000 N !↓

(2) Using the built-in conversion tool

Below we show how to use the built-in conversion tools. This may be useful when parameterizing data from measured specific heat or first-principles calculations.

Fitting with the Fitting Tool

٠

🚻 Curve Fitting To	ol			*
Paste	Clear	Data Converter !	Close	
XY-Values				
X Y	(30		
150 2	3.42572575	20		

After fitting using the Fitting Tool and saving the parameters with [Add Params], press the [Data Converter] button on the top of the Fitting Tool to start the conversion tool. The parameters are also transferred.

File Edit								
Phase	Formula	State	dH0(J/mol)	S0(J/molK)	Reference	MW(g)	Poisson's ratio	dE0(eV/atom)
	0	Q	\supset				(
O Fo	rmula 🔿 Atom							
T0(K)	T1(K)	C(0)	C(1)	C(-2)	C(2)	C(3)	C(-0.5)	C(-3)
0	20	0	0.11463708	0	0	0.0004143691	0	0
		54,449556	-0.072532194	4063.7403	0	0	-257.36478	0
20	100	34.449330	0.072002101	10001/100	-	-		-

• Enter Phase, Formula and State, and dE0 if the data were obtained from first principles calculations. Also, check the box depending on whether the Cp is per formula or atom. Then press the [Convert] button at the bottom to obtain the Gibbs energy function.

🕌 Data Con	vertor							
File Edit								
Phase	Formula	State	dH0(J/mol)	S0(J/molK)	Reference	MW(g)	Poisson's ratio	dE0(eV/atom)
МхО	MxO	S			2021RICT			-0.52826
O For	rmula 💿 Atom	ı						
T0(K)	T1(K)	C(0)	C(1)	C(-2)	C(2)	C(3)	C(-0.5)	C(-3)
0	20	0	0.11463708	0	0	0.0004143691	0	0
20	100	54.449556	-0.072532194	4063.7403	0	0	-257.36478	0
100	2000	21.904182	0.0041379413	-34832.016	0	0	30.172525	0
-9899	98.3937+645.469		194*T**2-4063.74	403*T**(-1)-2	058.91824*SQR	E-05*T**4; 20 Y RT(T)-108.899112* T(T)-43.808364*T		
			Convert		Copy parar	meters	(Quit

XI. Development of thermodynamic database

Optimization Steps

Usually, the following three steps are required:

- 1. Configuring Datafile
- 2. Summary of experimental data
- 3. Optimization through Assessment

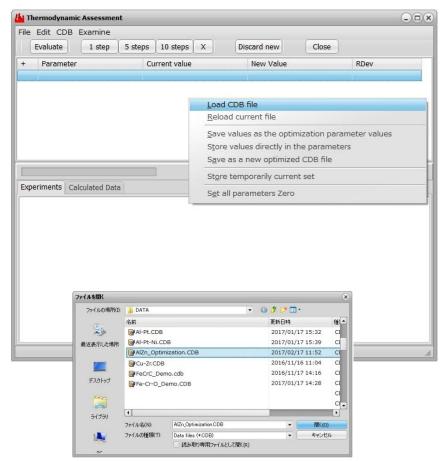
First, let's take an example of an Al-Zn system assessment.

Press the Assessment button in CaTCalc XE to open the Assessment module.

LaTCalc XE		*
File Edit Calculation Assessment Databases	Help	
Results	🔮 System 🔍 Data 🛛 🙀 Calculation 📾 Assessment 🚺 👩 Exit	
Project	Summary	
Project Phase Mapping for (AI-O-Si) #1 Phase Mapping for (AI-O-Si) #1 Phase Mapping for (Fe-C-C) #4 Phase Mapping for (Fe-C-C) #4 Phase Mapping for (Fe-C-C) #4 Phase Mapping for (Fe-C-C) #5 Phase Mapping for (Fe-C-C) #3 Phase Mapping for (Fe-C-C) #3 Phase Mapping for (Fe-C-C) #4 A projection Calc for (Fe-C-C) #3 Projection Calc for (Fe-C-C) #1 Phase Mapping for (Fe-C-C) #4 A projection Calc for (Fe-C-C) #1 Phase Mapping for (Fe-C-C) #4 Solidification for (Fe-C-C) #4 Phase Mapping for (Aj-C) #1 Phase Mapping for (Aj-C) #1 Phase Mapping for (Aj-C) #1 Phase Mapping for (Aj-C) #1 Phase Mapping for (Aj-C) #1 Solidification Cife (Fe-C-C) #3 Solidification for (Fe-C-C) #3 Solidification for (Fe-C-C) #4 Equilibrium Calc for (Fe-C-C) #1 Phase Mapping for (Aj-C) #1 Phase Mapping for (Fe-C-C) #1 Phase Mapping	Summary	

Loading Data

1. Press [Load CDB file] in the right button menu in the box above to bring up the File selection screen and load "AlZn_Optimization.CDB" in the data folder.



2. Select Al and Zn in the dialog that appears to select an element.

Elements		×
Select elements Al Zn		
	ОК	キャンセル

Reading DB files

le	Edit CDB E	Examine							
	Evaluate	1 step	5 steps	10 steps	X	Dis	card new	Close	
+	Parameter		Cu	rrent value	unana ang ang ang ang ang ang ang ang ang		New Value		RDev
+	FCC_H0		0						
+	FCC_S0		0						
+	FCC_H1		0						
+	FCC_S1		0						
+	FCC_H2		0						
+	FCC_S2		0						
+	HCP_H0		0						
+	HCP_S0		0						
+	LIQUID_H0		0						
+	LIQUID_S0		0						
+	LIQUID_H1		0						
+	LIQUID_S1		0						
				1		Dev	0		
Evr	periments Cal	ulated Dat					L		
EV	Call	ulateu Dat	.a						

- The data file is loaded and parameters to be optimized are displayed. Check the contents of the data file by pressing [CDB] in the menu.
- Next, open the file "AssessmentExample.xlsx" and open the Zn-Al sheet. This file is located in the data folder (/User/Documents/CaTCalcXE/DATA).

Editing experimental data

A	B C	D	E	F	G	Н	I
1 CaTCalc用の実験データ	PARROT	利のPOPファイ	JL				
2							
3 Tie-Line, Zn-Al, T(K)=656, X(FCC_A1,A)=0.33, X(LIQUID,AI)=0.11	ENTER_S	YIDX1=0.01,	DX2=0.01				
4 Tie-Line, Zn-Al, T(K)=675, X(FCC_A1,Al)=0.4, X(LIQUID,Al)=0.15	ENTER S	YIDT5=10.0,	DH = 100				
5 Tie-Line, Zn-Al, T(K)=699, X(FCC_A1,Al)=0.49, X(LIQUID,Al)=0.2							
6 Tie-Line, Zn-A, T(K)=800, X(FCC A1,AI)=0.85, X(LIQUID,AI)=0.59	\$ Tieline	between FC	C_A1#1 and	FCC_A1#2			
7 Tie-Line, Zn-Al, T(K)=656, X(LIQUID,AI)=0.11, X(HCP_A3,AI)=0.02	TABLE H	EAD	-	-			
8 Tie-Line, Zn-Al, T(K)=675, X(LIQUID,AI)=0.05, X(HCP_A3,AI)=0.012	CREATE	NEW EQUILI	BRIUM @@,1				
9 Tie-Line, Zn-A, T(K)=685, X(LIQUID,A)=0.02, X(HCP,A3,A)=0.006	CHANGE	STATUS PH	ASE * = S				
10 Tie-Line, Zn-Al, T(K)=400, X(FCC A1,A)=0.97, X(HCP A3,A)=0.003	CHANGE	STATUS PH	ASE FCC A	1#1. FCC A	1#2 = FIX 1		
11 Tie-Line, Zn-Al, T(K)=460, X(FCC_A1,Al)=0.94, X(HCP_A3,A)=0.006	SET CON	DITION P =	P0, T = @1				
12 Tie-Line, Zn-A, T(K)=500, X(FCC A1,A)=0.92, X(HCP A3,A)=0.01	EXPERIM	ENT X(FCC)	A1#1. AL)= (a3 : DX1. X	(FCC A1#2.	AL)= @2 :	DX1
13 Tie-Line, Zn-Al, T(K)=540, X(FCC A1,A)=0.873, X(HCP A3,Al)=0.014		RT VALUE Ÿ			/		
14 Tie-Line, Zn-Al, T(K)=550, X(FCC_A1,A)=0.86, X(HCP_A3,Al)=0.02		RT_VALUE Y					
15 Tie-Line, Zn-Al, T(K)=570, X(FCC A1,A)=0.39, X(HCP A3,A)=0.02		-	- /				
16 Tie-Line, Zn-Al, T(K)=610, X(FCC A1,A)=0.36, X(HCP A3,A)=0.02	TABLE_V	ALUES					
17 Tie-Line, Zn-Al, T(K)=650, X(FCC A1,A)=0.335, X(HCP A3,AI)=0.025		HE PHASE C	OMPOSITIO	N IN EOUI	LIBRIUM		
18 Tie-Line, Zn-Al, T(K)=654, X(FCC A1,A)=0.33, X(HCP A3,A)=0.02		X(FCC A1					
19 Tie-Line, Zn-Al, T(K)=552, X(FCC_A1,A)=0.86, X(FCC_A1,Al)=0.41	55		0.86		0.41		
20 Tie-Line, Zn-Al, T(K)=570, X(FCC A1,A)=0.83, X(FCC A1,Al)=0.445	57		0.83		0.445		
21 Tie-Line, Zn-Al, T(K)=599, X(FCC_A1,A)=0.78, X(FCC_A1,Al)=0.52	59	9	0.78		0.52		
22 Tie-Line, Zn-Al, T(K)=622, X(FCC_A1,A)=0.67, X(FCC_A1,A)=0.64	62	2	0.67		0.64		
23 HMR, Zn-Al, T(K)=953, X(LIQUID,A)=0.8, dH(J)=1568	TABLE_E	ND					
24 HMR, Zn-Al, T(K)=953, X(LIQUID,AI)=0.6, dH(J)=2430							
25 HMR, Zn-Al, T(K)=953, X(LIQUID,AI)=0.4, dH(J)=2508	\$ Tieline	between LIC	UID and FC	C A1			
26 HMR, Zn-Al, T(K)=953, X(LIQUID,AI)=0.2, dH(J)=1723	TABLE H						
27 Invariant-Reaction, Zn-Al, T(K)=550, X(FCC_A1,Zn)=0.1456, X(FCC_A1,Zn)=0.59, X(HCP_A3,Zn)=0.985		NEW EQUILI	BRIUM @@.1				
28 Invariant-Reaction, Zn-Al, T(K)=655, X(LIQUID,Zn)=0.89, X(FCC A1,Zn)=0.667, X(HCP A3,Zn)=0.977		STATUS PH					
29		STATUS PH		ECC A1 =	FIX 1		
30 TIE, Zn-Al, T(K)=550, X(FCC A1,Zn)=0.1456, X(FCC A1,Zn)=0.59		DITION P =					
31 TIE, Zn-Al, T(K)=550, X(FCC A1,Zn)=0.1456, X(HCP A3,Zn)=0.985		ENT X(LIQU		: DX1. X(FC	CC A1. AL)=	@2 : DX1	
32 TIE, Zn-Al, T(K)=550, X(FCC A1,Zn)=0.59, X(HCP A3,Zn)=0.985			-// -			C	
33 TIE, Zn-Al, T(K)=655, X(LIQUID,Zn)=0.89, X(FCC A1,Zn)=0.667	TABLE V	ALUES					
34 TIE, Zn-Al, T(K)=655, X(LIQUID,Zn)=0.89, X(HCP_A3,Zn)=0.977		HE PHASE C	OMPOSITIO	N IN FOUI	IBRIUM		
35 TIE, Zn-Al, T(K)=655, X(FCC_A1,Zn)=0.667, X(HCP_A3,Zn)=0.977		X(FCC_A1					
36	65		0.33	-,	0.11		
37	67		0.4		0.15		
38	69		0.49		0.2		
39	80		0.85		0.59		
40	TABLE E	-	0.00		0.00		
41	TADEL_D						

- The right-hand side of the figure above is a POP file of ThermoCalc-PARROT. Only the data in the POP file are extracted from the list, and this is the experimental data for CaTCalc. Select this part, and copy the data to the clipboard.
 - Spreadsheet software such as Excel is used to create and save the experimental data.

Loading experimental data

1	Edit CDB Examine			
	Evaluate 1 step	5 steps 10 steps X	Discard new	Close
+	Parameter	Current value	New Value	RDev
+	FCC_H0	0		
+	FCC_S0	0		
+	FCC_H1	0		
+	FCC_S1	0		
+	FCC_H2	0		
+	FCC_S2	0		
+	HCP_H0	0		
+	HCP_S0	0		
+	LIQUID_H0	0		
+	LIQUID_S0	0		
+	LIQUID_H1	0		
+	LIQUID_S1	0		
			Dev 0	
-	eriments Caculated Data			
LAP	eniments Caculated Data			
		Paste ClipBoard	Data I	
		Append ClipBoar		
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			u	
		A <u>d</u> d		
		Delete		
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e Edit CDB	ic Assessmen Examine		_		_	_	_	-
Evaluate	1 step	5 steps	10 steps	x	Discard new	/	Close	
+ Parameter		Cu	rrent value		New Va	lue		RDev
+ FCC_H0		0						
+ FCC_S0		0						
+ FCC_H1		0						
+ FCC_S1		0						
+ FCC_H2		0						
+ FCC_S2		0						
+ HCP_H0		0						
+ HCP_S0		0						
+ LIQUID_HO		0						
+ LIQUID_SO		0						
+ LIQUID_H1		0						
+ LIQUID_S1		0						
Experiments Ca 0: Tie-Line, Zn	lculated Data		 \1,Al)=0.33	3, X(LIQUI	Dev 0			
• • • • • • • • • • • • • • • • • • •	I-AI, T(K)=65 I-AI, T(K)=67 I-AI, T(K)=69 I-AI, T(K)=80 I-AI, T(K)=65 I-AI, T(K)=65 I-AI, T(K)=68 I-AI, T(K)=68 I-AI, T(K)=40 I-AI, T(K)=50 In-AI, T(K)=54	6, X(FCC_/ 9, X(FCC_/ 9, X(FCC_/ 0, X(FCC_/ 6, X(LIQUII 5, X(LIQUII 5, X(LIQUII 0, X(FCC_/ 0, X(FCC_/ 40, X(FCC_/ 40, X(FCC_/	A1,AI)=0.4, A1,AI)=0.49 A1,AI)=0.85 D,AI)=0.11, D,AI)=0.05, D,AI)=0.02, A1,AI)=0.97 A1,AI)=0.92 A1,AI)=0.92 A1,AI)=0.92 A1,AI)=0.8	X(LIQUID 9, X(LIQUI 5, X(LIQUI , X(HCP_A , X(HCP_A , X(HCP_A , X(HCP_A 4, X(HCP_A 2, X(HCP_A 7, X(HCP_A) 7, X(HCP_A 7, X(HCP_A) 7,	D,Al)=0.11 Al)=0.15),Al)=0.2),Al)=0.2 3,Al)=0.02 3,Al)=0.012 3,Al)=0.006 (3,Al)=0.003 (3,Al)=0.006 (3,Al)=0.01 _A3,Al)=0.014			

CaTCalc assessment module 1. Open the Experiments panel below and click on the menu that appears with the right

mouse button

2. Paste Clipboard data with Paste.

That's all you need to know.

You can optimize parameters by pressing the 1step, 5steps, or 10steps button.

ile	Edit	CDB Examine						
	Evalua	ate 1 step	5 steps 1	0 steps X	Di	scard new Clo	ose	
+	Para	ameter	Curre	nt value		New Value	RDev	
+	FCC	_но	7804.	50914661		7804.50911741	-3.74E-09	
+	FCC	_S0	-0.41	2798868469		-0.412798814462	1.31E-07	
+	FCC	_н1	6339.	57424204		6339.57423462	-1.17E-09	
+	FCC	_S1	-4.27	2578892		-4.272578877	3.51E-09	
+	FCC	_H2	-5404	.79083657		-5404.79080928	5.05E-09	
+	FCC	_S2	7.424	92294742		7.4249229049	-5.73E-09	
+	HCP	<u>-но</u>	14412	2.2967723		14412.2967581	-9.86E-10	
+	HCP	2_S0	0.328	439522225		0.328439550927	8.74E-08	
+	LIQU	UID_H0	9715.	40719726		9715.40714371	-5.51E-09	
+	LIQU	UID_S0	-2.67	039937979		-2.67039929263	3.26E-08	
+	LIQU	UID_H1	44.76	46553221		44.7646417346	-3.04E-07	
85								
+	LIQU	UID_S1		228512074	De	-1.23228510164 v 0.051580029	1.55E-08	
+ Expe	LIQU	its Calculated Dat				v 0.051580029		
+ Expe No.	LIQU erimen EN	Type	T	×/w	Weight	v 0.051580029 Exp. Value	Error	
+ Expe No.	LIQU erimen EN 0	Type TJE-LINE	T 656	x/w 0.33	Weight	v 0.051580029 Exp. Value dG/RT=0	Error -0.0059154540919234	200
+ Expe No. 0	LIQU erimen EN 0 0	Type TIE-LINE TIE-LINE	T 656 656	x/w 0.33 0.11	Weight 1 1	v 0.051580029 Exp. Value dG/RT=0 dG/RT=0	Error -0.0059154540919234 -0.0197668809725269	3
+ Expe No. 0 1 2	LIQU erimen EN 0 1	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE	T 656 656 675	x/w 0.33 0.11 0.4	Weight 1 1 1	 0.051580029 Exp. Value dG/RT=0 dG/RT=0 dG/RT=0 	Error -0.0059154540919234 -0.0197668809725269 0.02868790236632389	3
+ Expe No. 0 1 2 3	LIQU erimen EN 0 0 1 1	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE	T 656 656 675 675	x/w 0.33 0.11 0.4 0.15	Weight 1 1 1 1	v 0.051580029 Exp. Value dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0	Error -0.0059154540919234 -0.0197668809725269 0.02868790236632389 0.01214732740380724	3
+ Expe No. 0 1 2 3 4	LIQU Enimen 0 0 1 1 2	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE	T 656 656 675 675 699	x/w 0.33 0.11 0.4 0.15 0.49	Weight 1 1 1 1 1 1	<pre>v 0.051580029 Exp. Value dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0</pre>	Error -0.0059154540919234 -0.0197668809725269 0.02868790236632389 0.01214732740380724 0.02968307636206766	3
+ Expe No. 0 1 2 3 4 5	EN 0 0 1 1 2 2	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE	T 656 656 675 675 699 699	x/w 0.33 0.11 0.4 0.15 0.49 0.2	Weight 1 1 1 1 1 1 1 1 1 1	<pre>v 0.051580029 Exp. Value dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0</pre>	Error -0.0059154540919234 -0.0197668809725269 0.02868790236632385 0.01214732740380724 0.02968307636206766 -0.0112772344823836	3)
+ Expe No. 0 1 2 3 4	EN 0 1 1 2 2 3	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE	T 656 656 675 675 699 699 800	x/w 0.33 0.11 0.4 0.15 0.49 0.2 0.85	Weight 1 1 1 1 1 1 1 1 1 1 1 1	<pre>v 0.051580029 Exp. Value dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0</pre>	Error -0.0059154540919234 -0.0197668809725269 0.02868790236632389 0.01214732740380724 0.02968307636206766 -0.0112772344823836 0.03454931649738193	3)
+ Expe No. 0 1 2 3 4 5 6 7	EN EN 0 0 1 1 2 2 3 3	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE	T 656 656 675 675 699 699 800 800	x/w 0.33 0.11 0.4 0.15 0.49 0.2 0.85 0.85	Weight 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	 v 0.051580029 Exp. Value dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 	Error -0.0059154540919234 -0.0197668809725269 0.02868790236632389 0.01214732740380724 0.02968307636206766 -0.0112772344823836 0.03454931649738193 -0.0540941596221546	3) 1 8 3
+ Expe No. 0 1 2 3 4 5 6 7	LIQU erimen EN 0 0 1 1 2 2 3 3 4	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE	T 656 656 675 675 699 699 800 800 800 656	x/w 0.33 0.11 0.4 0.15 0.49 0.2 0.85 0.85 0.59 0.11	Weight 1 1 1 1 1 1 1 1 1 1 1 1	 0.051580029 Exp. Value dG/RT=0 	Error -0.0059154540919234 -0.0197668809725269 0.02868790236632389 0.01214732740380724 0.02968307636206766 -0.0112772344823836 0.03454931649738193 -0.0540941596221546 0.01582222345405665	3) 1 8 3
+ Expe No. 0 1 2 3 4 5 6 7 8 8 9	EN 0 0 1 1 2 2 3 3 4 4	TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE	T 656 656 675 675 699 699 800 800 656 656	x/w 0.33 0.11 0.4 0.15 0.49 0.2 0.85 0.59 0.11 0.02	Weight 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	 v 0.051580029 Exp. Value dG/RT=0 	Error -0.0059154540919234 -0.0197668809725269 0.02868790236632389 0.01214732740380724 0.02968307636206766 -0.0112772344823836 0.03454931649738193 -0.0540941596221546 0.01582222345405665 -0.142240854180252	3) 4 8 3 1
+ Expe No. 0 1 2 3 4 5 6 7	LIQU erimen EN 0 0 1 1 2 2 3 3 4	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE	T 656 656 675 675 699 699 800 800 800 656	x/w 0.33 0.11 0.4 0.15 0.49 0.2 0.85 0.85 0.59 0.11	Weight 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	 0.051580029 Exp. Value dG/RT=0 	Error -0.0059154540919234 -0.0197668809725269 0.02868790236632389 0.01214732740380724 0.02968307636206766 -0.0112772344823836 0.03454931649738193 -0.0540941596221546 0.01582222345405665	3 4 5 8 3 1 5

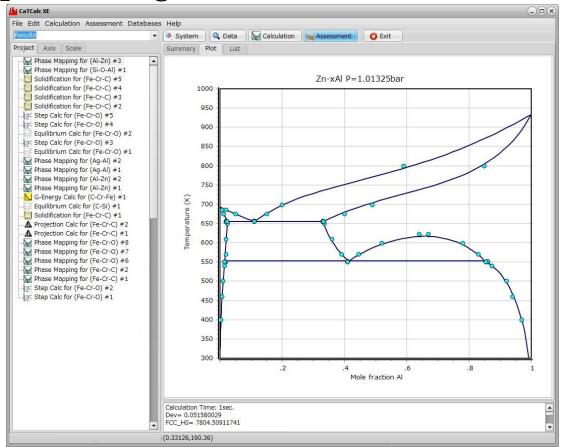
• The bottom panel switches to the list of Calculated Data, showing the differences between the experimental and calculated values. The experimental conditions T, x/w and weight can be edited.

In order of magnitude of error, they are colorized as colorless, blue, yellow, magenta and red. Colorless is the best, but if you have difficulty, some lines of yellow would be a good guide.

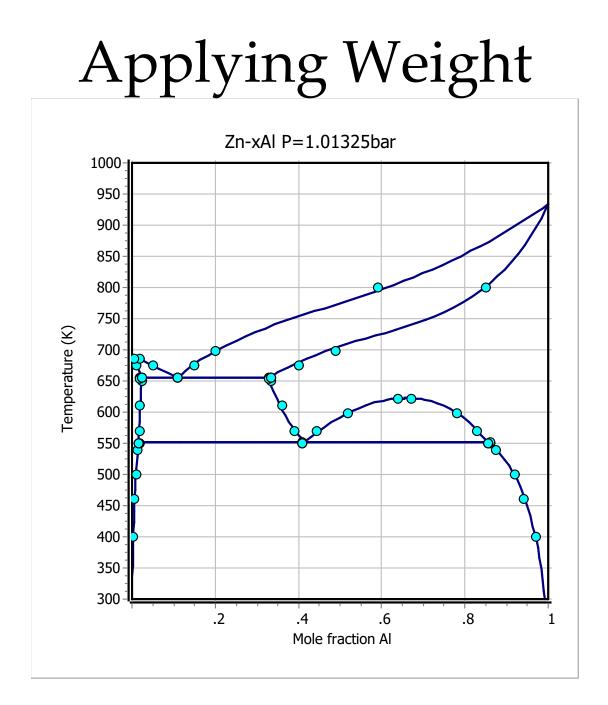
 Since experimental values are usually inconsistent, it may be better to adjust not only the weight, but also T and x/w (within the limits of experimental accuracy). Ideally, if there are a lot of data that are close to the average value, we can evaluate the data correctly, but it is not possible to obtain unbiased data that follow a Gaussian distribution. In the least-squares method, large deviations make a large contribution, which means that the data will have large errors. Therefore, it is better to correct the data. Of course, the correction must be within a reasonable range.

Confirmation of phase diagrams and other information

• Choose "Examine" menu and draw a phase diagram.



 In addition, the HMR and ACR should be checked.(If the calculations don't work, use normal equilibrium calculations.



 In the list of Calculated data, if the Weights of No. 36~39 are set to 1000 each, the vertices of the miscibility gap match the experimental values almost perfectly. Thus, we need to carefully decide which data to focus on by referring to the original experimental conditions and experimental data.

Related functions

Initialization of Parameters

100	Edit (CDB Examine						
	Evaluat	e 1 step	5 steps	10 steps X	D	iscard new	Close]
+	Parar	meter	Cu	rrent value		New Value		RDev
+	FCC_	H0	78	0 <mark>4.50911741</mark>				-3.74E-09
+	FCC_	S0	-0.	412798814462				1.31E-07
+	FCC_	<u>H1</u>	63	39.57423462				-1.17E-09
+	FCC_	S1	Load CDI	3 file				3.51E-09
+	FCC_	H2	1.	urrent file				5.05E-09
+	FCC_	S2						-5.73E-09
+	HCP_	HO				parameter val	ues	-9.86E-10
+	HCP_	.S0	S <u>t</u> ore val	ues directly in	the parar	neters		8.74E-08
+	LIQU	ID_H0	S <u>a</u> ve as a	a new optimiz	ed CDB fil	e		-5.51E-09
+	LIQUI	ID_S0	Store ter	nporarily curre	ent set			3.26E-08
+	LIQUI	ID_H1						-3.04E-07
+	LIQUI	ID_S1	S <u>e</u> t all pa	rameters Zero	\sim			1.55E-08
Expe	eriment	S Calculated D	ata			11.		
	eriment EN	s Calculated D	ata T	×/w	Weight	Exp. Value		Error
No.				×/w 0.445	Weight	Exp. Value dG/RT=0		Error -0.002824117820402956
No. 35	EN	Туре	T			201 (C201 (C201 (C201		
Exp(No. 35 36 37	EN 17	Type TIE-LINE	T 570	0.445	1	dG/RT=0		-0.002824117820402956
No. 35 36 37	EN 17 18	Type TIE-LINE TIE-LINE	T 570 599	0.445	1 1000	dG/RT=0 dG/RT=0		-0.002824117820402956 0.005269984190533915
No. 35 36 37 38	EN 17 18 18	Type TIE-LINE TIE-LINE TIE-LINE	T 570 599 599	0.445 0.78 0.52	1 1000 1000	dG/RT=0 dG/RT=0 dG/RT=0		-0.002824117820402956 0.005269984190533915 -0.003607270999909583
No. 35 36	EN 17 18 18 18	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE	T 570 599 599 622	0.445 0.78 0.52 0.67	1 1000 1000 1000	dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0		-0.002824117820402956 0.005269984190533915 -0.003607270999909583 0.000823996527196628
No. 35 36 37 38 39	EN 17 18 18 19 19	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE	T 570 599 599 622 622	0.445 0.78 0.52 0.67 0.64	1 1000 1000 1000 1000	dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0		-0.002824117820402956 0.005269984190533915 -0.003607270999909583 0.000823996527196628 -0.000854175725720552
No. 35 36 37 38 39 40	EN 17 18 18 19 19 20	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE HMR	T 570 599 622 622 953	0.445 0.78 0.52 0.67 0.64 0.8	1 1000 1000 1000 1000 1	dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dH=1568		-0.002824117820402956 0.005269984190533915 -0.003607270999909583 0.000823996527196628 -0.000854175725720552 -0.001165811481895896
No. 35 36 37 38 39 40 41	EN 17 18 18 19 19 20 21	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE HMR HMR	T 570 599 622 622 953 953	0.445 0.78 0.52 0.67 0.64 0.8 0.8	1 1000 1000 1000 1000 1 1	dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dH=1568 dH=2430		-0.002824117820402956 0.005269984190533915 -0.003607270999909583 0.000823996527196628 -0.000854175725720552 -0.001165811481895896 -0.01213497152825666
No. 35 36 37 38 39 40 41 42 43	EN 17 18 18 19 19 20 21 21 22	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE HMR HMR HMR	T 570 599 622 622 622 953 953 953	0.445 0.78 0.52 0.67 0.64 0.8 0.6 0.6 0.4	1 1000 1000 1000 1000 1 1 1 1	dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dH=1568 dH=2430 dH=2508		-0.002824117820402956 0.005269984190533915 -0.003607270999909583 0.000823996527196628 -0.000854175725720552 -0.001165811481895896 -0.01213497152825666 -0.02252123077903302
No. 35 36 37 38 39 40 41 42	EN 17 18 18 19 19 20 21 21 22 23	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE TIE-LINE HMR HMR HMR HMR	T 570 599 622 622 622 953 953 953 953	0.445 0.78 0.52 0.67 0.64 0.8 0.6 0.4 0.4 0.2	1 1000 1000 1000 1000 1 1 1 1 1 1	dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dH=1568 dH=2430 dH=2508 dH=1723		-0.002824117820402956 0.005269984190533915 -0.003607270999909583 0.000823996527196628 -0.000854175725720552 -0.001165811481895896 -0.01213497152825666 -0.02252123077903302 -0.02181212761568399
No. 35 36 37 38 39 40 41 42 43 44	EN 17 18 19 19 20 21 22 23 24	Type TIE-LINE TIE-LINE TIE-LINE TIE-LINE HMR HMR HMR HMR INVARIANT	T 570 599 622 622 622 953 953 953 953 550	0.445 0.78 0.52 0.67 0.64 0.8 0.6 0.4 0.2 0.8544	1 1000 1000 1000 1000 1 1 1 1 1 1 1 1 1	dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dH=1568 dH=2430 dH=2508 dH=1723 dG/RT=0		-0.002824117820402956 0.005269984190533915 -0.003607270999909583 0.000823996527196628 -0.000854175725720552 -0.001165811481895896 -0.01213497152825666 -0.02252123077903302 -0.02181212761568399 8.490162263524358E-06

Optimization

ile	Edit	CDB Examine						
	Evalua	te 1 step	5 steps 1	0 steps X	Dis	scard new C	lose	
+	Para	meter	Curre	nt value	umunananan	New Value		RDev
+	BCC	_A0	23532	2.8024165		23532.8024165		1.77E-12
+	BCC	_B0	-7.72	59668182		-7.72696681821		-1.31E-12
+	BCC	_A1	3258.	28540709		3258.28540707		-6.64E-12
+	LIQ_	<u>A0</u>	-2176	5.7934952		-21765.7934952		1.92E-12
+	LIQ	<u>B0</u>	15.21	52908428		15.2152908428		-2.5E-12
+	FCC	_A0	21985	5.3172086		21985.3172087		5.61E-12
+	FCC	_B0	-7.003	206438427		-7.00206438437		-1.44E-11
+	V1		20352	2.2795159		20352.2795159		-8.63E-13
+	V2		-29.44	448426251		-29.4448426251		-9.46E-13
1					Dev	0.00245590073		>
Evne	erimen	ts Calculated Data						
No.	EN	Type	Т	x/w	Weight	Exp. Value	Erro	ur.
0	0	INVARIANT	1193	.408	1	dG/RT=0	12.13	000688894354501602
1	0	INVARIANT	1193	0.13	1	dG/RT=0		01660766902403956
2	0	INVARIANT	1193	1/3	1	dG/RT=0	17.55	001214887981981031
3	1	CONGRUENT	1341	1/3	1	dG/RT=0	1	006691206284757573
4	2	HTR	1341	1/3	1	dH=3727	144	001309707511390672
5	3	INVARIANT	1049	0.73	1	dG/RT=0		00269362071344041
6	3	INVARIANT	1049	0.907	1	dG/RT=0	17.05	000667033690647252
7	3	INVARIANT	1049	1/3	1	dG/RT=0		004497352270948773
8	4	INVARIANT	1203	0.81	1	dG/RT=0	-0.0	000189722252227891
9	4	INVARIANT	1203	0.931	1	dG/RT=0	1.7	35378911739913E-05
10	4	INVARIANT	1203	0.94	1	dG/RT=0	-1.	579751158755762E-0
11	5	INVARIANT	726	0.037	1	dG/RT=0	0.0	001532301692186603
12	5	INVARIANT	726	0.886	1	dG/RT=0	0.0	00436108531258751
13	5	INVARIANT	726	1/3	1	dG/RT=0	9.6	95260749562062E-05
14	6	FORMATION	1594	0.98	1	dG/RT=0	-0.0	000675829004643517
15	7	FORMATION	1548	0.958	1	dG/RT=0		000399506419611256
16	8	FORMATION	1499	0.935	1	dG/RT=0	-0.0	000391344322505815
	-		100			and the second sec		

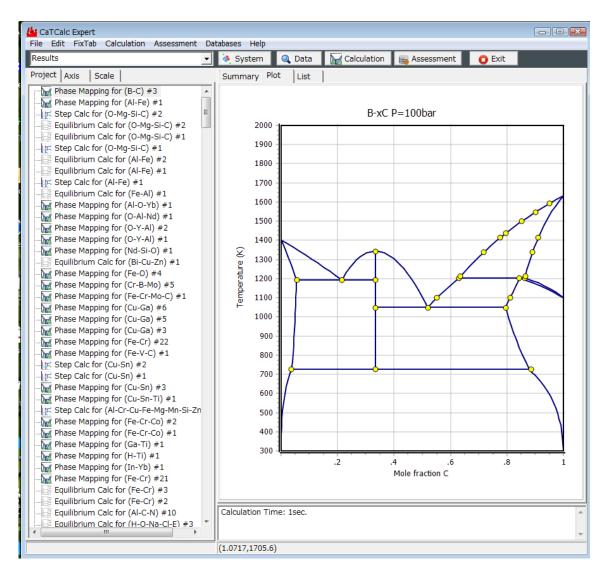
The data in the sheet of tcex36 in "AssessmentExample.xls" is loaded into the data file "tcex36.cdb", and the [1 Step] button is pressed 8 times. "RDev" in the parameter list indicates the amount of modification, which is almost converged, and "Dev" is the RMS of the error values in the experimental value list, which also converges when there is no change.

Phase diagram calculation

	Evalua	te 1 step	5 steps 10) steps X	Disca	ard new	Clo	se	
+	Para	meter	Curren	nt value	1	New Value			RDev
+	BCC	_A0	23532	.8024165					1.77E-12
+	BCC	_B0	-7.726	596681821					-1.31E-12
+	BCC	_A1	3258.2	28540707					-6.64E-12
+	LIQ	A0	-2176	5.7934952					1.92E-12
+	LIQ_	B0	Plot Co	ntrol			×		-2.5E-12
+	FCC_	_A0	1						5.61E-12
+	FCC	_B0	Calcu	ulation Type	hase Diagra	im	-		-1.44E-11
+	V1		Tem	perature (K)	300 2000	8	•		-8.63E-13
+	V2			sure (bar)	1.01325		•		-9.46E-13
			Corr	position (X)	0 1 0.02		-		
Expe	eriment	ts Calculated Data							
No.	EN	Туре	Phas	e				Erro	or [
	0	INVARIANT		as		Select A	All	-0.	000688894354501602
1	0	INVARIANT						0.0	01660766902403956
2	0	INVARIANT	- V L			Deselect	AII	-0.	001214887981981031
3	1	CONGRUENT				Details	,	0.0	006691206284757573
4	2	HTR		120		0		-0.	001309707511390672
5	3	INVARIANT				\sim		0.0	00269362071344041
6	3	INVARIANT	1		(Calculat	te)	-0.	000667033690647252
7	3	INVARIANT				\sim		0.0	004497352270948773
8	4	INVARIANT				Close		-0.	000189722252227891
9	4	INVARIANT		Plot experime	ital data	ciuse		1.7	35378911739913E-05
10	4	INVARIANT	1203	0.94	I	ug/KT=	0	-1.	579751158755762E-0
11	5	INVARIANT	726	0.037	1	dG/RT=	:0	0.0	001532301692186603
12	5	INVARIANT	726	0.886	1	dG/RT=	0	0.0	00436108531258751
13	5	INVARIANT	726	1/3	1	dG/RT=	:0	9.6	95260749562062E-05
14	6	FORMATION	1594	0.98	1	dG/RT=	:0	-0.	000675829004643517
15	7	FORMATION	1548	0.958	1	dG/RT=	:0		000399506419611256
16	8	FORMATION	1499	0.935	1	dG/RT=	:0	-0.	000391344322505815

[Plot Control] appears as shown in the above figure when [Examine] of the menu is clicked.

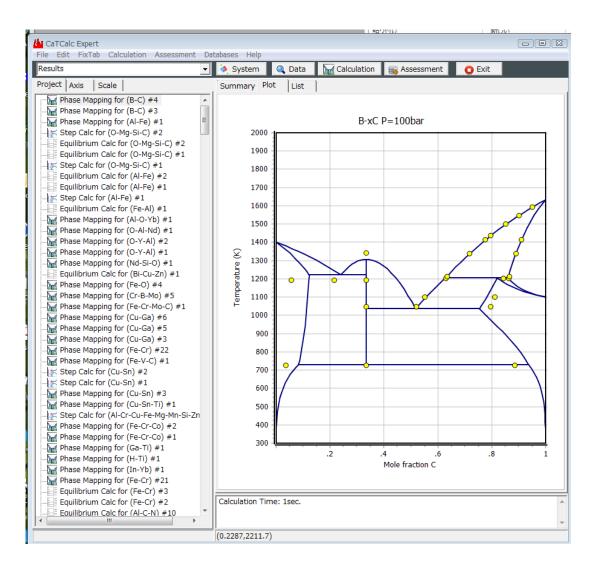
Display Results



Note: Since this system has a singularity problem, it is automatically recalculated including the gas phase. In this case, the pressure is automatically set to 100 bar, which is usually high enough to prevent the gas phase from being stabilized. If the gas phase appears, the pressure should be increased even higher. If the gas phase does not appear, the pressure may be reduced.

How to use the Weight Factor

Convergence to the Local Minimum



The above is a case where the values have converged to the local minimum. In such a case, it is effective to adjust the weight factor.

Manual Adjustment

File Edit CDB Examine									
	Evalua	te 1 step	5 steps	10 steps X	D	iscard new	Close		
+	Para	meter	Cu	irrent value		New Value		RDev	
+	BCC	_A0	27	087.9768361		23507.86436	87	-0.132	
+	BCC	_B0	-1	2.432909755		-7.89716815	032	0.365	
+	BCC	_A1	-6	21.276217424		2678.608367	74	5.31	
+	LIQ	A0	-2	1460.6705795		-21683.0149	591	-0.0104	
+	LIQ	B0	15	.1049359665		15.17649532	71	0.00474	
+	FCC	_A0	23	218.8460994		21918.25707		-0.056	
+	FCC	_B0	-7	.82032473767		-6.93335117	021	0.113	
+	V1		20	325.2997323		20433.30916	75	0.00531	
+	V2		-2	9.0850693484		-29.4720278	588	-0.0133	
-				-			2113 N		
-					De	o.01215512	51		
Expe	erimen	ts Calculated Da	ta		De	ev 0.01215512	51		
Expe No.	erimen EN	ts Calculated Da	ta T	x/w	De Weight	ev 0.01215512	51	Error	
			ta T 1193	a second second			51	Error 0.01355771434335934	
No.	EN	Туре	T	.408	Weight	ixp. Value	51		
No.	EN 0	Type INVARIANT	T 1193	.408 0.13	Weight 1	xp. Value cG/RT=0	.51	0.01355771434335934	
No. 0 1	EN O O	Type INVARIANT INVARIANT	T 1193 1193	.408 0.13 1/3	Weight 1 1	xp. Value dG/RT=0 dG/RT=0	.51	0.01355771434335934 -0.01527912207969434	
No. 0 1 2	EN 0 0 0	Type INVARIANT INVARIANT INVARIANT	T 1193 1193 1193	.408 0.13 1/3 1/3	Weight 1 1 1	txp. Value cG/RT=0 cG/RT=0 cG/RT=0	51	0.01355771434335934 -0.01527912207969434 0.017066747374663	9
No. 0 1 2 3	EN 0 0 0 1	Type INVARIANT INVARIANT INVARIANT CONGRUENT	T 1193 1193 1193 1341	.408 0.13 1/3 1/3 1/3	Weight 1 1 1 1	xp. Value dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0 dG/RT=0	.51	0.01355771434335934 -0.01527912207969434 0.017066747374663 -0.00981601534546316	9 1
No. 0 1 2 3 4	EN 0 0 1 2	Type INVARIANT INVARIANT INVARIANT CONGRUENT HTR	T 1193 1193 1193 1341 1341	.408 0.13 1/3 1/3 1/3 0.73	Weight 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	xp. Value	.51	0.01355771434335934 -0.01527912207969434 0.017066747374663 -0.00981601534546316 0.005578226435442694	9 1
No. 0 1 2 3 4 5	EN 0 0 1 2 3	Type INVARIANT INVARIANT INVARIANT CONGRUENT HTR INVARIANT	T 1193 1193 1193 1341 1341 1049	.408 0.13 1/3 1/3 1/3 0.73 0.907	Weight 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	txp. Value GG/RT=0 GG/RT=0 GG/RT=0 GG/RT=0 GG/RT=0 CH=3727 GG/RT=0	.51	0.01355771434335934 -0.01527912207969434 0.017066747374663 -0.00981601534546316 0.005578226435442694 -0.00863332302479417	9 1 7

In the list of calculated data, three columns of T, x/w and Weight are editable: T is the temperature, x/w is the molar percentage/weight percentage of components, and Weight is the weighting factor. In this optimization module, the comparison of these is made by that of the Gibbs energy. In this optimization method, better results are obtained when we give more weight to the phase diagram information. So we set the Weight of the data for Invariant, Formation and Tie-Line lines to 100.

Setting the Weight Factor

ile	Edit	CDB Examine						
	Evalua	te 1 step	5 steps 1	0 steps X	Di	scard new	Close	
+	Para	meter	Curre	ent <mark>value</mark>		New Value		RDev
+	BCC	_A0	2350	7.0114736		23532.2566096		0.00107
+	BCC	_B0	-7.71	045700721		-7.7267722543		-0.00212
+	BCC	_A1	3245	19262756		3257.42663453		0.00377
+	LIQ_	<u>A0</u>	-2172	74.7880303		-21765.7722017		0.000414
+	LIQ	B0	15.21	97023288		15.215292867		-0.00029
+	FCC	_A0	2182	6.2097396		21985.3537328		0.00729
+	FCC	_B0	-6.88	868134761		-7.00207399171		-0.0165
+	V1		2033	0.6018339		20352.0983898		0.00106
+	V2		-29.4	315179099		-29.4446549504		-0.000446
1					De	v 0.00257382462		
	<u> (27 - 2</u>		<u> </u>		De	0.00237302402		
Expe	erimen	ts Calculated Data						
No.	EN	Туре	Т	x/w	Weight	Exp. Value	Err	or
0	0	INVARIANT	1193	.408	100	dG/RT=0	-0.	.000601280566977995
1	0	INVARIANT	1193	0.13	100	dG/RT=0	0.0	00145311325590462
2	0	INVARIANT	1193	1/3	100	dG/RT=0	-0.	.001062630830163336
3	1	CONGRUENT	1341	1/3	1	dG/RT=0	0.0	000721640774381082
4	2	HTR	1341	1/3	1	dH=3727	-0.	000840895670931385
5	3	INVARIANT	1049	0.73	100	dG/RT=0	0.0	000325583646791767
6	3	INVARIANT	1049	0.907	100	dG/RT=0	-0.	.000806992370699523
7	3	INVARIANT	1049	1/3	100	dG/RT=0	0.0	000544387712759923
8	4	INVARIANT	1203	0.81	100	dG/RT=0	-0.	004101010168613751
9	4	INVARIANT	1203	0.931	100	dG/RT=0	0.0	000312823794756854
10	4	INVARIANT	1203	0.94	100	dG/RT=0	-0.	.000336270073343624
11	5	INVARIANT	726	0.037	100	dG/RT=0	0.0	000985919731762012
12	5	INVARIANT	726	0.886	100	dG/RT=0	0.0	001985371054235405
13	5	INVARIANT	726	1/3	100	dG/RT=0	0.0	000634655459253693
14	6	FORMATION	1594	0.98	100	dG/RT=0	-0.	.000714336659090607
15	7	FORMATION	1548	0.958	100	dG/RT=0	- <mark>0</mark> .	000459685728955584
16	8	FORMATION	1499	0.935	100	dG/RT=0	-0.	000455013547336714
1	1		Peri	110			100	•

Above figure shows the optimization. We can get the same optimization result as in page 78 by using Examine. Some parameters may give us an error in the equilibrium calculation, in this case, we should set the weight of the parameter to zero. When the parameters are somewhat better, the Weight is calculated back to the original value.

What to do when you're in trouble

(From Lukas et al. "Computational Thermodynamics")

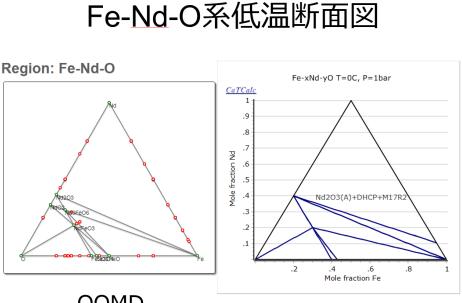
- Selection and exclusion of experimental data
 - Initially, as few experimental data as possible are used for general matching. It is usually a good idea to start with an invariant-reaction or a metastable state diagram that excludes some phases. The important point is that inconsistent experimental values do not allow for convergence. Therefore, it is necessary to exclude such experimental data. It is important to select a minimum number of experimental data sets that are consistent with each other. Let's call this group of conditions critical-set.
 - If the calculation of the invariant reaction including the intermediate phase is not successful, the intermediate phase should be removed and only the liquid phase and the important solution phase should be optimized. If good results are obtained, then the excluded phases are introduced, but the parameters of the liquid and solution phases are fixed and the additional phases are optimized. One important aspect of the optimization is not to consider conflicting data at the same time. After all, if they are truly contradictory, then at least one of them is not correct. If such a contradiction is seen, then one of them and the rest of the data must be used to optimize at once. In other words, the experimental data must also be optimized.
 - Other notes Systematic errors must be corrected. For example, there is the adjustment of the temperature scale. If you want to optimize the liquid phase and the end components at both ends, except for the intermediate phase, you should calculate a metastable diagram of just these two phases. There should not be any strange kinks and turns in the metastable state diagram. Such a metastable state diagram may be useful for later optimization. Note that the values of the optimization parameters stay in a reasonable range. If they start to vary by many orders of magnitude, the experimental data may be incorrectly weighted, or there may be too many optimization parameters.

Optimization of Specific Heat

- The specific heat needs to be optimized separately, and since it is a second derivative of Gibbs Energy, it needs to be fixed before optimizing the others.
- A standard function for the specific heat is built into the <u>fitting tool</u> in the menu of the unit.

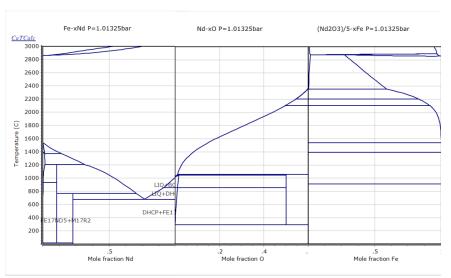
XII. How to use ab initio calculation data

* ab initio calculations and computational thermodynamics



OQMD

Ab initio calculations: fundamental information at low temperatures Practical information on room temperature and high temperature: Computational thermodynamics



Fe-Nd-O系縦断面図

(Nd,Fe)2O3固溶体

* Preparation for database creation

Taking BaTiO3 as an example, the Gibbs energy is obtained from the enthalpy of formation and the specific heat obtained by first-principles calculations, and the procedure for adding the data to the thermodynamic database is shown.

1. First, you need to prepare the database file to which you want to add data (not necessary if you want to add it to an existing file).

Δ.			hata	1.6	u c	alcui	lity	R	a Ti i	0		_	_			a	lose	
•	1		/unu	1.0	0.0	uncu	- and	11.		·								
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	Specify by Files
ł																Е	He	C Technic Technic Cons Constitut
1	Be											в	с	Ν	0	F	Ne	Include Ionic Gas Species
а	Mg											AI	Si	Ρ	s	CI	Ar	Include Aqueous Phase
¢	Ca	Sc	Tì	v	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	5e	Br	Кг	🗐 Include Extra Components
ь	Sr	Y	Zr	Nb	Mo	Тс	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те	I	Xe	Include Volume (if available)
s	Ba	+	Hf	Та	w	Re	Os	Ir	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn	✓ Max carbon in organics 2
r	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Ub							OR search
	٠	La	Ce	Pr	Nd	Pm	Sm	Eu	Gđ	Tb	Dy	Но	Er	Tm	Yb	Lu		
	••	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		Clear Load
1	DB N	lame					No	tes										
		1.0	adb				24	and a		narie	10.10	c 20	1812	181				

1.	As shown in the left figure, the
	data of Ba-Ti-O is read from the
	pure material database in the
	System screen.

🛛 🔍 Data 🖉	🛃 Calculate 🛛 Ba Ti	0	Close		
Phases	DataBase	Num	+ Solid Phases	5 T1(K)	T2(K)
Gas	IdealGas	10	+ Ba(s)	80	1000
Pure Liquids	PureLiq	8	+ BaO(s)	200	2246
Pure Solids	PureSol	8	+ Ti(s)	200	1944
			+ Ti2O3(s)	200	2110
			+ Ti305(s)	200	2050
			+ Ti407(s)	200	1960
			+ TiO(s)	200	2030
			+ TiO2(s)	200	2185

3		Data			Utility						
	<u> </u>	udta		🖌 Ci		ew Current Syst	em				c
0 :	1 2	3	4	5	Lis	st Species			•	15	16
н					Ι-	Range Check				h	Е
Li	Be				_		В	С	N	0	F

BaTiO3_Test.CDB - Xモ頓	
ファイル(E) 編集(E) 書式(Q) 表示(Y) ヘルプ(出)	
B DataBase_Info Ba-Ti-O system extracted from C:\USB Defined_System Ba-Ti-O !	ERS\SHOBU\DOCUMENTS\CATCALCXE\DATA\IdeaIGas.adb C:\USERS\SHOBU\DOCUMEI \$
\$ Element definitions	
Element Ba - 137.327 ! Element Ti - 47.88 ! Element 0 - 15.9994 ! S	s
-2485218.36-4715.14184-1-551.581611-1-11() 16277976.747438.101515-1812.74881=1-11()(1)- Parameter 6(Gas:Ba2:0) 200 355683.715+466.488929- 348156.961-178.886571+7-18.7384933+11()(1)- Parameter 6(Gas:Ba0:0) 200 -11027.6897-66.3367012 1597614.03+2907.58991+7-389.6796+1=11()(1)-546 -23292410.4-1821.64537+1102.788802+114()(1)	$\begin{array}{c} =& \\ =& \\ =& \\ =& \\ =& \\ =& \\ =& \\ =& $

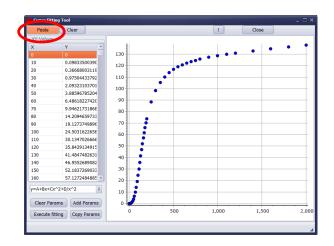
2. You can check the data on the Data screen.

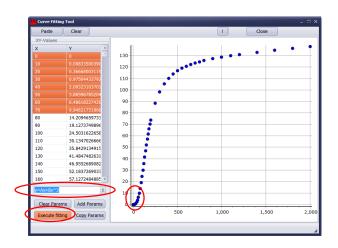
- 3. Select [Utility]-[View Current System] in the menu, and you will be asked to save the current system information, so save it as a file. Save it as a file named "BaTiO3-Test.CDB" for your convenience.
- 4. Editor will start up automatically. Add BaTiO3 data to this file afterwards.

Parameterization of Specific Heat and Gibbs Energy Functions

2. The enthalpy of formation and specific heat data are prepared by first principles calculations. Here we use the data from the BaTiO3 sheet of AssessmentExample.xlsx as an example (this data is not correct, and is for illustration purposes only).

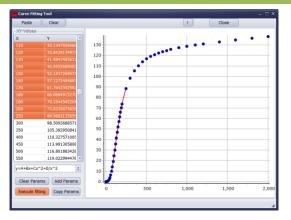
	А	в	C	U	E
1	変換係数	1 J/mol	1.04E-05	eV/atom	
2					
3					
4	BaTiO3	P4mm	-3.504	eV/atom	
5		H(T=0)	-3.38E+05	J/mol	
6		S(T=0)	0	J/molK	
7			\sim		
8	T(K)	Cp(J/molK	(2)		
9	0	0	\smile		
10	10	0.098335			
11	20	0.36668			
12	30	0.975044			
13	40	2.093231			





- ① in the figure on the left is the energy of formation, which can be converted to units of J/mol. Note that the value per atom is usually given in the first principle calculation, so do not forget to multiply by the number of atoms to get the value per Formula.
- 2. ② is the specific heat. This is also per Formula. Copy the values to the clipboard. (If you don't have specific heat data, you can use Kopp-Neumann method, which can be approximated by the sum of specific heat of the elements or compounds (BaO and TiO2 in the case of BaTiO3). (Usually, data above 298.15 K are sufficient.)
- 3. Open the Fitting Tool by clicking "Assessment" - "Fitting Tool" in the menu of CaTCalc, and paste the Cp data by clicking the "Paste" button.
- 4. Here, the approximate parameter is divided into three parts: 0~70K, 70~300K, and 300~2000K. (The best division method is usually determined by trial and error. First, select 0~70K as shown in the left figure. Next, choose Y=AX+BX^3 as the approximation function and click [Execute Fitting] button to find the approximation curve. A red curve is drawn in the right graph. If the approximation is good, click [Add Params] to save the parameters.

Parameterization of Specific Heat and Gibbs Energy Functions



T.S.	(3)	C	C(2)	-2)		C(1)	COL	T1	т0
	2.73E-05	0 2		0	846	0.008	0	76	0
	0	00168	-0.0	2822.23	193	1.06	-73.0147	250	70
	0	5E-06	-2.55	2131983	937	0.014	118,458	2000	250
							Cp_calc	Cp_ex	Т
							0	0	0
							0.11577	0.098335	10
							0.395419	0.36668	20
							1.002826	0.975044	30
							2.101869	2.093231	40
		- N					3.856427	3.885968	50
		\ \					6.430379	6.486182	60
							9.987604	9.946217	70
molK)	Cp(J/m	0					9.966722	9.946217	70
monty	- ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~						14.09711	14.20947	80
				1	160		19.13603	19.12737	90
					140		24.61122	24.50316	100
			-		120		30.25477	30.1347	110
				- -			35.90547	35.84291	120
				- F	100		41.46163	41.48475	130
<u> </u>				1	80		46.85653	46.95527	140
					60		52.04491	52.18373	150
							56.99519	57.12725	160
					40		61.68481	61.76423	170
\rightarrow				-	20		66.09729	66.08849	180
							70.22037	70.10445	190
2000	1500	1000	500	0 8	`		74.04477	73.82351	200
\					L		88.48503	88.56631	250
							87.92149	88.56631	250

- 5. For the next 70~250K, fitting is done using Y=A+BX+CX^2+D/X^2 as an approximation function and the parameters are added and saved with [Add Params]. 250~2000K is similar.
- 6. Finally, copy the parameters to the clipboard with [Copy Params].
- 7. Open and paste Excel (see AssessmentExample.xlsx) and check that the difference between the original Cp data and the approximation function is about 0.1 J/molK, which is a sufficiently accurate approximation.
- 8. Next, the resulting parameters are used to create the parameter set shown below.

C(3) Ref	0(0)										
C(3) Rei	C(2)	C(-2)	C(1)	C(0)	ST(J/molK	HT(J/mol)	T1	Т0	state	Formula	Phase
0 2.73E-05	0	0	0.008846	0	0	-3.38E+05	70	0	S	BaTiO3	BaTiO3
3 0	-0.00168	82822.23	1.06193	-73.0147	0	0	250	70	S	BaTiO3	BaTiO3
5 0	-2.55E-06	-2131983	0.014937	118.458	0	0	2000	250	S	BaTiO3	BaTiO3
-		82822.23	1.06193		0	0	250		s s	BaTiO3	BaTiO3

- 9. Copy this whole thing to the clipboard. You'll also need a title line.
- CaTCalcNE C Databases Help File Edit Calculation Data Assessment and Optimization Calculation 🛛 🙀 Assessme Project Image Digitizer Mi-xAl #1 Mi-xAl #1 Mi-xAl203-ysl Eitting Tool HSCp to GFuncion Function Fitting HSCp to ADB data BM4 fitting on ab-initio energy
 W 2203-xAl203-ySi

 Y203-xAl203-ySi

 Y203-xAl203-ySi

 W 2203-xAl203-ySi

 W 2203-xAl203-ySi

 Ca0-xAl203-ySi

 Ti-xN #1

 Ti-xAl-yN #4

 Ti-xAl-yN #3

 Ti-xAl-yN #3
 Debye Temperature from S298 GFunc to HSCp data Edit Base Functions Gibbs Energy Continuity Check Convert PV param Aqueous Utility Programs Calc Debye Cp Ti-xAl-yN #2
 - 10. Click [Assessment]-[Convert Thermodynamic Data]-[HSCp to Phase data] in the menu to convert the data to Gibbs energy function. Paste the result into your first file, BaTiO3-Test.CDB and add the data. That's all.

⁽²⁾ Gibbs energy of mixing

3. When the mixed enthalpies of the solid solution phase are obtained by SQS in the ab initio calculations, the method for determining the interaction coefficient is the same as the usual thermodynamic database assessment method. Here we use the data from the Cu-Si sheet of AssessmentExample.xlsx as an example.

HMR, Cu-Si, T(K)=298.15, X(FCC,Si)=0.25, dH=-9851.8 HMR, Cu-Si, T(K)=298.15, X(FCC,Si)=0.5, dH=-7169.6 HMR, Cu-Si, T(K)=298.15, X(FCC,Si)=0.75, dH=-1062.4

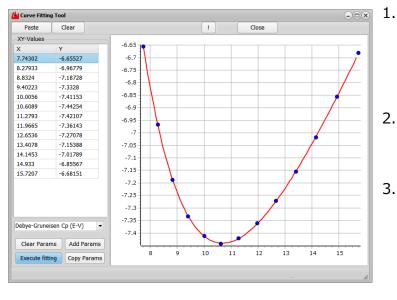
💾 Thermodynamic Assessment 💷 🗆 🗙									
File Data Edit CDB Examine									
	Evaluate 1 step	5 steps 10 steps X	Discard new	Close					
+	Parameter	Current value	New Value	RDev					
+	V11	0							
	V12	0							
+	V13	0							
	V14	0							
+	V15	0							
	V16	0							
			Dev 1.4471970	03E-12					
Ехре	eriments Calculated Data								
0:	HMR, Cu-Si, T(K)=298.15	5, X(FCC,Si)=0.25, dH=-98	351.8						
		5, X(FCC,Si)=0.5, dH=-716							
		5, X(FCC,Si)=0.75, dH=-10							
-									
				A.					

		· ·	Assessme		-	-	-	-	_ 🗆 X
	Evalu		1 step	5 step:	s 10 ste	ps X	Disc	ard new	Close
+ Parameter				Currer	nt value		New Value		RDev
+ V11			-28678	-28678.4012153				-6.07E-13	
	V12			0	0				
+	V13			-46876	5.7997801				8.58E-14
	V14			0					
+	V15				53495376				1.96E-12
	V16			0					
							Dev	5.2955454	49E-16
Exp	erime	ents Cal	culated Dat	a					
No.	EN	Туре		т	x/w	Weight	Exp. Value	En	ror
0	0	HMR		298.15	0.25	1	dH=-9851.8 0		
1	1	HMR		298.15	0.5	1	dH=-7169.6 -7.3		.33772308E-16
2	2	HMR		298.15	0.75	1	dH=-1062.4 -5.5		5.50329231E-16
4	11								P

- In this example, we will only focus on the FCC phase in the Cu-Si system; please use the Cu-Fe-FCC.CDB file. The left figure shows the mixed enthalpies of the FCC phase obtained by the SQS method in the experimental format used in the CaTCalc assessment. This is used to obtain the interaction coefficient.
- 2. Open the assessment module of CaTCalc. Open Cu-Si-FCC.CDB as a CDB file to be optimized. Copy and paste the above experimental values into the Experiments panel of the assessment module.
- 3. Since there are only three experimental values, the maximum number of parameters that can be determined is three. Therefore, only V11, V13 and V15 are considered here.
- Press the [5 steps] button, etc. to optimize the result. Save the result with the right button menu. For details, please refer to "<u>XI.</u> <u>Development of thermodynamic</u> <u>database</u>" in this manual.

③ Debye-Gruneisen model

CaTCalc incorporates thermodynamic parameter development capabilities based on the quasi-harmonic Debye-Gruneisen model of FP calculations. This method can be used to estimate temperature-dependent Cp, volume, elastic modulus, etc. Please refer to the EOS manual for more details. Below we show how to use it.



- Numerical data of the volume dependence of Energy from FP calculations are loaded into the Fitting tool, as shown on the left. It is per atom.
- Select Debye-Gruneisen Cp(E-V) as the fitting function, as shown on the left.
- 3. Execute fitting, and you will be asked for the effective mass, Poisson ratio, and the number of temperature divisions up to 3000 K. Enter the values as appropriate. Enter the number of temperature divisions as appropriate.
- 4. After pressing Add Params, use Copy Params to transfer the data to the clipboard and paste it into Excel, etc. to obtain the data shown in the figure below.

	Α	В	С	D	E	F	G	Н	I
1	E-mass(g)	Poisson's ra	Debye-T(K	Gruneisen	Param				
2	19.44025	0.24	938.4114	1.419765					
3									
4	т(к)	ET(eV/ator	VT(m^3/m	VK(1/Pa)	VN	Cv(J/mol_a	VA(/K)	Cp(J/mol_a	tomK)
5	10	-7.34506	6.49E-06	5.39E-12	3.842768	0.002457	2.90E-09	0.002457	
6	30	-7.34507	6.49E-06	5.39E-12	3.842788	0.066342	7.82E-08	0.066342	
7	60	-7.34509	6.49E-06	5.39E-12	3.843086	0.530448	6.25E-07	0.530476	
8	100	-7.34527	6.49E-06	5.39E-12	3.84471	2.350731	2.77E-06	2.351656	
9	150	-7.34607	6.49E-06	5.40E-12	3.84822	6.276822	7.41E-06	6.286731	
10	210	-7.34847	6.49E-06	5.42E-12	3.852152	11.12154	1.32E-05	11.16521	
11	280	-7.35376	6.50E-06	5.44E-12	3.855278	15.32095	1.82E-05	15.43186	
12	360	-7.3632	6.51E-06	5.48E-12	3.857606	18.37529	2.19E-05	18.58136	
13	450	-7.37789	6.53E-06	5.52E-12	3.859588	20.44197	2.45E-05	20.76245	
14	550	-7.39873	6.54E-06	5.56E-12	3.861595	21.81208	2.63E-05	22.26069	
15	660	-7.4265	6.56E-06	5.62E-12	3.86383	22.72381	2.76E-05	23.31191	
16	780	-7.46183	6.58E-06	5.68E-12	3.866386	23.33927	2.86E-05	24.07768	
17	910	-7.5053	6.61E-06	5.74E-12	3.869292	23.7624	2.93E-05	24.6623	
18	1050	-7.55743	6.64E-06	5.81E-12	3.872552	24.05895	2.99E-05	25.13229	
19	1200	-7.61867	6.67E-06	5.89E-12	3.876159	24.27072	3.05E-05	25.53033	
20	1360	-7.68945	6.70E-06	5.98E-12	3.880102	24.42461	3.10E-05	25.88435	

- 5. This is the temperature-dependent volume, elastic modulus, and specific heat estimated by the Debye-Gruneisen model, where VT, VK, and VN are, respectively, the volume parameter VT, the compressibility parameter VK, and the pressure derivative of the elastic modulus in the Birch-Murnaghan EOS. It corresponds to the parameter VN.
- First, for Cp, the 0~298.15K part does not require an entropy value to be entered if the fitting is also done. For actual fitting and parameterization, please refer to <u>the Fitting Tool</u> and <u>the Thermodynamic Data Conversion</u> <u>Method (2)</u>.
- 7. Next, parameters for VT, VK, and VN can be obtained by fitting with the VT function of the Fitting Tool. For practical use, for example, fitting data above 280 K should be sufficient. Since these are parameterized directly, they should be written in the data file as they are. However, it is necessary to edit the phase names and component formulas. For VK and VN, it is necessary to change the parameter names.