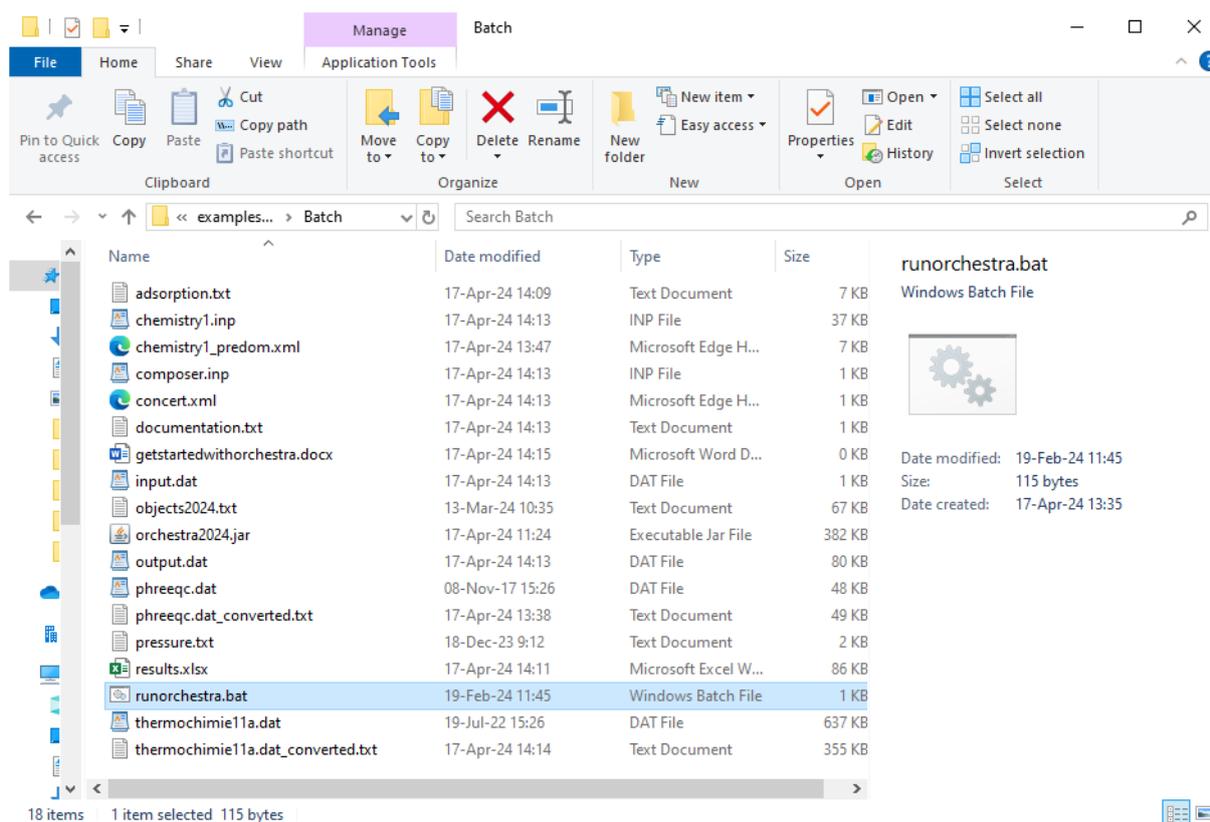


A quick tutorial to get started with ORCHESTRA

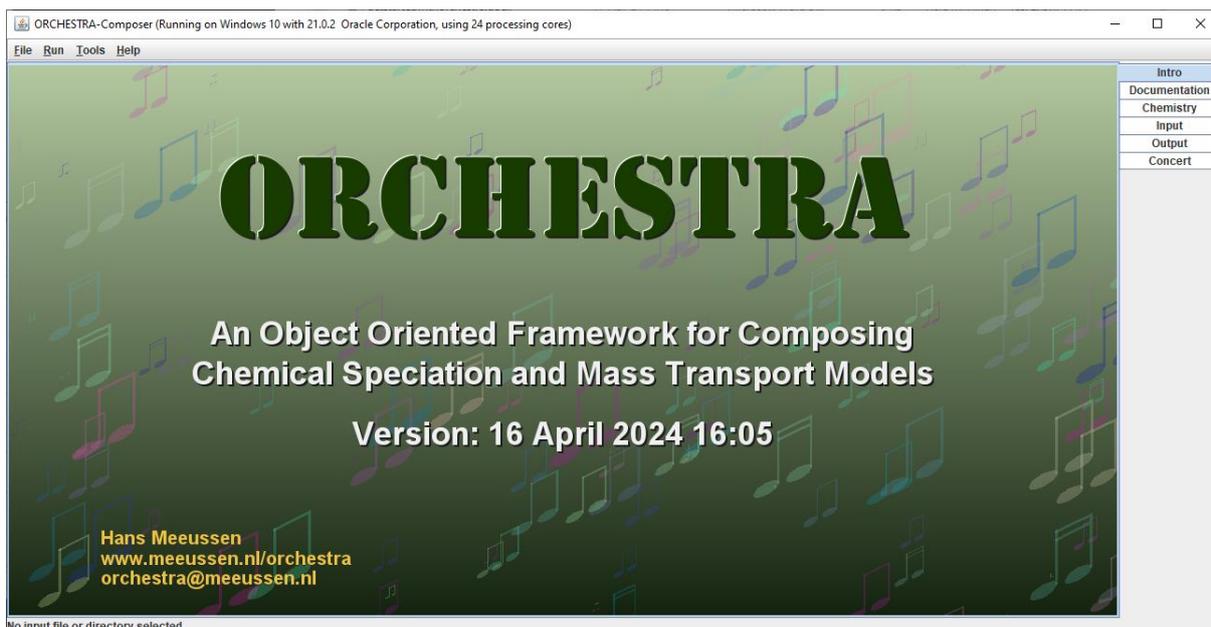
Hans Meeussen 17/4/2024

This document describes how to get started with performing chemical equilibrium calculations with ORCHESTRA.

- 1) Make sure that you have a Java virtual machine installed on your machine (available for free from <https://openjdk.org/> or <https://www.graalvm.org/>)
- 2) Download the complete self-contained zipped folder with ORCHESTRA executable, database and input files from: www.meeussen.nl/orchestra/getstarted.zip
- 3) Unzip this folder on your machine and (under Windows) click the runorchestra.bat file or from a command window/console opened in this folder give the command: `java -cp orchestra2024.jar orchestra2.composer` under Linux or MacOS



- 4) This will start up the orchestra composer



- 5) In the chemistry editor define you system by selecting substances from the thermodynamic database (in this case Pb)

chemistry1.inp

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

Selectable Primary Entities/ Master Species in Database

tot	diss	min	gas
R	I	A	P
S	K	B	Pa
T	L	C	Pa[+4]
U	M	E	Pa[+5]
Z	N	F	Pb
	O	G	Pd
P	H		Phthalat

Include Database

Include	Database
<input checked="" type="checkbox"/>	thermochimie11a.dat
<input checked="" type="checkbox"/>	adsorption.bt

Selected Primary Entities/ Master Species

Incl.	Primary entity	Phase	Input variable	Fix log activity	Log activity	Concentration	Phase	Expression
<input checked="" type="checkbox"/>	Cl	tot		<input type="checkbox"/>		0.1	tot	
<input checked="" type="checkbox"/>	E	tot	pe	<input type="checkbox"/>	-7.0			E.logact = -pe
<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"/>		0.1	tot	
<input checked="" type="checkbox"/>	O	tot	H2O.logact	<input checked="" type="checkbox"/>	0.0			O.logact = H2O.logact

Balance Charge pe

ORCHESTRA-Composer (Running on Windows 10 with 21.0.2 Oracle Corporation, using 24 processing cores)

File Run Tools Help

chemistry1.inp

Read Write GUI View

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

Selectable Primary Entities/ Master Species in Database

tot	diss	min	gas
R	I	A	P
S	K	B	Pa
T	L	C	Pa[+4]
U	M	E	Pa[+5]
Z	N	F	Pd
	O	G	Phthalat
	P	H	Pu

Include	Database
<input checked="" type="checkbox"/>	thermochimie11a.dat
<input checked="" type="checkbox"/>	adsorption.bt

Select Primary Entities/ Master Species

Incl.	Primary entity	Phase	Input variable	Fix log activity	Log activity	Concentration	Phase	Expression
<input checked="" type="checkbox"/>	Cl	tot		<input type="checkbox"/>		0.1	tot	
<input checked="" type="checkbox"/>	E	tot	pe	<input checked="" type="checkbox"/>	-7.0		tot	E.logact = -pe
<input checked="" type="checkbox"/>	H	tot	pH	<input checked="" type="checkbox"/>	-6.0		tot	H.logact = -pH
<input checked="" type="checkbox"/>	Na	tot		<input type="checkbox"/>		0.1	tot	
<input checked="" type="checkbox"/>	O	tot	H2O.logact	<input checked="" type="checkbox"/>	0.0		tot	O.logact = H2O.logact
<input checked="" type="checkbox"/>	Pb	tot		<input type="checkbox"/>		0.1	tot	

Balance Charge pe

No input file or directory selected.

- Lead (Pb) will appear in the list of selected primary entities (also called Master species or independent components in other codes).
- So we now have a system with water, (H, O and E) and Na Cl and Pb present.
- For the Pb primary entity we can select either a given log activity or a given amount or “mass balance” in any of the phases in the system. Here we select a given total amount, so Pb.tot in “tot” phase (total amount) and not a fixed log activity.
- Under the phases & reactions tab we can now see all the possible lead reactions that can be selected from the selected set of primary entities to be included in the chemical system. By default all dissolved species are automatically selected, but mineral phases have to be specifically selected. Lead can form complexes with Cl⁻ and OH⁻, and also can precipitate in different solid phases.

ORCHESTRA-Composer (Running on Windows 10 with 21.0.2 Oracle Corporation, using 24 processing cores)

File Run Tools Help

chemistry1.inp

Read Write GUI View

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

Phase Hierarchy and Entities

Reactions in all phases

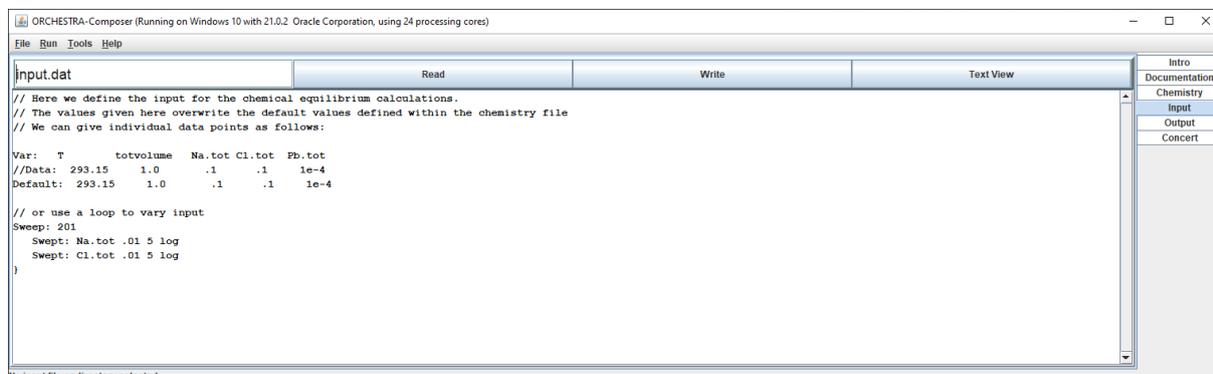
Formation reactions in phase: all, depending on primary entity: Pb and: all

Hide unselected Alphabetical Select all listed Select all recursive

Incl.	Name	Log K (25C)	Phase	Coef.	Reactant	Coef.	Reactant
<input checked="" type="checkbox"/>	Cotunnite[s]	4.810000	min	2.0	Cl-	1.0	Pb+2
<input checked="" type="checkbox"/>	Exch_X2-Pb	4.500000e-1	Exch_X	2.0	Exch_X	1.0	Pb+2
<input checked="" type="checkbox"/>	Laurionite[s]	-6.200000e-1	min	1.0	Cl-	-1.0	H+
<input checked="" type="checkbox"/>	Liltharge[s]	-12.63000	min	-2.0	H+	1.0	H2O
<input checked="" type="checkbox"/>	Massicot[s]	-12.74000	min	-2.0	H+	1.0	H2O
<input checked="" type="checkbox"/>	Minum[s]	-73.53000	min	-8.0	H+	4.0	H2O
<input checked="" type="checkbox"/>	Paralaunonite[s]	-6.200000e-1	min	1.0	Cl-	-1.0	H+
<input checked="" type="checkbox"/>	Pb+2	0.0	diss	1.0	Pb		
<input checked="" type="checkbox"/>	Pb2[OH]3	-7.180000	diss	-1.0	H+	1.0	H2O
<input checked="" type="checkbox"/>	Pb4[OH]4+4	-20.63000	diss	-4.0	H+	4.0	H2O
<input checked="" type="checkbox"/>	Pb6[OH]8+4	-42.68000	diss	-8.0	H+	8.0	H2O
<input checked="" type="checkbox"/>	PbCl+	1.440000	diss	1.0	Cl-	1.0	Pb+2
<input checked="" type="checkbox"/>	PbCl2	2.000000	diss	2.0	Cl-	1.0	Pb+2
<input checked="" type="checkbox"/>	PbCl3-	1.690000	diss	3.0	Cl-	1.0	Pb+2
<input checked="" type="checkbox"/>	PbCl4-2	1.400000	diss	4.0	Cl-	1.0	Pb+2
<input checked="" type="checkbox"/>	Pb[OH]+	-7.510000	diss	-1.0	H+	1.0	H2O
<input checked="" type="checkbox"/>	Pb[OH]2	-16.95000	diss	-2.0	H+	2.0	H2O
<input checked="" type="checkbox"/>	Pb[OH]3[s]	-13.61000	min	-2.0	H+	2.0	H2O
<input checked="" type="checkbox"/>	Pb[OH]3-	-27.20000	diss	-3.0	H+	3.0	H2O
<input checked="" type="checkbox"/>	Pb[OH]4-2	-38.90000	diss	-4.0	H+	4.0	H2O
<input checked="" type="checkbox"/>	Pb[cr]s	-4.250000	min	-1.0	Pb+2	2.0	e-
<input checked="" type="checkbox"/>	Plattinote[s]	-49.60000	min	-4.0	H+	2.0	H2O

No input file or directory selected.

10) Next we can define our (set of) input conditions in the input file. This can be single or multiple datapoints. The values given here overrule the default values given within the chemistry file. So here you can give a list of concentrations for e.g. Cl, Na or Pb. The values of Pb.tot, Na.tot and Cl.tot given here will overrule the values given in the graphical user interface. In this case we want to perform a series of calculations for a range of NaCl concentrations (Sweep) and a constant total concentration of Pb (1e-4 mol)



```

input.dat
// Here we define the input for the chemical equilibrium calculations.
// The values given here overrule the default values defined within the chemistry file
// We can give individual data points as follows:
Var: T      totvolume Na.tot Cl.tot Pb.tot
//Data: 293.15 1.0 .1 .1 1e-4
Default: 293.15 1.0 .1 .1 1e-4
// or use a loop to vary input
Sweep: 201
Sweep: Na.tot .01 5 log
Sweep: Cl.tot .01 5 log
}

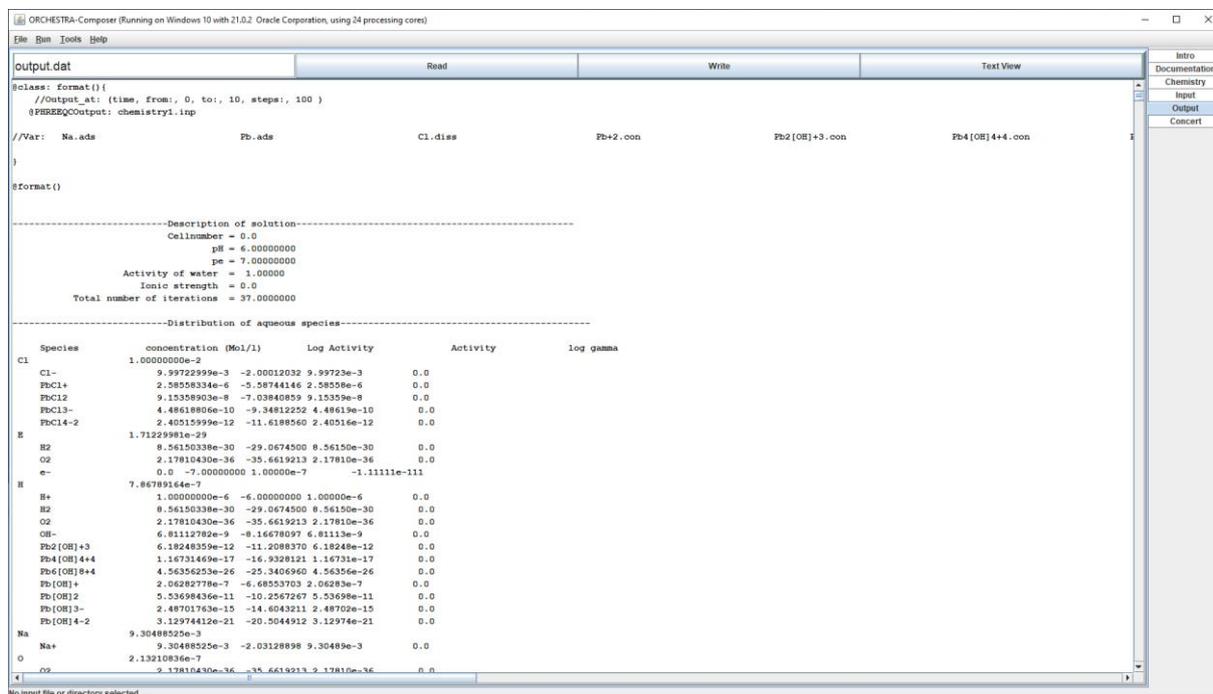
```

11) Now we can perform the calculation by clicking the “run” button in the GUI.

12) When the run is finished, the calculated results will be written to the output text file, which is automatically reloaded.

13) In the output file you can define the type of output you want. This can be either an automatic set of variables, similar to PHREEQC, or a list of individual variables in any order you specify.

14) So the type of output is actually defined in the output file itself, and this file is read before a run to determine which output needs to be generated.



```

output.dat
@class: Format()
//Output_at: (time, from:, 0, to:, 10, steps:, 100)
@PREEQCOutput: chemistry1.inp
//Var: Na.ads Pb.ads Cl.diss Pb+2.con Pb2[OH]+3.con Pb4[OH]4+4.con
}
@format()
-----Description of solution
Cellnumber = 0.0
pH = 6.00000000
pe = 7.00000000
Activity of water = 1.00000
Ionic strength = 0.0
Total number of iterations = 37.0000000
-----Distribution of aqueous species-----
Species concentration (Mol/l) Log Activity Activity log gamma
Cl 1.00000000e-2
Cl- 9.99722999e-3 -2.00012032 9.99723e-3 0.0
FBCl+ 2.98598334e-6 -5.59744146 2.98598e-6 0.0
FBCl2 9.15308930e-8 -7.03848059 9.15309e-8 0.0
FBCl3- 4.48618806e-10 -9.34812252 4.48619e-10 0.0
FBCl4-2 2.40515999e-12 -11.6188560 2.40516e-12 0.0
E 1.71229981e-29
E2 8.56150338e-30 -29.0674500 8.56150e-30 0.0
O2 2.17810430e-36 -35.6619213 2.17810e-36 0.0
e- 0.0 -7.00000000 1.00000e-7 -1.11111e-111
H 7.86789164e-7
H+ 1.00000000e-6 -6.00000000 1.00000e-6 0.0
H2 8.56150338e-30 -29.0674500 8.56150e-30 0.0
O2 2.17810430e-36 -35.6619213 2.17810e-36 0.0
OH- 6.81112782e-9 -8.16678097 6.81113e-9 0.0
Pb2[OH]+3 6.18248359e-12 -11.2088370 6.18248e-12 0.0
Pb4[OH]4+4 1.16731469e-17 -16.9328121 1.16731e-17 0.0
Pb6[OH]8+4 4.56356253e-26 -25.3406960 4.56356e-26 0.0
Pb[OH]+ 2.06282778e-7 -6.6853703 2.06283e-7 0.0
Pb[OH]2 5.53698436e-11 -10.2567267 5.53698e-11 0.0
Pb[OH]3- 2.48701763e-15 -14.6043211 2.48702e-15 0.0
Pb[OH]4-2 3.12974412e-21 -20.5044912 3.12974e-21 0.0
Na 9.30488525e-3
Na+ 9.30488525e-3 -2.03128898 9.30489e-3 0.0
O 2.13210836e-7
O2 2.13210836e-7 -35.6619213 2.13210e-36 0.0
}

```

15) Or you can ask for individual variables by writing them in the column headers, and re-run the model

```

ORCHESTRA-Composer (Running on Windows 10 with 21.0.2 Oracle Corporation, using 24 processing cores)
File Run Tools Help

output.dat                                Read                                Write                                Text View
-----
@class: format()
//Output_at: (time, from: 0, to: 10, steps: 100)
//@PBRREQOutput: chemistry1.inp

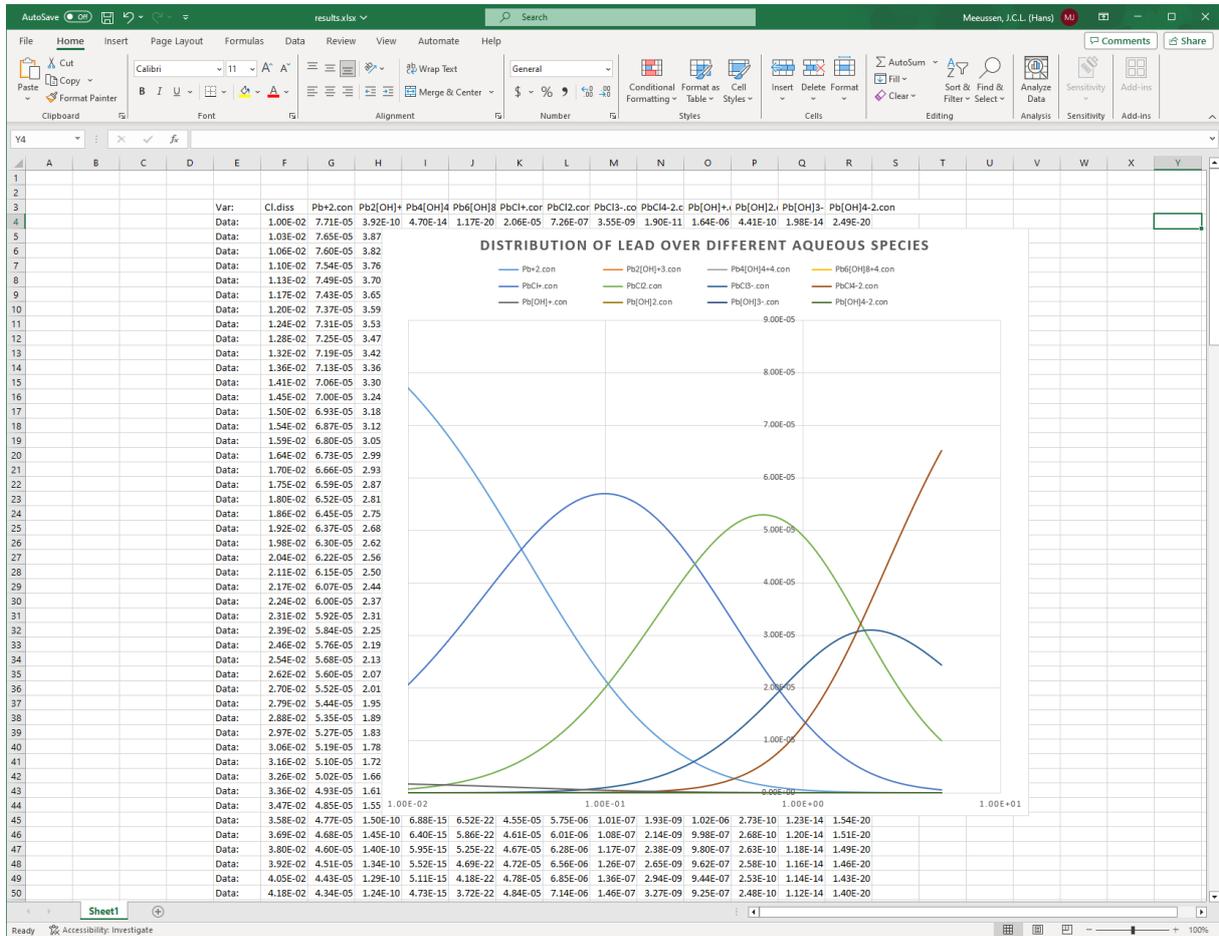
Var:  Na_ads      Pb_ads      Cl_diss      Pb+2_con      Pb2[OH]+3_con      Pb4[OH]4+4_con
]

@format()
// The column headers in this file can be edited and determine the output for the next run.
Var:  Na_ads      Pb_ads      Cl_diss      Pb+2_con      Pb2[OH]+3_con      Pb4[OH]4+4_con
Data:  6.35114746e-4  8.74426271e-5  1.00000000e-2  9.67345231e-6  6.13244835e-12  1.16721469e-17
Data:  6.96666625e-4  8.66666675e-5  1.03156085e-2  1.02001377e-5  6.87404018e-12  1.44306581e-17
Data:  6.98294786e-4  8.58562071e-5  1.06411778e-2  1.07460733e-5  7.62956182e-12  1.77771116e-17
Data:  7.00009946e-4  8.49959031e-5  1.09770224e-2  1.13110480e-5  8.45289914e-12  2.18209362e-17
Data:  7.01768649e-4  8.41659757e-5  1.13234665e-2  1.18947453e-5  9.34781305e-12  2.66859458e-17
Data:  7.03653761e-4  8.31313196e-5  1.16808447e-2  1.24967376e-5  1.03179472e-11  3.25129638e-17
Data:  7.05602931e-4  8.21855347e-5  1.20459021e-2  1.31164795e-5  1.13667045e-11  3.94576432e-17
Data:  7.07635325e-4  8.11823374e-5  1.24297945e-2  1.37533033e-5  1.24972381e-11  4.76968939e-17
Data:  7.09751657e-4  8.01241136e-5  1.28220894e-2  1.44066447e-5  1.37123479e-11  5.74229704e-17
Data:  7.11923264e-4  7.90239126e-5  1.32267454e-2  1.50748888e-5  1.50144087e-11  6.88457619e-17
Data:  7.14237584e-4  7.78812079e-5  1.36442133e-2  1.57576680e-5  1.64052892e-11  8.21920455e-17
Data:  7.16607144e-4  7.66964796e-5  1.40748362e-2  1.64535605e-5  1.78862701e-11  9.7015771e-17
Data:  7.19060535e-4  7.54697327e-5  1.45190500e-2  1.71612399e-5  1.94579608e-11  1.16263076e-16
Data:  7.21598996e-4  7.42015522e-5  1.49772835e-2  1.78792460e-5  2.12021816e-11  1.38625630e-16
Data:  7.24215003e-4  7.28924986e-5  1.54499792e-2  1.86059880e-5  2.28720701e-11  1.64961803e-16
Data:  7.26913254e-4  7.15437316e-5  1.59375937e-2  1.93397461e-5  2.47116382e-11  1.86494093e-16
Data:  7.29689658e-4  7.01551709e-5  1.64405976e-2  2.00786783e-5  2.66360760e-11  2.16671852e-16
Data:  7.32541828e-4  6.87290959e-5  1.69594769e-2  2.08208259e-5  2.86415096e-11  2.50526893e-16
Data:  7.35469705e-4  6.72665126e-5  1.74947322e-2  2.15641210e-5  3.07231928e-11  2.88263059e-16
Data:  7.38461904e-4  6.57690479e-5  1.80468808e-2  2.23063960e-5  3.28744742e-11  3.30049923e-16
Data:  7.41523018e-4  6.42384908e-5  1.86164557e-2  2.30453937e-5  3.50887795e-11  3.76009252e-16
Data:  7.44646319e-4  6.26768405e-5  1.92040068e-2  2.37877890e-5  3.73576116e-11  4.26206638e-16
Data:  7.47827413e-4  6.10849346e-5  1.98101015e-2  2.45340452e-5  3.96715673e-11  4.80648096e-16
Data:  7.51061525e-4  5.94629373e-5  2.04353251e-2  2.52839620e-5  4.20201752e-11  5.39254544e-16
Data:  7.54343510e-4  5.78282450e-5  2.1082012e-2  2.59210233e-5  4.43919530e-11  6.01825393e-16
Data:  7.57667869e-4  5.61606535e-5  2.17455928e-2  2.66075269e-5  4.67748571e-11  6.68159346e-16
Data:  7.61020776e-4  5.44589121e-5  2.24319021e-2  2.72760672e-5  4.91542921e-11  7.37885054e-16
Data:  7.64402095e-4  5.27899256e-5  2.31398719e-2  2.79241496e-5  5.15181087e-11  8.10553765e-16
Data:  7.67835417e-4  5.10822344e-5  2.38701859e-2  2.85493137e-5  5.38506989e-11  8.85614447e-16
Data:  7.71268086e-4  4.93565959e-5  2.46235491e-2  2.91491511e-5  5.61373389e-11  9.62222366e-16
Data:  7.74711246e-4  4.7643770e-5  2.54006892e-2  2.9723241e-5  5.83682925e-11  1.04024296e-15
Data:  7.78157862e-4  4.59210699e-5  2.62023565e-2  3.02639489e-5  6.05118920e-11  1.118261179e-15
Data:  7.81600782e-4  4.41939920e-5  2.70293250e-2  3.07737922e-5  6.25640636e-11  1.19560046e-15
Data:  7.85032775e-4  4.24636125e-5  2.78829342e-2  3.12499332e-5  6.45205685e-11  1.27133023e-15
Data:  7.88446581e-4  4.07767094e-5  2.87623854e-2  3.16901369e-5  6.63511160e-11  1.34449276e-15
Data:  7.91834969e-4  3.90835188e-5  2.96701506e-2  3.20926833e-5  6.80425242e-11  1.41421301e-15
]

No input file or directory selected.

```

16) The tabular output in this format can be directly copied and pasted into a spreadsheet program to make graphs.

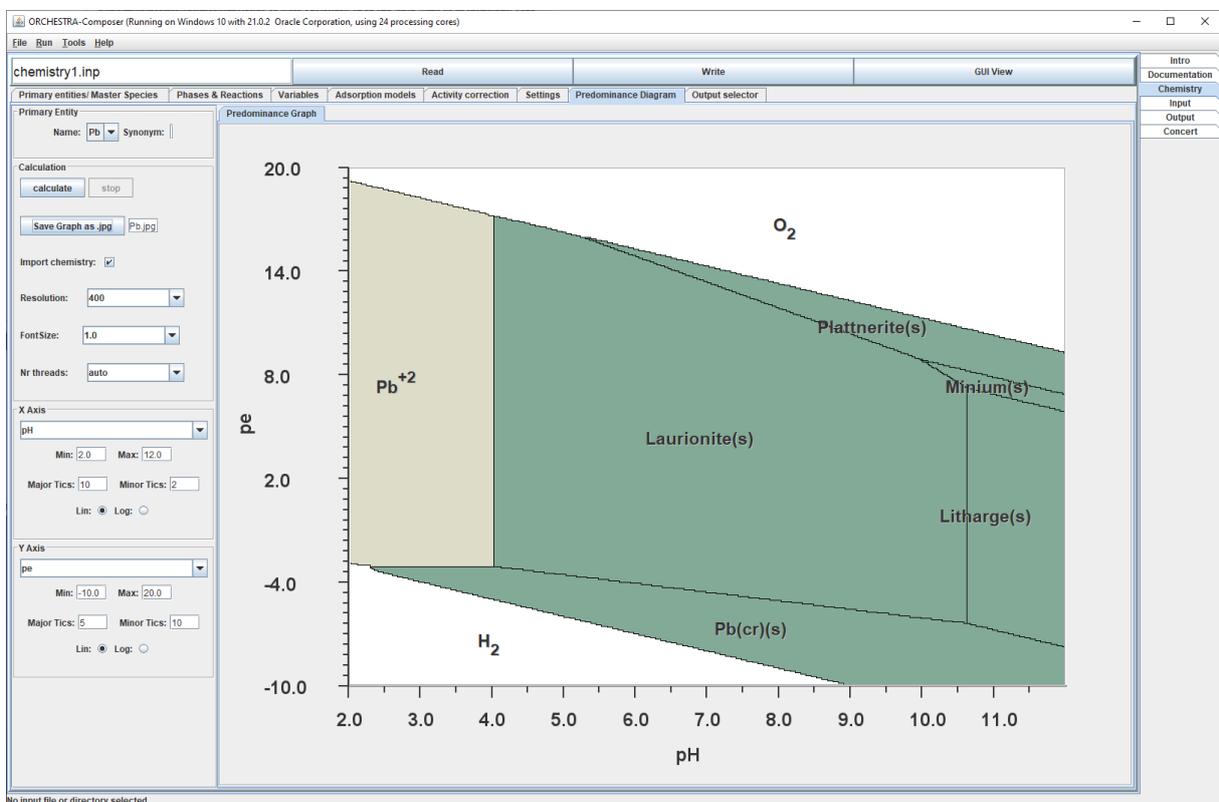


Stability predominance diagrams

Apart from numerical output that can be used in spreadsheet programs to make graphs, ORCHESTRA also can create so called predominance plots for the currently selected chemical system.

This option can be found in the chemical editor under the “PredominanceDiagram” tab.

In contrast with other codes that analytically derive the equations for the area boundaries, ORCHESTRA simply calculates the chemical composition at each grid point to find the predominant species/phase there. This is more computationally intensive, but can take into account arbitrary non linear chemical models (adsorption, activity corrections) for which it would be impossible to derive analytical expressions for area boundaries. Furthermore on modern computers, with multiple calculation cores, calculation of a complete grid is only a matter of seconds.



Differences with PHREEQC

- The chemical system is defined interactively by selecting reactions from a (PHREEQC format) thermodynamic database.
- This database is only used during the selection process, so by the GUI. But once the system is defined, it is written to a text file (e.g. chemistry.inp) that is used by the calculations. The database file is thus not required during the calculations anymore.
- In contrast with PHREEQC, an ORCHESTRA system is calculated in a single pass, so no separate calculations of solution and solid / adsorbed / gas phases that are combined in a second step.

- In ORCHESTRA the total amounts of primary entities/master species (summed over all possible phases) are given as input. So e.g. system with 1 mol of Halite (NaCl) per liter water is defined by adding 1 mol Na and 1 mol of Cl.
- ORCHESTRA works moles, so no conversion from gram/l to mol/l
- Solid pure phases are called minerals in ORCHESTRA, and when selected standard these automatically precipitate when supersaturated.
-