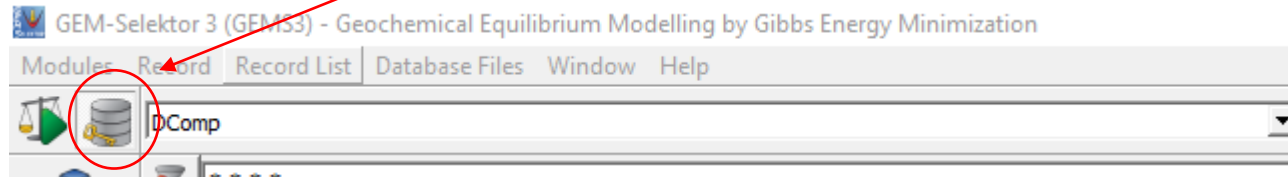


Adding a DCOMP phase in GEMS

Background

1. In GEMS, it is not recommended (disabled by default) to make changes to the parent thermodynamic database.
2. When a project is created, an editable copy of the database is made by GEMS.
3. It is recommended to make changes on this database.
4. This walkthrough assumes that you already have a project setup.
5. Open an existing project and select the “Database mode” button.



Adding a DCOMP phase in GEMS

1. We will add anorthite as a DCOMP phase.
2. The thermodynamic parameters for anorthite can be adopted from literature and databases (e.g. MINES; <http://tdb.mines.edu/>)
3. A screenshot of the required thermodynamic parameters for anorthite (from MINES database) is shown in figure below.
4. Save the screenshot of Page 1 and Page 2.

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Anorthite
CaAl₂Si₂O₈

M0	278.207	Zz	0	ab	0.05	---
V0d	10.079		0			
G0d	-4007510		---			
H0d	-4233480		---			
S0d	200		---			
Cp0d	211.836		0			
PrTr	1		25			
LamST	---		---			
BetAlp	919		2.38e-005			

H&P:1998:phaseq: MINES17

Page 1 | **Page 2** | 27/06/2019, 16:13

C H E M U J b C + - - - Feb2017 1 0 1 0

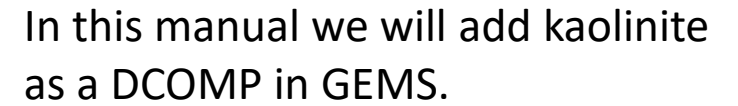
Tcint	
0	0
1	1000

a1CpT	
0	371.6
1	0.012615
2	-4.1102e+006
3	-2038.4
4	0
5	0
6	0
7	0
8	0
9	0
10	0
11	0

Hf pb	
0	2026.85
1	11
2	0.05

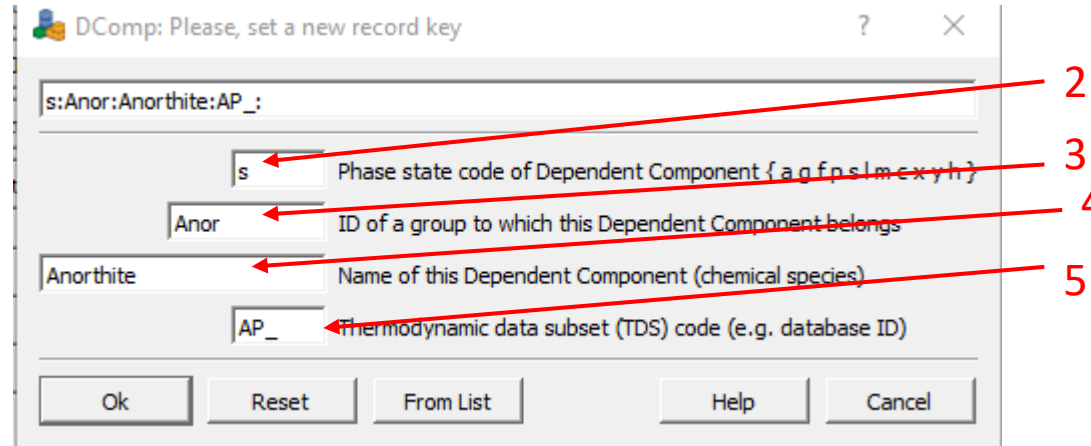
Required thermodynamic parameters for a DCOMP phase

1



1: Select Record → New Record

STEP 2



The screenshot shows a Windows-style dialog box titled "DComp: Please, set a new record key". It contains five input fields with corresponding labels and five red arrows pointing to them, numbered 2 through 6. The input fields contain the following text: "s:Anor:Anorthite:AP_".

- 2: Points to the first input field containing "s".
- 3: Points to the second input field containing "Anor".
- 4: Points to the third input field containing "Anorthite".
- 5: Points to the fourth input field containing "AP_".
- 6: Points to the fifth input field, which is empty.

The labels for the input fields are:

- Phase state code of Dependent Component {a g f p s l m e x y h}
- ID of a group to which this Dependent Component belongs
- Name of this Dependent Component (chemical species)
- Thermodynamic data subset (TDS) code (e.g. database ID)
- (Label is partially obscured by the arrow)

At the bottom of the dialog box are five buttons: "Ok", "Reset", "From List", "Help", and "Cancel".

2: Select the phase state code. For crystalline solids (e.g. Anorthite), select s. You can refer to the complete list of available codes by selecting the Help button (bottom right).

3: Enter a ID.

4: Enter the name of the phase

5: This is for the reference of the user. It is recommended to enter a unique identifier (e.g. your initials). You can use the identifier to locate phases that were added by you. It is really helpful if there is an error.

STEP 3

Step 1 - Defining the Dependent Component (DC) type and the calculation method codes

Select here to which class this Dependent Component belongs

This class code will be copied into Phase definition as default for this DC

Dependent Component of a single-component condensed phase

The codes selected below will configure the DComp record data fields, and tell the program how thermodynamic properties of this DC (per mole) will be corrected for T and P of interest.

Select here the codes of methods for temperature T and pressure P corrections

General method code for T (temperature) corrections of thermodynamic properties:

Calculation on the basis of standard S0 and Cp0 integration

Method variant code for EoS T (temperature) corrections of thermodynamic properties:

Calculation using Landau contribution to Cp(T) (Holland and Powell 1998)

Method code for P (pressure) corrections of thermodynamic properties:

Pressure correction using dV (T,P) from Birch-Murnaghan EoS (Holland and Powell 1998)

Codes for species-dependent EoS (Equation-of-State) subroutines:

No fluid model routine

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TCint	
0	0
1	1000

a1CpT	
0	371.6
1	0.012615
2	-4.1102e+006
3	-2038.4
4	0
5	0
6	0
7	0
8	0
9	0
10	0
11	0

FT pb	
0	2026.85
1	11
2	0.05

Use the screenshot as reference
to select the calculation method
codes

STEP 4

Step 2 - Specific dimensions and settings

Dimensions to change only in special cases

1 Number of sets of coefficients of $C_p=f(T)$ equation can be changed here, if available for several temperature intervals. Default is 1, maximum 5 sets (intervals).

0 Number of phase transitions can be changed here, if necessary (usually one less than the number of sets of $C_p=f(T)$ coefficients). Default is 0, maximum 4.

0 Number of EoS coefficients can be set here for certain EoS models of fluids (default: 0). Coefficients will be collected automatically into Phase record, if this DC is included.

☐ Check here to allocate the $V_m = f(P, T)$ vector of coefficients (reserved)

Units of measurement (cannot be changed in this version of GEMS)

j J/mol/(K) Units of energy (default: j)

j J/bar = 0.1 cm³/mol Units of volume (default: j)

b bar = 10⁵ Pa Units of pressure (default: b)

C Celsius Units of temperature (default: C)

[Learn more](#) < Back **Next>** Cancel

Step 3 - Useful hints

Optional

1 Set here the number of links to bibliography SDref records (default 0)

What will happen after you click "Finish"

(1) Page 1 of "DComp" window appears. Fill out the DCname field, and (essential!) enter DC formula into DCform field.

(2) Enter standard molar properties of DC into V0d, G0d, H0d, S0d, Cp0d cells. If unknown, enter the 'empty' value ('---'). Any two of three values G0, H0 and S0 must be known; the third one (if given as 'empty') will be retrieved upon re-calculation.

(3) Switch to Page 2 and enter values into TCint, then ai_Cp or aiHKF arrays, whatever appropriate. In some cases, fluid EoS coefficients, critical parameters, or V(T,P) coefficients may need to be entered.

(4) Go back to Page 1 and click the 'Calculate' toolbar button. Missing DC properties will appear. If $C_p=f(T)$ (or HKF) coefficients were entered, Cp0 (and V0) values will also be calculated. Save the record. To test T,P corrections, create a RTParm tabulator for this DComp record.

[Learn more](#) < Back **Finish** Cancel

- For most phases, it is usually not necessary to change the default values in this step. Select “**Next**” on the “Step 2 - Specific dimensions and settings dialogue box” followed by “**Finish**” on the Step 3 – Useful hints dialogue box.
- Select “**Learn more**” if you are not sure.

STEP 5

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Anorthite
CaAl₂Si₂O₈

M0	278.207	Zz	0	ab	0.05	---
----	---------	----	---	----	------	-----

V0d	10.079	0
G0d	-4007510	---
H0d	-4233480	---
S0d	200	---
Cp0d	211.836	0
PrTr	1	25
LamST	---	---
BetAlp	919	2.38e-005

H&P:1998:phaseq: MINES17



DComp :: Remake of the new record finished OK. It is recommended to re-calculate the data

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Anorthite

M0	---	Zz	---	ab	---	---
----	-----	----	-----	----	-----	-----

V0d	---	---
G0d	---	---
H0d	---	---
S0d	---	---
Cp0d	---	---
PrTr	1	25
LamST	---	---
BetAlp	---	---

--	--

- Manually enter the database parameters.
- In this example we use the parameters from MINES database for anorthite.

STEP 6

Page 1 Page 2 27/06/2019, 16:13

C H E N O j j b C + - - - Feb2017 1 0 1 0

TCint	
0	0
1	1000

aiCpT	
0	371.6
1	0.012615
2	-4.1102e+006
3	-2038.4
4	0
5	0
6	0
7	0
8	0
9	0
10	0
11	0

FI pb	
0	2026.85
1	11
2	0.05



DComp :: Remake of the new record finished OK. It is recommended to re-calculate the data

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C H E N O j j b C + - - - 21/02/20 1 0 1 0

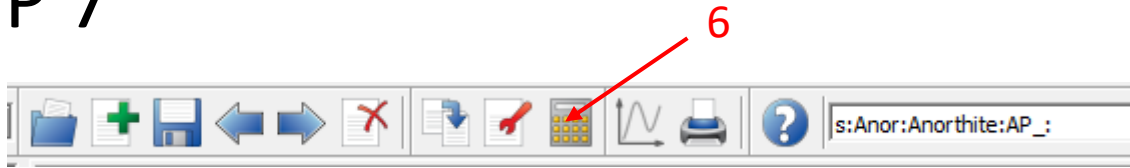
TCint	
0	0
1	0

aiCpT	
0	0
1	0
2	0
3	0
4	0
5	0
6	0
7	0
8	0
9	0
10	0
11	0

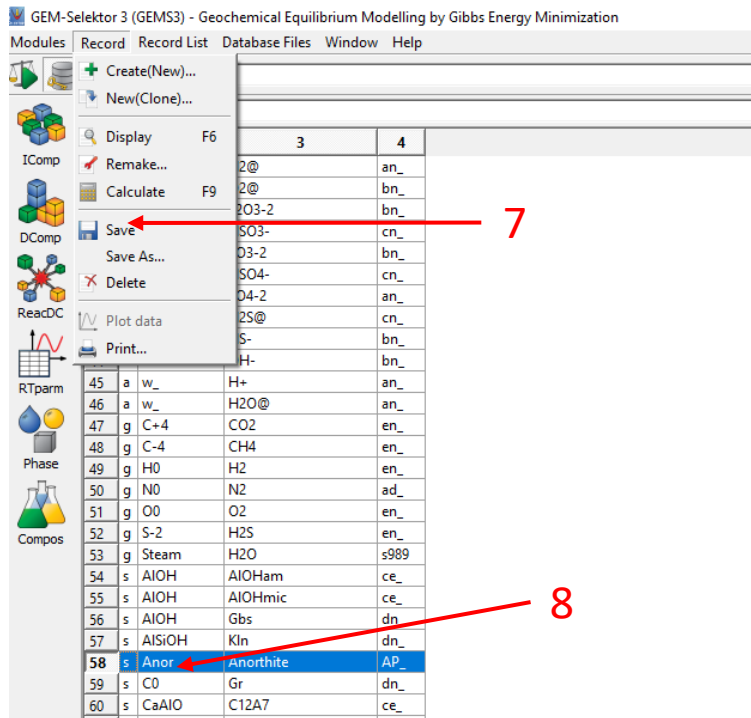
FI pb	
0	0
1	0
2	0

- Manually enter the database parameters.
- In this example we use the parameters from MINES database for anorthite.

STEP 7



Select the calculate record button (6).



- Select Record → Save (7)
- Check DCOMP list for anorthite (8)

STEP 8

1. It is important to open the same project again.
2. A dialogue box will pop up when the project is opened.
 - Select “Yes” Add for all. (This will add the DCOMP phase to the project)
3. Run a recipe with the DCOMP and check for convergence.