A quick tutorial to get started with ORCHESTRA

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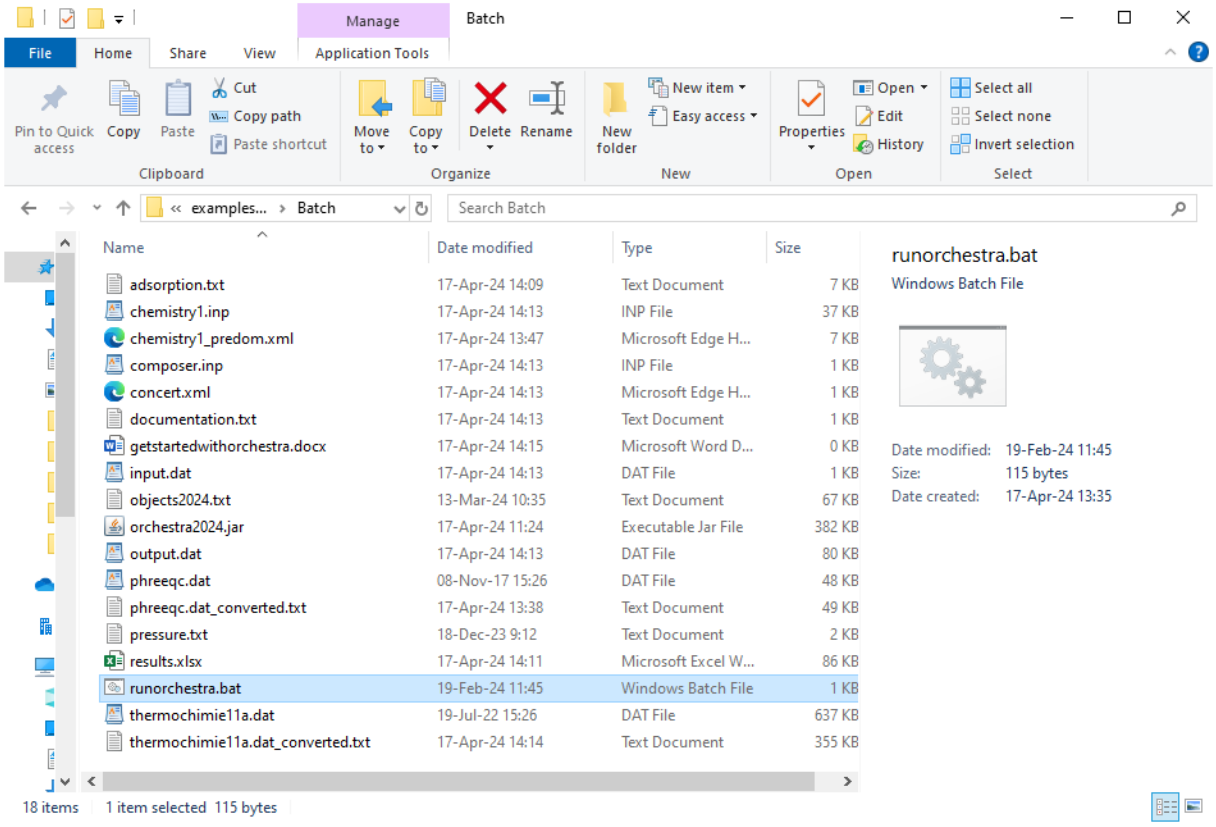
This document describes how to get started with performing chemical equilibrium calculations with ORCHESTRA.

1) Make sure that you have a Java virtual machine installed on your machine (available for free from or https://www.graalvm.org/)

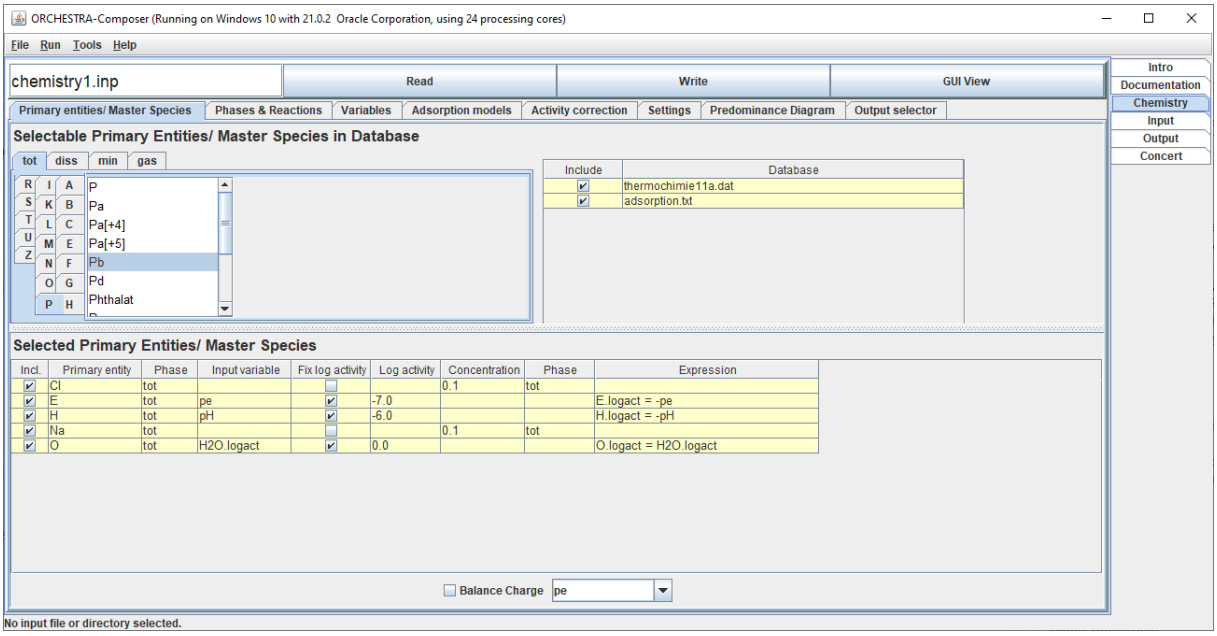
2) Download the complete self-contained zipped folder with ORCHESTRA executable, database and input files from: www.meeussen.nl/orchestra/getstarted.zip

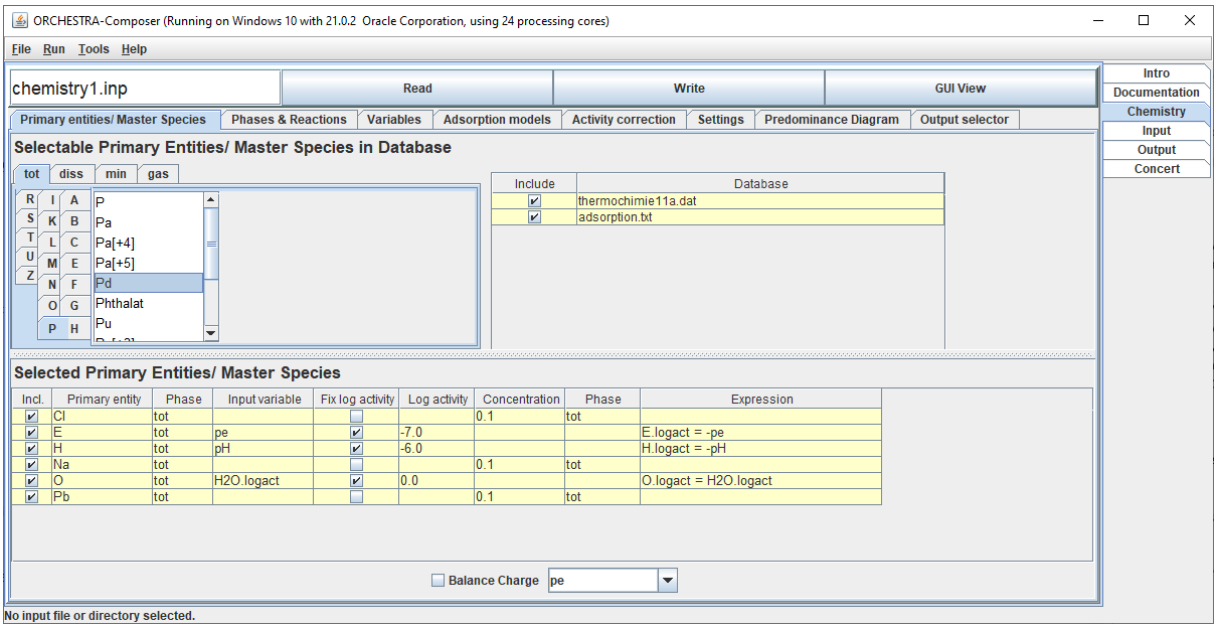
3) Unzip this folder on your machine and (under Windows) click the runorchestra.bat file or from a command window/console opened in this folder give the command: java -cp orchestra2024.jar orchestra2.composer under Linux or MacOS



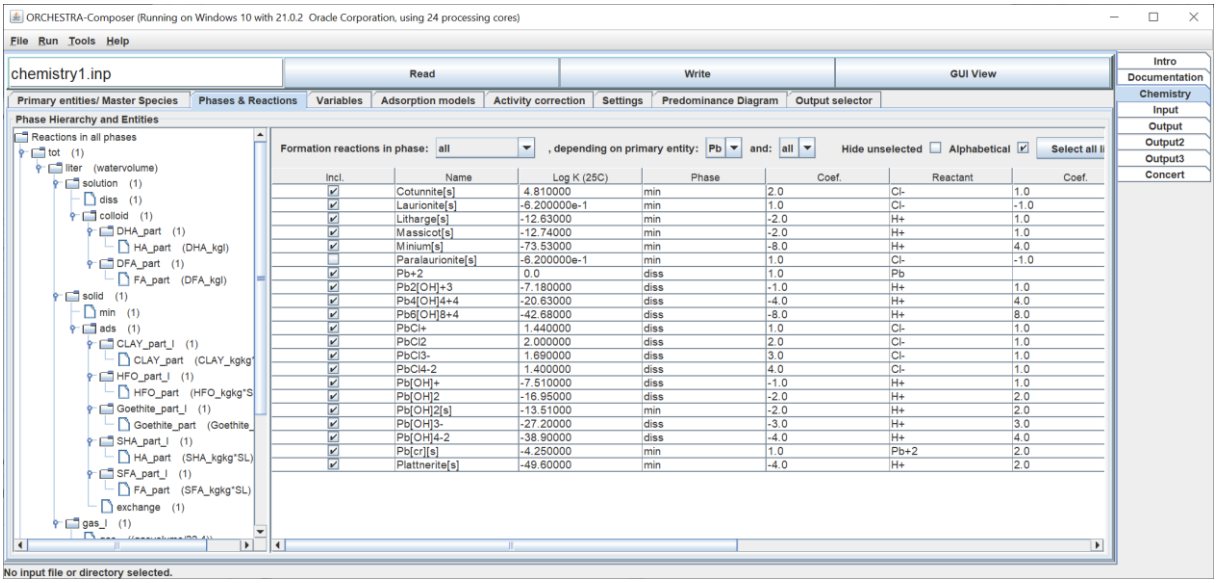
4) This will start up the orchestra composer

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

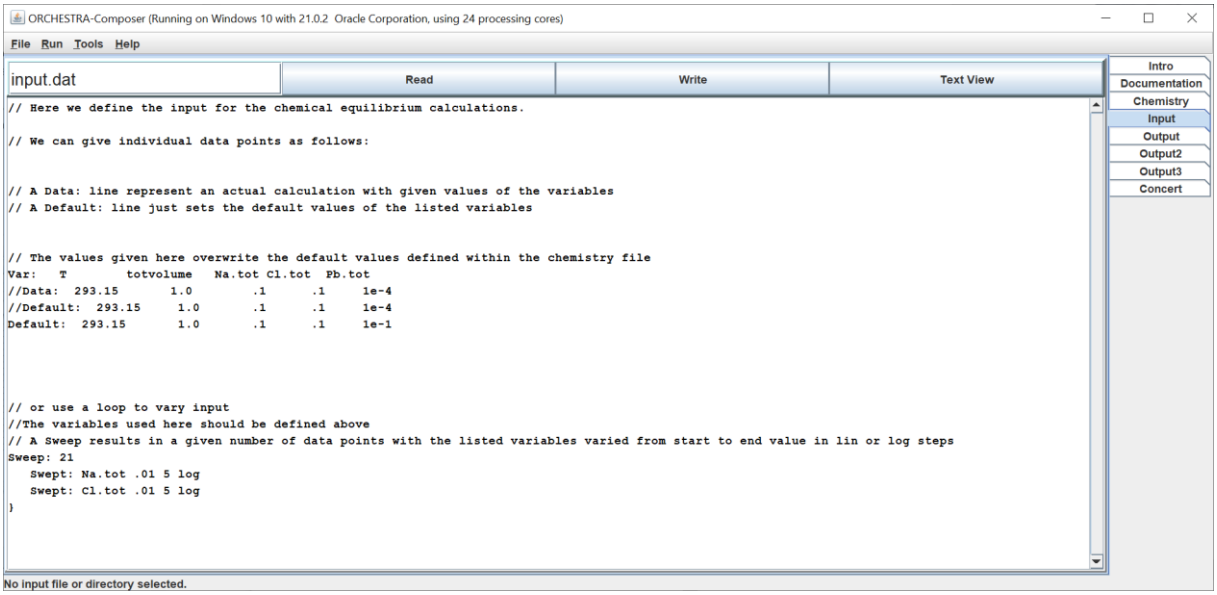




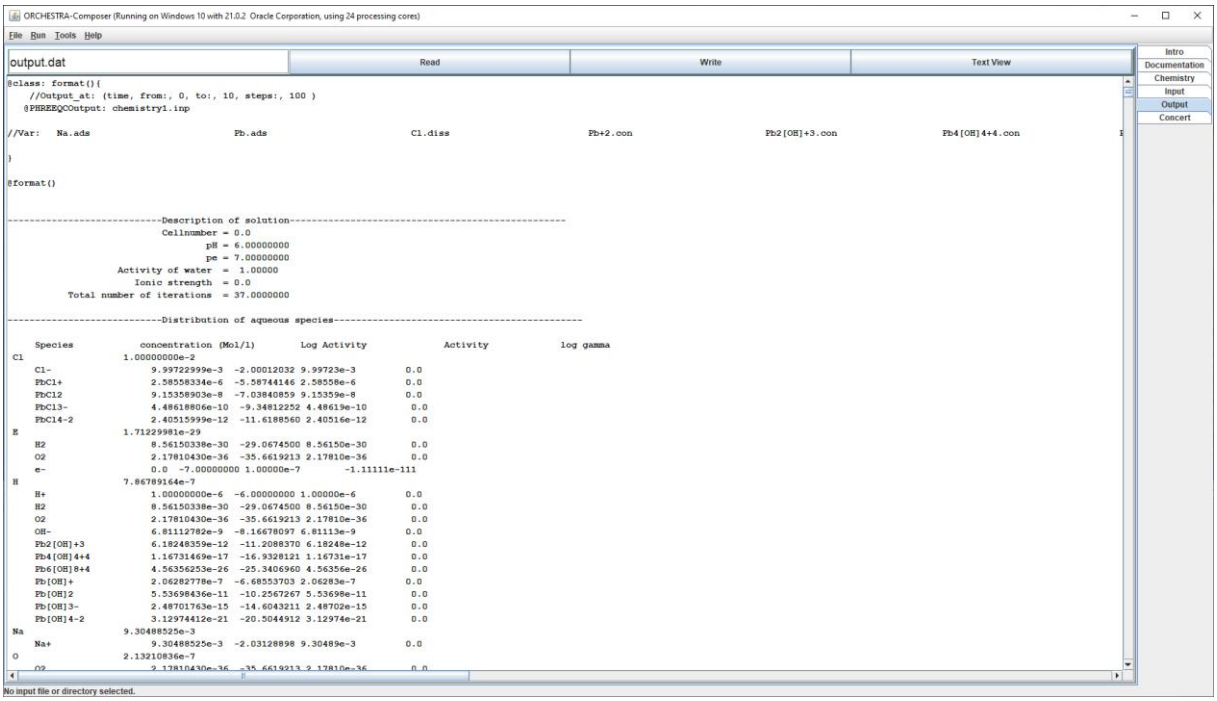
6) Lead (Pb) will appear in the list of selected primary entities (also called Master species or independent components in other codes).
7) For this Pb primary entity we can select either a given log activity or a given amount or “mass balance” in any of the phases in the system. Here we select a given total amount, so Pb.tot in “tot” phase (total amount) and not a fixed log activity.
8) 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.



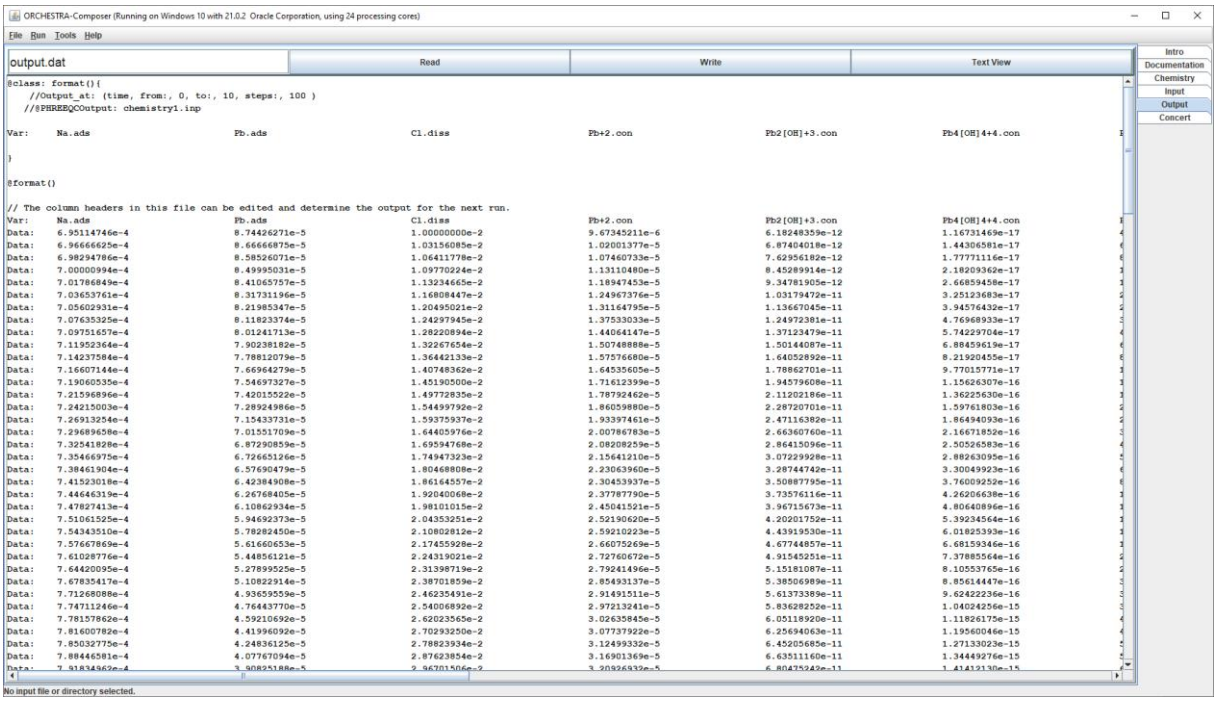
9) Next we can define our (set of) input conditions in the input file. This can be single or multiple datapoints. The values given here overrule the default values given within the chemistry file. So here you can give a list of concentrations for Cl, Na or Pb. The values of Pb.tot, Na.tot and Cl.tot given here will overrule the values given in the graphical user interface.



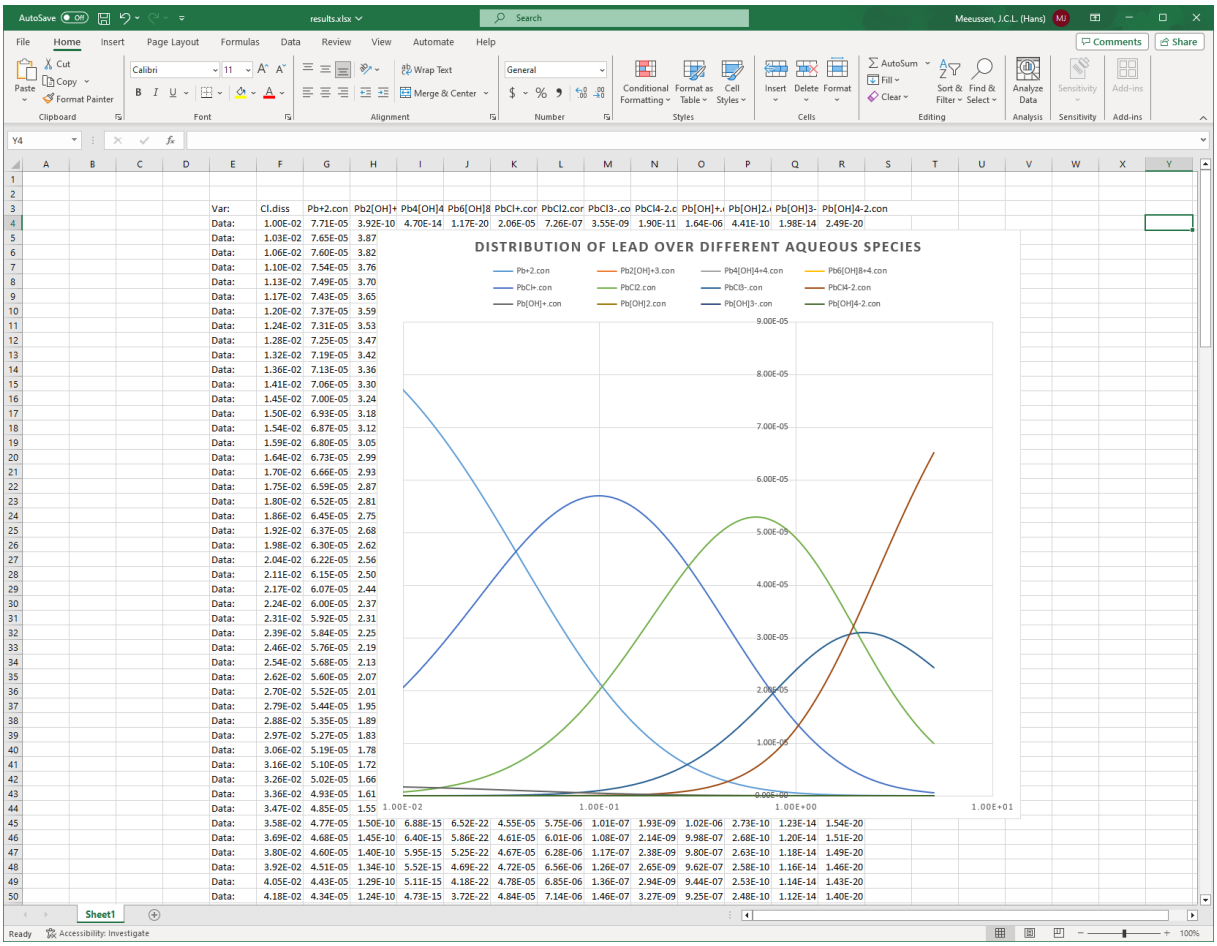
10) Now we can perform the calculation by clicking the “run” button in the GUI.
11) When the run is finished, the calculated results will be written to the output text file, which is automatically reloaded.
12) In the output file you can define the type of output you want. This can be either an automatic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



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



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



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y
1																									
2																									
3					Var:	Cl.diss	Pb+2.con	Pb2[OH]+	Pb4[OH]4	Pb6[OH]8	PbCl+.cor	PbCl2.cor	PbCl3-.co	PbCl4-2.c	Pb[OH]+.(	Pb[OH]2.(	Pb[OH]3-	Pb[OH]4-2.con							
4					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							
5					Data:	1.03E-02	7.65E-05	3.87																	
6					Data:	1.06E-02	7.60E-05	3.82																	
7					Data:	1.10E-02	7.54E-05	3.76																	
8					Data:	1.13E-02	7.49E-05	3.70																	
9					Data:	1.17E-02	7.43E-05	3.65																	
10					Data:	1.20E-02	7.37E-05	3.59																	
11					Data:	1.24E-02	7.31E-05	3.53																	
12					Data:	1.28E-02	7.25E-05	3.47																	
13					Data:	1.32E-02	7.19E-05	3.42																	
14					Data:	1.36E-02	7.13E-05	3.36																	
15					Data:	1.41E-02	7.06E-05	3.30																	
16					Data:	1.45E-02	7.00E-05	3.24																	
17					Data:	1.50E-02	6.93E-05	3.18																	
18					Data:	1.54E-02	6.87E-05	3.12																	
19					Data:	1.59E-02	6.80E-05	3.05																	
20					Data:	1.64E-02	6.73E-05	2.99																	
21					Data:	1.70E-02	6.66E-05	2.93																	
22					Data:	1.75E-02	6.59E-05	2.87																	
23					Data:	1.80E-02	6.52E-05	2.81																	
24					Data:	1.86E-02	6.45E-05	2.75																	
25					Data:	1.92E-02	6.37E-05	2.68																	
26					Data:	1.98E-02	6.30E-05	2.62																	
27					Data:	2.04E-02	6.22E-05	2.56																	
28					Data:	2.11E-02	6.15E-05	2.50																	
29					Data:	2.17E-02	6.07E-05	2.44																	
30					Data:	2.24E-02	6.00E-05	2.37																	
31					Data:	2.31E-02	5.92E-05	2.31																	
32					Data:	2.39E-02	5.84E-05	2.25																	
33					Data:	2.46E-02	5.76E-05	2.19																	
34					Data:	2.54E-02	5.68E-05	2.13																	
35					Data:	2.62E-02	5.60E-05	2.07																	
36					Data:	2.70E-02	5.52E-05	2.01																	
37					Data:	2.79E-02	5.44E-05	1.95																	
38					Data:	2.88E-02	5.35E-05	1.89																	
39					Data:	2.97E-02	5.27E-05	1.83																	
40					Data:	3.06E-02	5.19E-05	1.78																	
41					Data:	3.16E-02	5.10E-05	1.72																	
42					Data:	3.26E-02	5.02E-05	1.66																	
43					Data:	3.36E-02	4.93E-05	1.61																	
44					Data:	3.47E-02	4.85E-05	1.55	1.00E-02				1.00E-01					1.00E+00				1.00E+01				
45					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							
46					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							
47					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							
48					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							
49					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							
50					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							