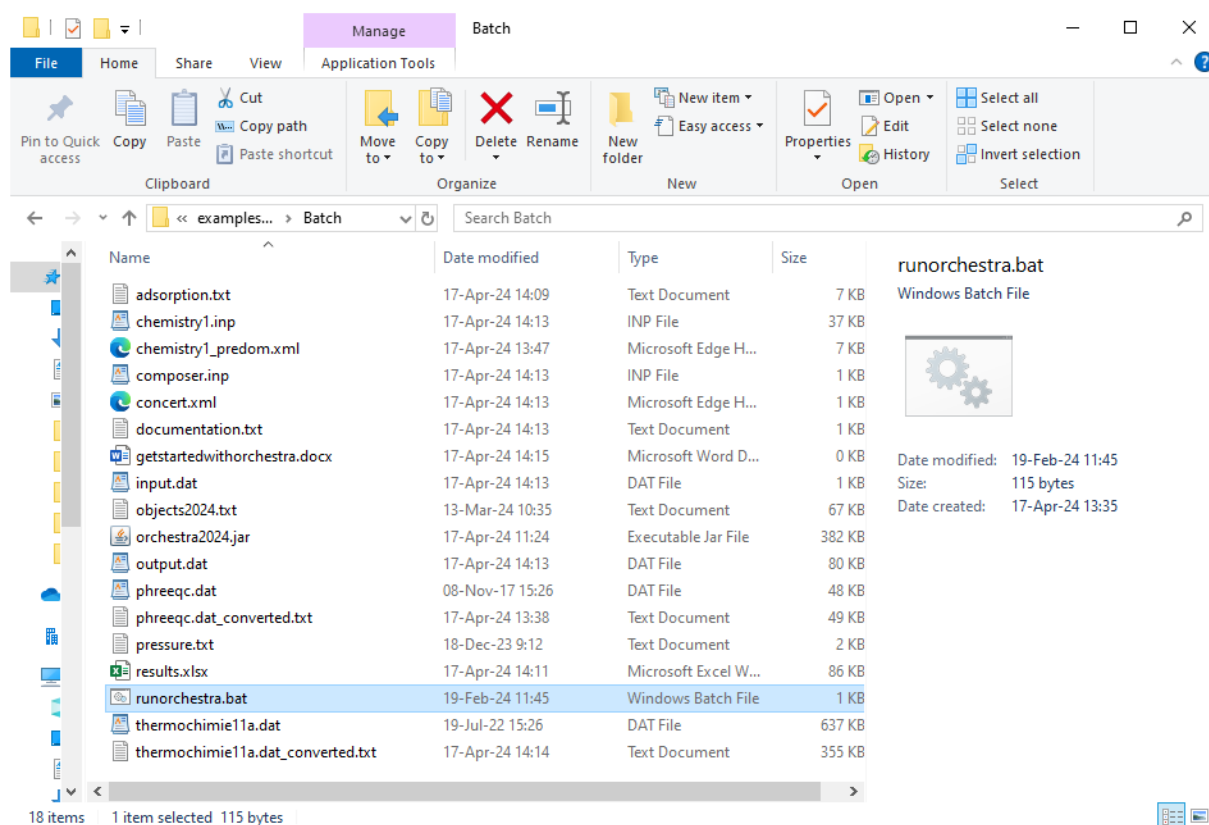


A quick tutorial to get started with ORCHESTRA

Hans Meeussen 17/8/2024

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 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

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	dis	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
<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 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

Balance Charge pe

No input file or directory selected.

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	Include	Database
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	thermochimie11a.dat
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<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"/>			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).
- For this 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.

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

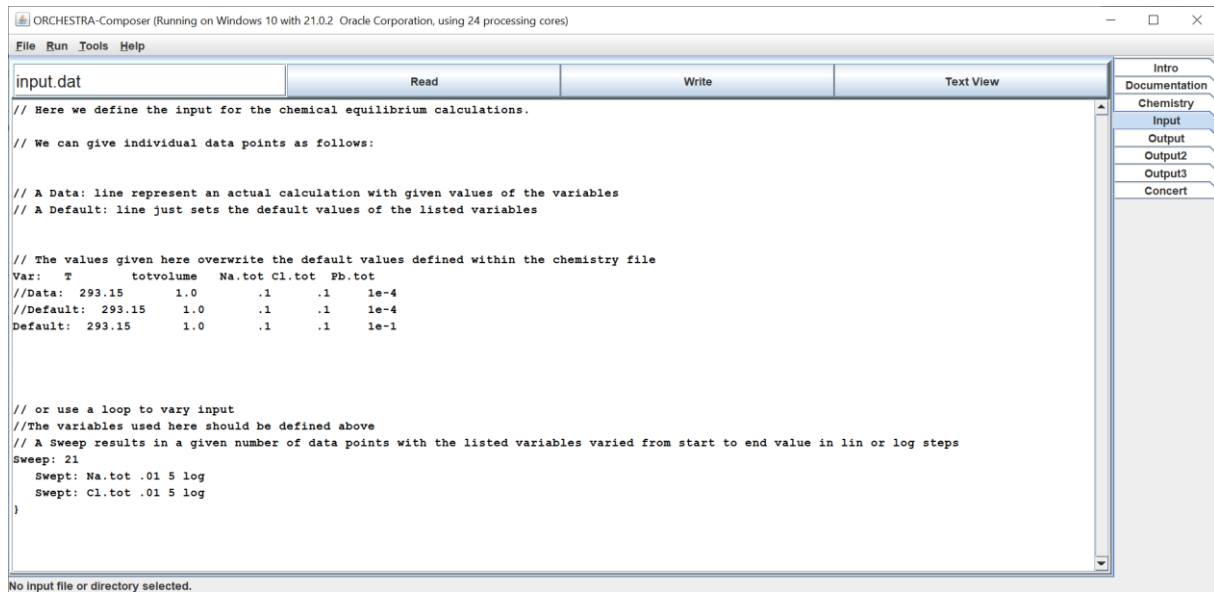
Reactions in all phases

Formation reactions in phase: all, depending on primary entity: Pb and: all Hide unselected Alphabetical Select all

Incl.	Name	Log K (25C)	Phase	Coef.	Reactant	Coef.
<input checked="" type="checkbox"/>	Cotunnite[s]	4.810000	min	2.0	Cl-	1.0
<input checked="" type="checkbox"/>	Laurionite[s]	-6.200000e-1	min	1.0	Cl-	-1.0
<input checked="" type="checkbox"/>	Litharge[s]	-12.63000	min	-2.0	H+	1.0
<input checked="" type="checkbox"/>	Massicot[s]	-12.74000	min	-2.0	H+	1.0
<input checked="" type="checkbox"/>	Minium[s]	-73.53000	min	-8.0	H+	4.0
<input checked="" type="checkbox"/>	Paralaurionite[s]	-6.200000e-1	min	1.0	Cl-	-1.0
<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
<input checked="" type="checkbox"/>	Pb4[OH]+4	-20.63000	diss	-4.0	H+	4.0
<input checked="" type="checkbox"/>	Pb6[OH]+4	-42.68000	diss	-8.0	H+	8.0
<input checked="" type="checkbox"/>	PbCl+	1.440000	diss	1.0	Cl-	1.0
<input checked="" type="checkbox"/>	PbCl2	2.000000	diss	2.0	Cl-	1.0
<input checked="" type="checkbox"/>	PbCl3-	1.690000	diss	3.0	Cl-	1.0
<input checked="" type="checkbox"/>	PbCl4-2	1.400000	diss	4.0	Cl-	1.0
<input checked="" type="checkbox"/>	Pb[OH]+	-7.510000	diss	-1.0	H+	1.0
<input checked="" type="checkbox"/>	Pb[OH]2	-16.95000	diss	-2.0	H+	2.0
<input checked="" type="checkbox"/>	Pb[OH]2[s]	-13.51000	min	-2.0	H+	2.0
<input checked="" type="checkbox"/>	Pb[OH]3-	-27.20000	diss	-3.0	H+	3.0
<input checked="" type="checkbox"/>	Pb[OH]4-2	-38.90000	diss	-4.0	H+	4.0
<input checked="" type="checkbox"/>	Pb[Cl]s	-4.250000	min	1.0	Pb+2	2.0
<input checked="" type="checkbox"/>	Plattnerite[s]	-49.60000	min	-4.0	H+	2.0

No input file or directory selected.

- 9) 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 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.



```
// Here we define the input for the chemical equilibrium calculations.

// We can give individual data points as follows:

// A Data: line represent an actual calculation with given values of the variables
// A Default: line just sets the default values of the listed variables

// The values given here overwrite the default values defined within the chemistry file
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
Default: 293.15    1.0      .1    .1    1e-1

// or use a loop to vary input
//The variables used here should be defined above
// A Sweep results in a given number of data points with the listed variables varied from start to end value in lin or log steps
Sweep: 21
  Swept: Na.tot .01 5 log
  Swept: Cl.tot .01 5 log
}
```

- 10) Now we can perform the calculation by clicking the “run” button in the GUI.
- 11) When the run is finished, the calculated results will be written to the output text file, which is automatically reloaded.
- 12) In the output file you can define the type of output you want. This can be either an automatic set of variable, similar to PHREEQC.
- 13) 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.

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)
@PBRBQOutput: 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 = 6.0000000
pe = 7.0000000
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
Cl-          9.99722999e-3         -2.00012032      9.99723e-3        0.0
PbCl+       2.98598334e-6         -5.58744146      2.98598e-6        0.0
PbCl2       9.15358903e-8         -7.03840059      9.15359e-8        0.0
PbCl3-      4.48618806e-10        -9.34812252      4.48619e-10       0.0
PbCl4-2     2.40515999e-12        -11.6188560     2.40516e-12       0.0
E
H2          1.71229981e-29
H2         8.56150339e-30       -29.0674500     8.56150e-30       0.0
O2         2.17810430e-36       -35.6619213     2.17810e-36       0.0
e-         0.0 -7.0000000 1.00000e-7       -1.11111e-11
H
H+         1.00000000e-6        -6.00000000     1.00000e-6        0.0
H2         8.56150339e-30       -29.0674500     8.56150e-30       0.0
O2         2.17810430e-36       -35.6619213     2.17810e-36       0.0
OH-        6.8111782e-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       -16.9398121     1.16731e-17       0.0
Pb6[OH]8+4 4.56356263e-26       -25.3405960     4.56356e-26       0.0
Pb[OH]+    2.06282778e-7        -6.6855303     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
Na+        9.30488525e-3        -2.03128898     9.30489e-3        0.0
O
O2         2.13210836e-7
O2         2.17810430e-36       -35.6619213     2.17810e-36       0.0

```

No input file or directory selected.

14) 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)
@PBRBQOutput: 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: 6.95114746e-4      8.74426271e-5      1.00000000e-2      9.67345211e-6      6.18248359e-12      1.16731469e-17
Data: 6.9666625e-4      8.6666675e-5      1.03156085e-2      1.02001377e-5      6.87404018e-12      1.44306581e-17
Data: 6.98294786e-4      8.58526071e-5      1.06411778e-2      1.07460733e-5      7.62956182e-12      1.77771116e-17
Data: 7.00009394e-4      8.49950531e-5      1.09770224e-2      1.13110480e-5      8.45899914e-12      2.18209362e-17
Data: 7.01768494e-4      8.41650737e-5      1.13234665e-2      1.18947453e-5      9.34878190e-12      2.68859458e-17
Data: 7.03653761e-4      8.31311966e-5      1.16808447e-2      1.24967376e-5      1.03177472e-11      3.25123683e-17
Data: 7.05602931e-4      8.21985474e-5      1.20495021e-2      1.31164795e-5      1.13667045e-11      3.94576432e-17
Data: 7.07635325e-4      8.11823074e-5      1.24297945e-2      1.37533033e-5      1.24972381e-11      4.76968933e-17
Data: 7.09751657e-4      8.01814113e-5      1.28220994e-2      1.44056147e-5      1.37121247e-11      5.74229704e-17
Data: 7.11952364e-4      7.90238182e-5      1.32267654e-2      1.50744888e-5      1.50144087e-11      6.88459619e-17
Data: 7.14237584e-4      7.78812079e-5      1.36442133e-2      1.57576680e-5      1.64052892e-11      8.21920455e-17
Data: 7.16607144e-4      7.6694479e-5      1.40748362e-2      1.64535605e-5      1.78862701e-11      9.77015771e-17
Data: 7.19060530e-4      7.54697374e-5      1.45190500e-2      1.71612399e-5      1.94579609e-11      1.15626307e-16
Data: 7.21598954e-4      7.42015526e-5      1.49728335e-2      1.78792452e-5      2.11202186e-11      1.36225650e-16
Data: 7.24215003e-4      7.28942986e-5      1.54499792e-2      1.86059880e-5      2.28720701e-11      1.597481803e-16
Data: 7.26913254e-4      7.15433731e-5      1.59375937e-2      1.93397461e-5      2.47116382e-11      1.86494093e-16
Data: 7.29689658e-4      7.0151109e-5      1.64400976e-2      2.00786783e-5      2.66360760e-11      2.16671892e-16
Data: 7.32541828e-4      6.87290859e-5      1.69594768e-2      2.08208295e-5      2.86413096e-11      2.50524583e-16
Data: 7.35466975e-4      6.72651266e-5      1.74947323e-2      2.15641210e-5      3.07229928e-11      2.88243095e-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      1.86144557e-2      2.30453937e-5      3.50887795e-11      3.76009252e-16
Data: 7.44646319e-4      6.26769405e-5      1.92040068e-2      2.37879790e-5      3.73576116e-11      4.26266638e-16
Data: 7.47827413e-4      6.10862934e-5      1.98101015e-2      2.45401521e-5      3.96715673e-11      4.80640896e-16
Data: 7.51061525e-4      5.94629735e-5      2.04353251e-2      2.52919620e-5      4.20201752e-11      5.39245644e-16
Data: 7.54343510e-4      5.7828210e-5      2.10820812e-2      2.59210223e-5      4.43919530e-11      6.01825393e-16
Data: 7.57667869e-4      5.61640653e-5      2.17455928e-2      2.66075269e-5      4.67744857e-11      6.68159346e-16
Data: 7.61028776e-4      5.44856121e-5      2.24319021e-2      2.72765872e-5      4.91545251e-11      7.37885564e-16
Data: 7.64420095e-4      5.2789525e-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      5.38506898e-11      8.86144474e-16
Data: 7.71268088e-4      4.9365959e-5      2.46235491e-2      2.91491511e-5      5.61373389e-11      9.6422236e-16
Data: 7.74711246e-4      4.7643705e-5      2.54006892e-2      2.97212414e-5      5.83682925e-11      1.04024256e-15
Data: 7.78157862e-4      4.59216592e-5      2.62023565e-2      3.02630845e-5      6.05118920e-11      1.11826175e-15
Data: 7.81600782e-4      4.41966092e-5      2.70293250e-2      3.07737922e-5      6.25694063e-11      1.19560046e-15
Data: 7.85032775e-4      4.24836125e-5      2.78823934e-2      3.12499332e-5      6.45205685e-11      1.27133023e-15
Data: 7.88446281e-4      4.07767094e-5      2.87622854e-2      3.16901369e-5      6.63511160e-11      1.34449276e-15
Data: 7.91834662e-4      3.90825188e-5      2.96701506e-2      3.20926835e-5      6.80435264e-11      1.41431330e-15

```

No input file or directory selected.

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

AutoSave results.xlsx Meussen, J.C.L. (Hans)

File Home Insert Page Layout Formulas Data Review View Automate Help

Calibri 11 A' A'

General

Conditional Formatting Format as Table Cell Styles Insert Delete Format AutoSum Fill Sort & Filter Find & Select Analyze Data Sensitivity Add-ins

Clipboard Font Alignment Number Styles Cells Editing Analysis Sensitivity Add-ins

Y4

Var:	Cl.diss	Pb+2.con	Pb2(OH)+	Pb4(OH)4	Pb6(OH)8	PbCl+.con	PbCl2.con	PbCl3-.co	PbCl4-2.c	Pb(OH)+.c	Pb(OH)2.c	Pb(OH)3-.c	Pb(OH)4-2.con
Data:	1.00E-02	7.71E-05	3.92E-10	4.70E-14	1.17E-20	2.06E-05	7.26E-07	3.55E-09	1.90E-11	1.64E-06	4.41E-10	1.98E-14	2.49E-20
Data:	1.03E-02	7.65E-05	3.87										
Data:	1.06E-02	7.60E-05	3.82										
Data:	1.10E-02	7.54E-05	3.76										
Data:	1.13E-02	7.49E-05	3.70										
Data:	1.17E-02	7.43E-05	3.65										
Data:	1.20E-02	7.37E-05	3.59										
Data:	1.24E-02	7.31E-05	3.53										
Data:	1.28E-02	7.25E-05	3.47										
Data:	1.32E-02	7.19E-05	3.42										
Data:	1.36E-02	7.13E-05	3.36										
Data:	1.41E-02	7.06E-05	3.30										
Data:	1.45E-02	7.00E-05	3.24										
Data:	1.50E-02	6.93E-05	3.18										
Data:	1.54E-02	6.87E-05	3.12										
Data:	1.59E-02	6.80E-05	3.05										
Data:	1.64E-02	6.73E-05	2.99										
Data:	1.70E-02	6.66E-05	2.93										
Data:	1.75E-02	6.59E-05	2.87										
Data:	1.80E-02	6.52E-05	2.81										
Data:	1.86E-02	6.45E-05	2.75										
Data:	1.92E-02	6.37E-05	2.68										
Data:	1.98E-02	6.30E-05	2.62										
Data:	2.04E-02	6.22E-05	2.56										
Data:	2.11E-02	6.15E-05	2.50										
Data:	2.17E-02	6.07E-05	2.44										
Data:	2.24E-02	6.00E-05	2.37										
Data:	2.31E-02	5.92E-05	2.31										
Data:	2.39E-02	5.84E-05	2.25										
Data:	2.46E-02	5.76E-05	2.19										
Data:	2.54E-02	5.68E-05	2.13										
Data:	2.62E-02	5.60E-05	2.07										
Data:	2.70E-02	5.52E-05	2.01										
Data:	2.79E-02	5.44E-05	1.95										
Data:	2.88E-02	5.35E-05	1.89										
Data:	2.97E-02	5.27E-05	1.83										
Data:	3.06E-02	5.19E-05	1.78										
Data:	3.16E-02	5.10E-05	1.72										
Data:	3.26E-02	5.02E-05	1.66										
Data:	3.36E-02	4.93E-05	1.61										
Data:	3.47E-02	4.85E-05	1.55	1.00E-02									
Data:	3.58E-02	4.77E-05	1.50E-10	6.88E-15	6.52E-22	4.55E-05	5.75E-06	1.01E-07	1.93E-09	1.02E-06	2.73E-10	1.23E-14	1.54E-20
Data:	3.69E-02	4.68E-05	1.45E-10	6.40E-15	5.86E-22	4.61E-05	6.01E-06	1.08E-07	2.14E-09	9.98E-07	2.68E-10	1.20E-14	1.51E-20
Data:	3.80E-02	4.60E-05	1.40E-10	5.95E-15	5.25E-22	4.67E-05	6.28E-06	1.17E-07	2.38E-09	9.80E-07	2.63E-10	1.18E-14	1.49E-20
Data:	3.92E-02	4.51E-05	1.34E-10	5.52E-15	4.69E-22	4.72E-05	6.56E-06	1.26E-07	2.65E-09	9.62E-07	2.58E-10	1.16E-14	1.46E-20
Data:	4.05E-02	4.43E-05	1.29E-10	5.11E-15	4.18E-22	4.78E-05	6.85E-06	1.36E-07	2.94E-09	9.44E-07	2.53E-10	1.14E-14	1.43E-20
Data:	4.18E-02	4.34E-05	1.24E-10	4.73E-15	3.72E-22	4.84E-05	7.14E-06	1.46E-07	3.27E-09	9.25E-07	2.48E-10	1.12E-14	1.40E-20

DISTRIBUTION OF LEAD OVER DIFFERENT AQUEOUS SPECIES

Legend:

- Pb+2.con
- PbCl+.con
- Pb(OH)+.con
- Pb2(OH)+
- Pb4(OH)4
- Pb6(OH)8
- PbCl2.con
- PbCl3-.con
- PbCl4-2.con
- Pb(OH)2.con
- Pb(OH)3-.con
- Pb(OH)4-2.con
- Pb(OH)4+4.con
- Pb(OH)8+4.con
- PbCl2-2.con

Sheet1

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