

A short tutorial how to implement a PHREEQC equilibrium and reaction example in ORCHESTRA

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This document describes how to implement a simple PHREEQC equilibrium and reaction example in ORCHESTRA. The example was taken from the very useful PHREEQC site by Tony Appelo and can be found here:

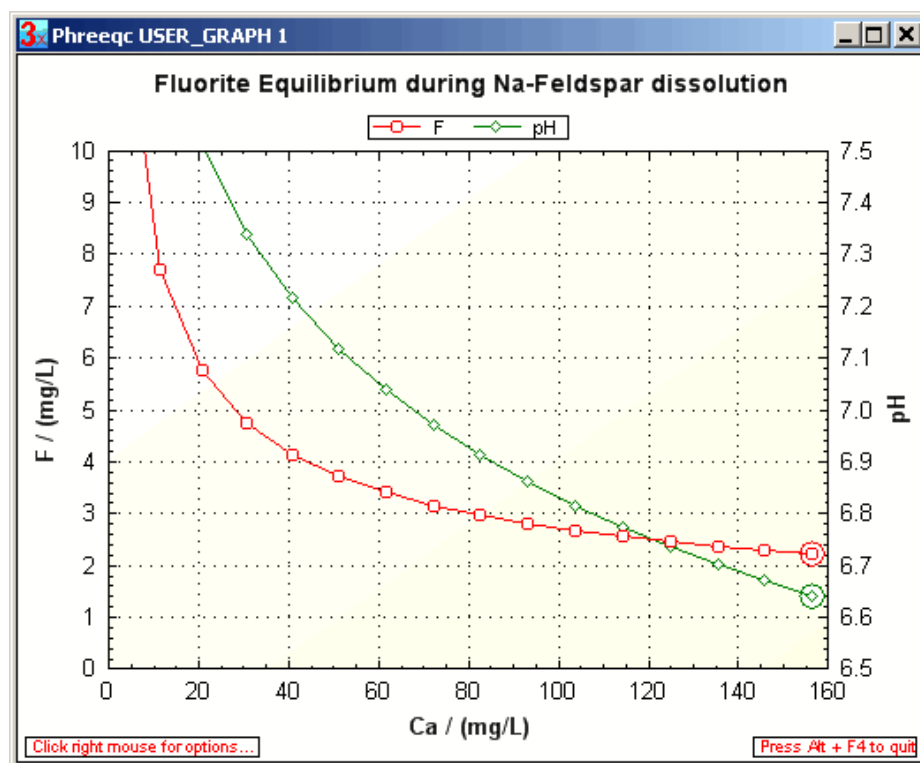
https://hydrochemistry.eu/exmpls/ca_f.html

The example demonstrates how to calculate the composition of a solution first in equilibrium with calcite, fluorite and a fixed CO_2 pressure, and subsequently let this solution react with $\text{NaAlSi}_3\text{O}_8$ (Na-Feldspar).

The PHREEQC simulation starts with calculating water (SOLUTION 1), with a CO_2 pressure of 0.1 atm, and Ca and F concentrations in equilibrium with calcite and fluorite, respectively. This is the encircled composition in the graph, with (right-click on the chart calculated by PHREEQC, and select 'Show Point Values') 157 mg Ca/L and 2.3 mg F/L.

Next, 7.5 mmol Na-feldspar dissolve in 15 steps (keyword REACTION), while calcite, fluorite, kaolinite and quartz react to equilibrium (keyword EQUILIBRIUM_PHASES).

The graph shows the increase of F (red line) and pH (green line) as a result of the reactions.



In PHREEQC the complete definition of the simulation is very compact:

```
SOLUTION 1
pH 7 charge
C 1 CO2(g) -1
Ca 1 Calcite
F 1 Fluorite

REACTION
NaAlSi3O8 1
7.5e-3 in 15

EQUILIBRIUM_PHASES 1
Fluorite
Calcite
Quartz 0 0
Kaolinite 0 0
```

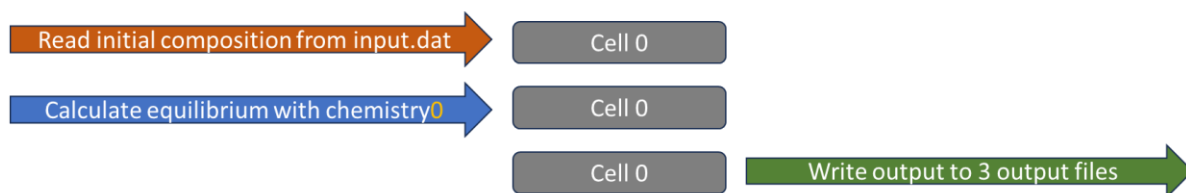
This short description is very elegant, but to reproduce it with another code it is necessary to understand what is going on behind the screen!

[ORCHESTRA implementation of initial solution calculation](#)

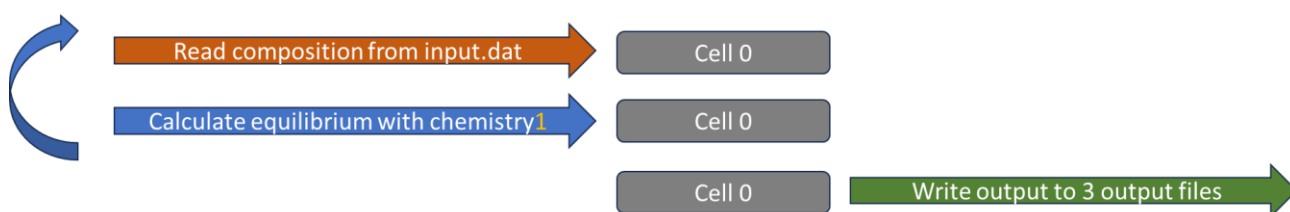
For the ORCHESTRA implementation we need a single cell, that is first equilibrated with the solid phases and fixed CO₂ pressure. Subsequently 7.5e-3 M of NaAlSi₃O₈ is added in 15 steps and equilibrated (and output generated) at each step. A graphical representation of the order of things

looks as follows:

Initialization of solution



Loop 16 times



In the ORCHESTRA concert.xml file we can find the definition of a single cell, an input file for this cell, two chemical solvers that operate on this cell and three different output files (to demonstrate different output formats). The order of actions during a run is defined in the “run” task at the bottom of the concert.xml file.



This XML file does not appear to have any style information associated with it. The document tree is shown below.

```
<?xml version="1.0" encoding="UTF-8" ?>
<Concert>
  <!-- **** The nodes that are used in the system. -->
  // in this case just a single node
  <Nodes TypeFile="input.dat" NrNodes="1"/>
  <!-- **** The list of Tasks that are used in the system. -->
  <Task Name="Equilibrate node0" Type="NodeGroup" Threads="1">
    <Calculator>chemistry0</Calculator>
    <Nodes>(0)</Nodes>
  </Task>
  <Task Name="Equilibrate node" Type="NodeGroup" Threads="1">
    <Calculator>chemistry1</Calculator>
    <Nodes>(0)</Nodes>
  </Task>
  <Task Name="Read node" Type="InstreamGroup">
    <File>input.dat</File>
    <Nodes>(0)</Nodes>
  </Task>
  <Task Name="Write output" Type="OutstreamGroup">
    <File>output.dat</File>
    <Nodes>(0)</Nodes>
  </Task>
  <Task Name="Write output2" Type="OutstreamGroup">
    <File>output2.dat</File>
    <Nodes>(0)</Nodes>
  </Task>
  <Task Name="Write output3" Type="OutstreamGroup">
    <File>output3.dat</File>
    <Nodes>(0)</Nodes>
  </Task>
  <Task Name="Each Step" Type="RepeatingTaskGroup">
    <DoTask Name="Read node"/>
    <DoTask Name="Equilibrate node"/>
    <DoTask Name="Write output"/>
    <DoTask Name="Write output2"/>
    <DoTask Name="Write output3"/>
  </Task>
  <Task Name="Run" Type="TaskGroup">
    <DoTask Name="Read node"/>
    <DoTask Name="Equilibrate node0"/>
    <DoTask Name="Write output"/>
    <DoTask Name="Write output2"/>
    <DoTask Name="Write output3"/>
    <DoTask Name="Each Step"/>
  </Task>
</Concert>
```

To calculate the composition of a solution in equilibrium with calcite, fluorite and 0.1 atmosphere $\text{CO}_2[\text{g}]$, we first need to interactively define a chemical system. We do this by selecting $\text{CO}_2[\text{g}]$, Ca and F as primary entities from the PHREEQC.dat database. The H, O and E primary entities are standard (PHREEQC) entities that together represent water. In PHREEQC these are selected by default, in

ORCHESTRA these have to be selected manually as shown in the graph below. For Ca and F we select given amounts in the tot phase (given total amount). For CO₂ we select a given log activity (partial pressure). In case of PHREEQC the primary entities are called master species, and are defined as such in the PHREEQC database.

In case of ORCHESTRA species or entities are made primary or master species at the moment they are selected as such in the user interface, regardless how they are defined in the database.

The user interface automatically rewrites formation reactions in terms of the selected primary entity, and also detects which species / entities are dependent (can be formed out of selected primary entities via reactions). Only independent entities can be selected as primary.

So for example in this case we could select either C (= PHREEQC default) , or e.g. CO₃⁻², or HCO₃⁻ or CO₂[g] as primary entity. Selection of any of these entities as primary, will make the other ones dependent, so not available for selection as primary.

For the first calculation we want to use a fixed partial pressure for CO₂[g], which we can define by choosing CO₂[g] as primary entity with a fixed log activity (which is equal to the log of the partial pressure).

(Alternatively it would be possible to use C as primary entity and to define CO₂[g] as a pure phase or “mineral” with given log solubility constant of -1, which is the common PHREEQC approach to obtain the same result.)

We also select given log activities for O, E and H. But the pH is adapted by the charge balancing procedure to reach electroneutrality. (Balance charge on pH).

Note that the default values of 1E-9 given here for the total amounts of Ca and F are overwritten by values in the input file!

chemistry0.inp

File Run Tools Help

Read Write GUI View

Adsorption models Activity correction Settings Predominance Diagram Output selector

Primary entities/ Master Species Phases & Reactions Variables Extra Text

Selectable Primary Entities/ Master Species in Database

tot diss min gas

Z P N L H C A Al
S O M K F B Amm

Include Database

PHREEQC_old.dat

Selected Primary Entities/ Master Species

Incl.	Primary entity	Phase	Input variable	Fix log activity	Log activity	Concentration	Phase	Expression
<input checked="" type="checkbox"/>	CO2[g]	gas		<input checked="" type="checkbox"/>	-9.0			
<input checked="" type="checkbox"/>	Ca	tot		<input checked="" type="checkbox"/>		1.0E-9	tot	
<input checked="" type="checkbox"/>	E	tot	pe	<input checked="" type="checkbox"/>	-7.0			E.logact = -pe
<input checked="" type="checkbox"/>	F	tot		<input checked="" type="checkbox"/>		1.0E-9	tot	
<input checked="" type="checkbox"/>	H	tot	pH	<input checked="" type="checkbox"/>	-6.0			H.logact = -pH
<input checked="" type="checkbox"/>	O	tot	H2O.logact	<input checked="" type="checkbox"/>	0.0			O.logact = H2O.logact

☒ Balance Charge pH

No input file or directory selected.

We have the following aqueous ions present (in the diss phase) :

ORCHESTRA-Composer (Running on Windows 10 with 20.0.2 Oracle Corporation, using 8 processing cores)

File Run Tools Help

chemistry0.inp

Read Write GUI View

Primary entities/ Master Species Phases & Reactions Variables Extra Text Adsorption models Activity correction Settings Predominance Diagram Output selector

Phase Hierarchy and Entities

Reactions in all phases

Formation reactions in phase: **diss**, depending on primary entity: **all** and: **all** Hide unselected ☐ Alphabetical ☒

Incl.	Name	Log K (25C)	Phase	Coef.	
<input checked="" type="checkbox"/>	CH4	0.0	diss	1.0	C[-4]
<input checked="" type="checkbox"/>	CO2	-1.468000	diss	1.0	CO2[g]
<input checked="" type="checkbox"/>	CO3-2	-16.68100	diss	1.0	CO3-2
<input checked="" type="checkbox"/>	Ca+2	0.0	diss	1.0	Ca
<input checked="" type="checkbox"/>	CaCO3	3.224000	diss	1.0	CO3-2
<input checked="" type="checkbox"/>	CaHCO3+	11.43500	diss	1.0	CO3-2
<input checked="" type="checkbox"/>	CaOH+	-12.78000	diss	1.0	Ca+2
<input checked="" type="checkbox"/>	F-	0.0	diss	1.0	F
<input checked="" type="checkbox"/>	H+	0.0	diss	1.0	H[+1]
<input checked="" type="checkbox"/>	H2	0.0	diss	1.0	H[+0]
<input checked="" type="checkbox"/>	HCO3-	10.32900	diss	1.0	CO3-2
<input checked="" type="checkbox"/>	HF	3.180000	diss	1.0	F-
<input checked="" type="checkbox"/>	HF2-	3.760000	diss	2.0	F-
<input checked="" type="checkbox"/>	O2	0.0	diss	1.0	O[+0]
<input checked="" type="checkbox"/>	OH-	-13.99475	diss	-1.0	H+
<input checked="" type="checkbox"/>	[CO2]2	-1.736241	diss	2.0	CO2
<input checked="" type="checkbox"/>	e-	0.0	diss	1.0	E

No input file or directory selected.

And calcite and fluorite are switched on as potentially precipitating minerals/phases.

ORCHESTRA-Composer (Running on Windows 10 with 20.0.2 Oracle Corporation, using 8 processing cores)

File Run Tools Help

chemistry0.inp

Read Write GUI View

Primary entities/ Master Species Phases & Reactions Variables Extra Text Adsorption models Activity correction Settings Predominance Diagram Output selector

Phase Hierarchy and Entities

Reactions in all phases

Formation reactions in phase: **min**, depending on primary entity: **all** and: **all** Hide unselected ☐ Alphabetical ☒

Incl.	Name	Log K (25C)	Phase	Coef.	
<input checked="" type="checkbox"/>	Aragonite[s]	8.338000	min	1.0	CO3-2
<input checked="" type="checkbox"/>	Calcite[s]	8.480000	min	1.0	CO3-2
<input checked="" type="checkbox"/>	Fluorite[s]	10.60000	min	1.0	Ca+2

No input file or directory selected.

In the input file the molar amounts of the primary entities Ca, F and the (log) partial pressure of CO2[g] is given. The variables for Al, Si and Na are already there, but these are ignored by the calculation with the first solver. Note that values given in the input file overwrite the default values present in the chemistry files!

```

// Here we define the input for the chemical equilibrium calculations.
//
// In the concert.xml file this file is used repetitively to read input for cell/node 0
//
// First a line with the names of the variables that we want to use as column headers starting with Var:
//
// Subsequently we can give one or more data lines with values for all the listed variables (in the same order)
//
// For each data line a calculation will be performed
// So we want to initialize a system with 1 mol of CaCO3 (Calcite) and 1 mol of CaF2(Fluorite) in contact with a fixed CO2 pressure of 0.1 atm
// In chemistry0 we have selected Ca, F and CO2[g] as primary entities.
// With for Ca and F a given total amount, and for CO2[g] a given log activity (partial pressure)
// So we can now give the appropriate input variables the wanted values
// Values given here overwrite the default values defined in the chemistry file.
//
// We do not have to specify the amount of protons in the system, as this is automatically done by chargebalancing on the pH
// So the amount of protons and pH is adjusted to result in an electroneutral system.
//
Var:  T      totvolume  Ca.tot  F.tot  CO2[g].logact  Si.tot  Al.tot  Na.tot
Data: 298.15  1.0      2      2      -1.0          1e-12  1e-12  1e-12

//
// After this first calculation, which is carried out with chemistry0 (see concert file),

```

With this we have defined the initial conditions for the simulation.

In the output file we can check the pH and total dissolved F (F.diss) and Ca (Ca.diss)

```

// The column headers in this file can be edited and determine the output for the next run.
Factor: 1          19000          40078
Var:    pH          F.diss          Ca.diss
Data:   6.64439142  2.17171369  1.55577072e2

```

Output 3 shows an automatic full overview of the system composition, very similar to that of PHREEQC.

ORCHESTRA-Composer (Running on Windows 10 with 20.0.2 Oracle Corporation, using 8 processing cores)

File Run Tools Help

output3.dat Read Write Text View

```
@class: format() {
  //Output_at: (time, from:, 0, to:, 10, steps:, 100 )
  @PHREEQCOutput: chemistry1.inp
}

@format()
```

-----Description of solution-----

Cellnumber = 0.0
 pH = 6.64439142
 pe = 7.00000000
 Activity of water = 9.99748e-1
 Ionic strength = 1.11781446e-2
 Total number of iterations = 93.0000000

-----Distribution of aqueous species-----

Species	concentration (Mol/l)	Log Activity	Activity	log gamma
Al	0.0			
Al+3	0.0 0.0 1.00000	0.0		
AlF+2	0.0 0.0 1.00000	0.0		
AlF2+	0.0 0.0 1.00000	0.0		
AlF3	0.0 0.0 1.00000	0.0		
AlF4-	0.0 0.0 1.00000	0.0		
AlOH+2	0.0 0.0 1.00000	0.0		
Al[OH]2+	0.0 0.0 1.00000	0.0		
Al[OH]3	0.0 0.0 1.00000	0.0		
Al[OH]4-	0.0 0.0 1.00000	0.0		
CO2[g]	1.10377744e-2			
CH4	5.83403970e-88	-87.2329128	5.84908e-88	1.11781e-3
CO2	3.39533152e-3	-2.46800000	3.40408e-3	1.11781e-3
CO3-2	2.09557503e-6	-5.86032645	1.37935e-6	-1.81630e-1
CaCO3	5.53200018e-6	-5.25600000	5.54626e-6	1.11781e-3
CaHCO3+	2.26585938e-4	-3.68939142	2.04460e-4	-4.46244e-2
HCO3-	7.40780504e-3	-2.17571787	6.67240e-3	-4.54074e-2
NaCO3-	0.0 0.0 1.00000	0.0		
NaHCO3	0.0 0.0 1.00000	0.0		
[CO2]2	2.12149100e-7	-6.67224099	2.12696e-7	1.11781e-3
Ca	3.88185717e-3			

No input file or directory selected.

ORCHESTRA implementation of PHREEQC “reaction” simulation

After the first equilibration of a solution, the simulation continues by adding stepwise 7.5 mmol 7.5e-3 M of NaAlSi₃O₈ to the solution. In PHREEQC this is defined as follows:

REACTION

NaAlSi308 1

7.5e-3 in 15

For these subsequent calculations the CO₂[g] pressure is no longer fixed, but instead the total amount of CO₂[g] in the system resulting from the first calculation is kept constant. This requires a change of the chemical equilibrium settings. In ORCHESTRA it is not possible to adapt an existing solver, so we simply create a second one.

We simply copy the first one and change the settings for the CO₂[g] primary entity from fixed partial pressure to given total amount (CO₂[g].tot). We also add the Na, Al and Si primary entities with given total amounts.

ORCHESTRA-Composer (Running on Windows 10 with 20.0.2 Oracle Corporation, using 8 processing cores)

File Run Tools Help

chemistry1.inp Read Write GUI View

Adsorption models Activity correction Settings Predominance Diagram Output selector

Primary entities/ Master Species Phases & Reactions Variables Extra Text

Selectable Primary Entities/ Master Species in Database

tot diss min gas

Z A Amm

Include Database

☒ PHREEQC_old.dat

Add database file

Selected Primary Entities/ Master Species

Incl.	Primary entity	Phase	Input variable	Fix log activity	Log activity	Concentration	Phase	Expression
<input checked="" type="checkbox"/>	Al	tot		<input type="checkbox"/>		1.0E-9	tot	
<input checked="" type="checkbox"/>	CO2[g]	gas		<input type="checkbox"/>		1.0E-9	tot	
<input checked="" type="checkbox"/>	Ca	tot		<input type="checkbox"/>		1.0E-9	tot	
<input checked="" type="checkbox"/>	E	tot	pe	<input type="checkbox"/>		1.0E-9	tot	E.logact = -pe
<input checked="" type="checkbox"/>	F	tot		<input type="checkbox"/>		1.0E-9	tot	
<input checked="" type="checkbox"/>	H	tot	pH	<input checked="" type="checkbox"/>	-6.0			H.logact = -pH
<input checked="" type="checkbox"/>	Na	tot		<input type="checkbox"/>		1.0E-9	tot	
<input checked="" type="checkbox"/>	O	tot	H2O.logact	<input checked="" type="checkbox"/>	0.0			O.logact = H2O.logact
<input checked="" type="checkbox"/>	Si	tot		<input type="checkbox"/>		1.0E-9	tot	

☒ Balance Charge pH

No input file or directory selected.

We select the Quartz and Kaolinite as solid phases:

ORCHESTRA-Composer (Running on Windows 10 with 20.0.2 Oracle Corporation, using 8 processing cores)

File Run Tools Help

chemistry1.inp Read Write GUI View

Adsorption models Activity correction Settings Predominance Diagram Output selector

Primary entities/ Master Species Phases & Reactions Variables Extra Text

Phase Hierarchy and Entities

Reactions in all phases

- tot (1)
 - liter (watervolume)
 - solution (1)
 - diss (1)
 - colloid (1)
 - DHA_part (1)
 - HA_part (1)
 - DFA_part (1)
 - FA_part (1)
 - solid (1)
 - min (1)
 - ads (1)
 - CLAY_part_1
 - CLAY_part_2

Formation reactions in phase: min, depending on primary entity: all and: all

| Incl. | Name | Log K (25C) | Phase | Cov |
|-------------------------------------|-----------------------|-------------|-------|------|
| <input type="checkbox"/> | Al[OH]3[a][s] | -10.80000 | min | 1.0 |
| <input type="checkbox"/> | Albite[s] | 18.00200 | min | 1.0 |
| <input type="checkbox"/> | Anorthite[s] | 19.71400 | min | 2.0 |
| <input type="checkbox"/> | Aragonite[s] | 8.336000 | min | 1.0 |
| <input type="checkbox"/> | Ca-Montmorillonite[s] | 45.02700 | min | 2.33 |
| <input checked="" type="checkbox"/> | Calcite[s] | 8.480000 | min | 1.0 |
| <input type="checkbox"/> | Chalcedony[s] | 3.550000 | min | -2.0 |
| <input checked="" type="checkbox"/> | Fluorite[s] | 10.60000 | min | 1.0 |
| <input type="checkbox"/> | Gibbsite[s] | -8.110000 | min | 1.0 |
| <input checked="" type="checkbox"/> | Kaolinite[s] | -7.435000 | min | 2.0 |
| <input checked="" type="checkbox"/> | Quartz[s] | 3.980000 | min | -2.0 |
| <input type="checkbox"/> | SiO2[a][s] | 2.710000 | min | -2.0 |

No input file or directory selected.

And keep all the automatically selected aqueous ions:

ORCHESTRA-Composer (Running on Windows 10 with 20.0.2 Oracle Corporation, using 8 processing cores)

File Run Tools Help

chemistry1.inp

Read Write GUI View

Adsorption models Activity correction Settings Predominance Diagram Output selector

Primary entities/ Master Species Phases & Reactions Variables Extra Text

Phase Hierarchy and Entities

Reactions in all phases

tot (1)

liter (watervolume)

solution (1)

diss (1)

colloid (1)

DHA_part (1)

HA_part (1)

DFA_part (1)

FA_part (1)

solid (1)

min (1)

ads (1)

CLAY_part_I (1)

CLAY_part (1)

HFO_part_I (1)

HFO_part (1)

Goethite_part_I (1)

Goethite_part (1)

SHA_part_I (1)

HA_part (1)

SFA_part_I (1)

FA_part (1)

exchange (1)

gas_I (1)

gas (gasvolume*(1))

kg (1)

liter (1/SL)

solution (1)

diss (1)

colloid (1)

DHA_part (1)

DFA_part (1)

solid (1)

Formation reactions in phase: **diss**, depending on primary entity: **all** and: **all**

| Incl. | Name | Log K (25C) | Phase |
|-------------------------------------|----------|--------------|-------|
| <input checked="" type="checkbox"/> | Al+3 | 0.0 | diss |
| <input checked="" type="checkbox"/> | AlF+2 | 7.000000 | diss |
| <input checked="" type="checkbox"/> | AlF2+ | 12.700000 | diss |
| <input checked="" type="checkbox"/> | AlF3 | 16.800000 | diss |
| <input checked="" type="checkbox"/> | AlF4- | 19.400000 | diss |
| <input checked="" type="checkbox"/> | AlOH+2 | -6.000000 | diss |
| <input checked="" type="checkbox"/> | Al[OH]2+ | -10.100000 | diss |
| <input checked="" type="checkbox"/> | Al[OH]3 | -16.900000 | diss |
| <input checked="" type="checkbox"/> | Al[OH]4- | -22.700000 | diss |
| <input checked="" type="checkbox"/> | CH4 | 0.0 | diss |
| <input checked="" type="checkbox"/> | CO2 | -1.468000 | diss |
| <input checked="" type="checkbox"/> | CO3-2 | -16.68100 | diss |
| <input checked="" type="checkbox"/> | Ca+2 | 0.0 | diss |
| <input checked="" type="checkbox"/> | CaCO3 | 3.224000 | diss |
| <input checked="" type="checkbox"/> | CaHCO3+ | 11.43500 | diss |
| <input checked="" type="checkbox"/> | CaOH+ | -12.78000 | diss |
| <input checked="" type="checkbox"/> | F- | 0.0 | diss |
| <input checked="" type="checkbox"/> | H+ | 0.0 | diss |
| <input checked="" type="checkbox"/> | H2 | 0.0 | diss |
| <input checked="" type="checkbox"/> | H2SiO4-2 | -23.00000 | diss |
| <input checked="" type="checkbox"/> | H3SiO4- | -9.830000 | diss |
| <input checked="" type="checkbox"/> | H4SiO4 | 0.0 | diss |
| <input checked="" type="checkbox"/> | HCO3- | 10.32900 | diss |
| <input checked="" type="checkbox"/> | HF | 3.180000 | diss |
| <input checked="" type="checkbox"/> | HF2- | 3.760000 | diss |
| <input checked="" type="checkbox"/> | Na+ | 0.0 | diss |
| <input checked="" type="checkbox"/> | NaCO3- | 1.270000 | diss |
| <input checked="" type="checkbox"/> | NaF | -2.400000e-1 | diss |
| <input checked="" type="checkbox"/> | NaHCO3 | -2.500000e-1 | diss |
| <input checked="" type="checkbox"/> | NaOH | -10.00000 | diss |
| <input checked="" type="checkbox"/> | O2 | 0.0 | diss |
| <input checked="" type="checkbox"/> | OH- | -13.99475 | diss |
| <input checked="" type="checkbox"/> | SiF6-2 | 30.18000 | diss |
| <input checked="" type="checkbox"/> | [CO2]2 | -1.736241 | diss |
| <input checked="" type="checkbox"/> | e- | 0.0 | diss |

No input file or directory selected.

Now we define the addition of NaAlSi3O8 in the input file:

ORCHESTRA-Composer (Running on Windows 10 with 20.0.2 Oracle Corporation, using 8 processing cores)

File Run Tools Help

input.dat

Read Write Text View

```
// Now we want to add 7.5 mmol NaAlSi3O8 in 15 steps
// This can be done by adding a loop in which we add the amounts of constituent primary entities in NaAlSi3O8
// We do not have to add the O/H+, as this is automatically done via the charge balance on protons.
// A Sweep results in a given number of data points with the listed variables varied from start to end value
// Because the start point is included in the calculations, we specify one extra point to get the same 15 add
// as in the PHREEQC example.
//-----

// PHREEQC statement:
//REACTION
// NaAlSi3O8 1
// 7.5e-3 in 15

Sweep{ 16
  Swept: Na.tot 1e-12 7.5e-3 lin
  Swept: Al.tot 1e-12 7.5e-3 lin
  Swept: Si.tot 3e-12 22.5e-3 lin
}
```

No input file or directory selected.

In the concert file we define a first calculation with chemistry0 to initialize the system with fixed CO2 pressure:

The screenshot shows the ORCHESTRA-Composer application window. The title bar indicates it is running on Windows 10 with version 20.0.2, using 8 processing cores. The menu bar includes File, Run, Tools, and Help. The main window has three tabs: Read, Write, and Text View. The Text View tab is active, displaying the content of concert.xml. The XML code defines a single node for chemistry0, followed by a task group for equilibration. The right sidebar contains a navigation menu with links to Intro, Documentation, Chemistry0, Chemistry1, Input, Output, Output2, Output3, and Concert. The bottom status bar indicates "No input file or directory selected."

```

concert.xml
// in this case just a single node
<Nodes TypeFile="input.dat" NrNodes="1" />

<!--**** The list of Tasks that are used in the system.-->
<Task Name="Equilibrate node0" Type="NodeGroup" Threads="1">
  <Calculator>chemistry0</Calculator>
  <Nodes>(0)</Nodes>
</Task>

<Task Name="Equilibrate node" Type="NodeGroup" Threads="1">
  <Calculator>chemistry1</Calculator>
  <Nodes>(0)</Nodes>
</Task>

<Task Name="Read node" Type="InstreamGroup">
  <File>input.dat</File>
  <Nodes>(0)</Nodes>
</Task>

<Task Name="Write output" Type="OutstreamGroup">

```

No input file or directory selected.

The screenshot shows the ORCHESTRA-Composer application window with the same title bar and menu bar. The main window now has four tabs: Read, Write, Text View, and a new tab for output3.dat. The Text View tab is active, displaying the updated content of concert.xml. The XML code now includes a task group for "Each Step" which repeats the "Read node", "Equilibrate node", and "Write output" tasks. The right sidebar navigation menu is the same. The bottom status bar indicates "No input file or directory selected."

```

concert.xml
<File>output3.dat</File>
<Nodes>(0)</Nodes>
</Task>

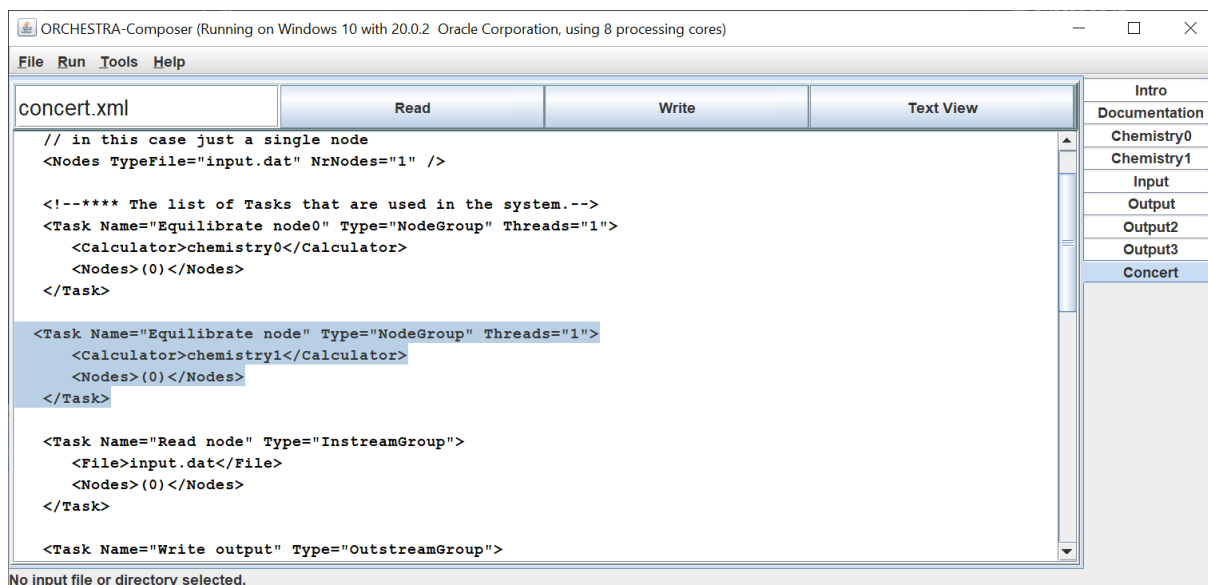
<Task Name="Each Step" Type="RepeatingTaskGroup">
  <DoTask Name="Read node" />
  <DoTask Name="Equilibrate node" />
  <DoTask Name="Write output" />
  <DoTask Name="Write output2" />
  <DoTask Name="Write output3" />
</Task>

<Task Name="Run" Type="TaskGroup">
  <DoTask Name="Read node" />
  <DoTask Name="Equilibrate node0" />
  <DoTask Name="Write output" />
  <DoTask Name="Write output2" />
  <DoTask Name="Write output3" />
  <DoTask Name="Each Step" />
</Task>

```

No input file or directory selected.

After that the same cell 0 is used in the “Each Step” task to be equilibrated with chemistry1 (given total amount of CO2[g])



Note that after each calculation, output is written to three different output files.

The output of output2.dat can be directly pasted in Excel to compare the results with PHREEQC.

ORCHESTRA-Composer (Running on Windows 10 with 20.0.2 Oracle Corporation, using 8 processing cores)

File Run Tools Help

output2.dat Read Write Text View

// The column headers in this file can be edited and determine the output for the next run.

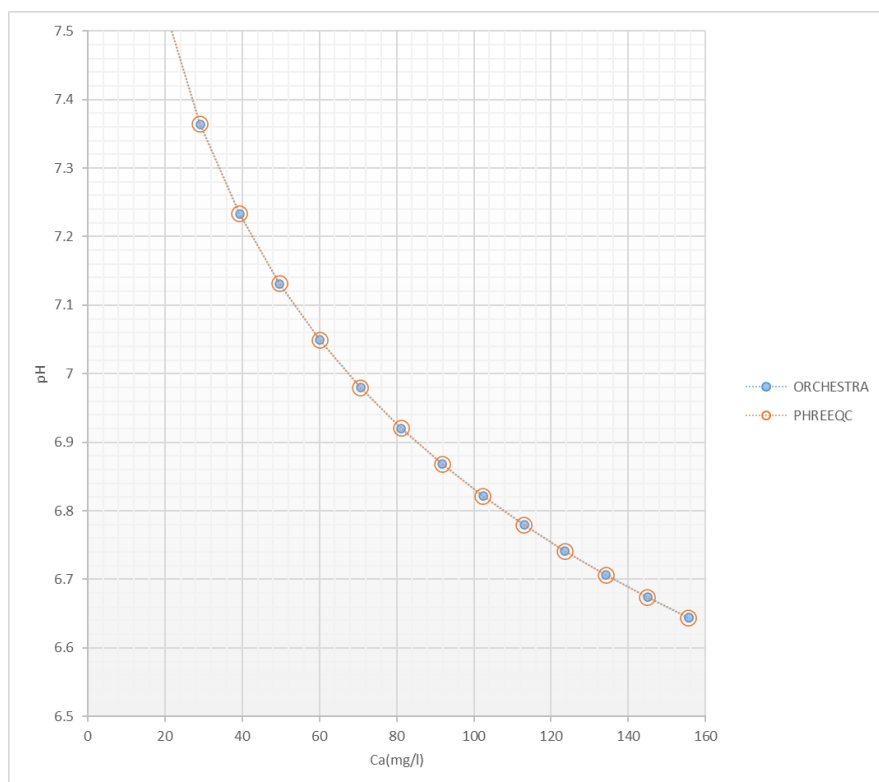
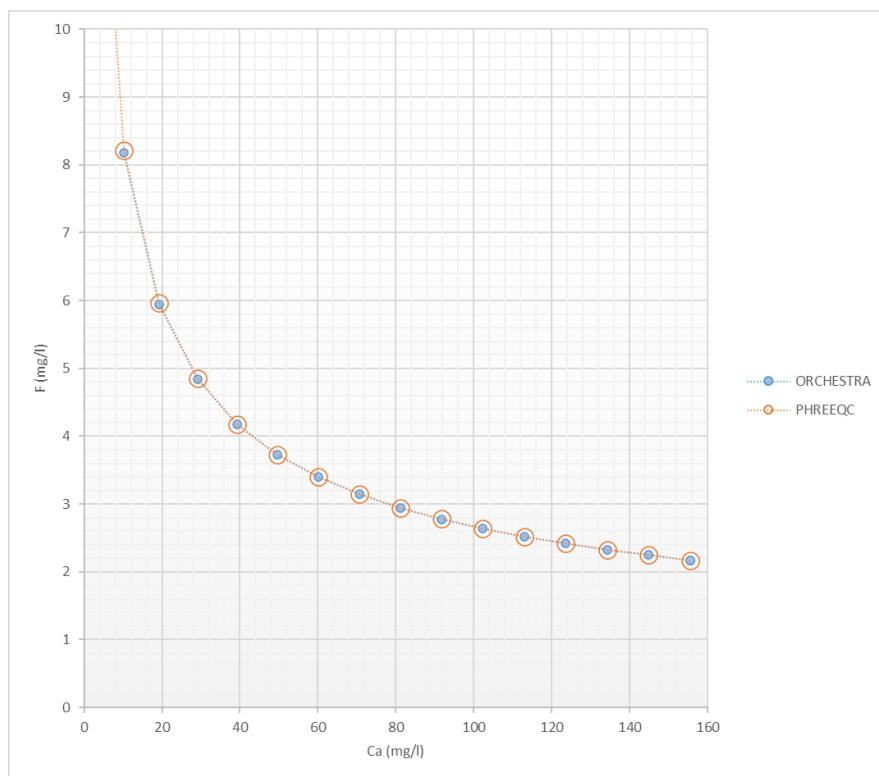
| | | | |
|---------|------------|------------|--------------|
| Factor: | 1 | 19000 | 40078 |
| Var: | pH | F.diss | Ca.diss |
| Data: | 6.64439142 | 2.17171369 | 1.55577072e2 |
| Data: | 6.64439142 | 2.17171374 | 1.55577072e2 |
| Data: | 6.67429476 | 2.24662443 | 1.44917716e2 |
| Data: | 6.70651679 | 2.32639975 | 1.34265067e2 |
| Data: | 6.74144203 | 2.41650710 | 1.23620826e2 |
| Data: | 6.77955241 | 2.51931118 | 1.12987346e2 |
| Data: | 6.82146970 | 2.63800206 | 1.02367645e2 |
| Data: | 6.86801486 | 2.77700326 | 91.7656962 |
| Data: | 6.92030236 | 2.94265483 | 81.1868896 |
| Data: | 6.97989696 | 3.14441864 | 70.6388416 |
| Data: | 7.04908952 | 3.39714821 | 60.1329093 |
| Data: | 7.13141688 | 3.72572562 | 49.6872961 |
| Data: | 7.23273030 | 4.17558108 | 39.3342071 |
| Data: | 7.36364160 | 4.84010250 | 29.1390218 |
| Data: | 7.54585824 | 5.94648345 | 19.2632319 |
| Data: | 7.82895191 | 8.18479909 | 10.2281275 |
| Data: | 8.28187827 | 13.5855614 | 3.85827416 |

No input file or directory selected.

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Data and graphs can be found in results.xls in the zipped folder.

The PHREEQC and ORCHESTRA results appear to match very closely.



The zipped folder contains all the necessary files (PHREEQC input file, ORCHESTRA complete model and input files) to reproduce the calculations yourself.