UMass Dartmouth/Lowell - Chemical Oceanography – Spring Dr. David K. Ryan

MINEQL+ Version 4.6 User Guide

System Requirements

- PC (running Windows XP, Windows 7 or Windows 8 in any of its versions Home, Pro, etc.)
- At least 4 MB of RAM
- At least 2.5 MB of hard disk space

Installation

- Start Windows
- Double click on MINEQL.exe file
- Follow instructions on the screen

Launch MINEQL+ Program

- Click on Start | Program | MINEQL+ | MINEQL+
- MINEQL+ program should open on your screen

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Tutorial

Please note that this is only intended to be a basic instructional guide to set up simple ionic equilibrium problems. Please consult the **HELP** wizard for more details. This guide will consider MgSO₄ at pH 8.2 at 25°C as an example. Launch **MINEQL**+ by going to **Start | Programs | MINEQL**+ | **MINEQL**+

Chemical Components Selection Module should launch automatically. Select the components in the system by clicking Mg^{2+} and SO_4^{2-} and they should be highlighted in blue. (Note, H₂O and H⁺ are highlighted by default)

🚆 Chemical Components Selection Module								
Scan THERMO	G New	💪 Return	Edit Mode					
Select Components for Calculation								
🗆 e(-)	🔽 H20	∨ H	[+]	PSI0	🗖 PSIB	_		
🗖 SOH	🗌 Ag(+)		(3+) 🗆	As03(3-)	🗌 As04(3-)			
🗖 Au(+)	🗌 🛛 🖂 🖂	E Be	e(2+)	Br(-)	🗌 B(OH)3			
🗖 Ca(2+)	🗌 Cd(2+)	🗖 Ce	e(3+) 🗆	CI(-)	🗖 CN(-)			
🗖 OCN(-)	🗌 SCN(-)		03(2-) 🗆	Co(2+)	🗌 Co(3+)			
🗖 CrO4(2-)	🗌 Cr(2+)	🗖 Ci	(OH)2(+) 🗌	Cs(+)	🗌 Cu(2+)			
🗖 Cu(+)	🗌 Fe(2+)	🗖 Fe	*(3+) 🗆	F(-)	🗌 Hg2(2+)			
🗖 Hg(OH)2	🗆 I(-)	🗆 K.	[+]	La(3+)	🗌 Li(+)			
✓ Mg(2+)	🗌 Mn(2+)	П М	n(3+) 🗆	MoO4(2-)	🗌 Na(+)			
NH20H	🔲 NH4(+)	🗖 N	i(2+) 🗆	NO2(-)	🗖 NO3(-)			
🗖 P207(4-)	🗖 P3010	(5-) 🗌 PI	b(2+) 🗆	PO4(3-)	🗖 Rb(+)			
🗖 S(0)	🗖 \$203(2	?-) 🗆 🗆 SI	6(OH)3 🗆	Sb(OH)6(-)	🗌 Sc(3+)			
🗆 SeO4(2-)	🗖 HSeO3	(-) 🗆 H:	Se(-) 🗆	Si(OH)4	🗌 Sn(2+)			
🗆 Sn(4+)	🗖 SO3(2-) <mark>V</mark> SI	D4(2-)	Sr(2+)	🗖 HS(-)	-		

After selecting all the components, click **Scan THERMO**.

After clicking **Scan THERMO**, the **Aqueous Species Module** should appear on screen and it shows the aqueous species selected and their thermodynamic data (built within **MINEQL**+), which can be altered if desired.

🖀 Type II - Aqueous Species							
🕂 Insert 🖌 Delete 🗍	Move 🕻	Close	/izard 🧖 Helj	p			
Name	H20	H(+)	Mg(2+)	SO4(2-)	Log K	Delta H	
OH- (-1)	1	-1	0	0	-13.997	13.339	
MgOH+ (+1)	1	-1	1	0	-11.397	16.207	
HS04- (-1)	0	1	0	1	1.9900	5.2580	
MgSO4 (aq)	0	0	1	1	2.2600	1.3860	
							-
Total Conc. (M)>	0.000E+00	0.000E+00	0.000E+00	0.000E+0			
		a		Þ			

For this example, no change is made. Click Close.

After clicking **Close**, the **Tableau Switch Module** appears on screen. This allows the user to jump and view different species types. View and make necessary modifications if desired. Again for this example, no modification will be made. Click **NO** to launch **Run Time Manager**.

Species Type: O Aqueous Complexes Fixed Entities O Dissolved Solids O Species Not Considered
 Aqueous Complexes Fixed Entities Dissolved Solids Species Not Considered
 Fixed Entities Dissolved Solids Species Not Considered
© Dissolved Solids © Species Not Considered
C Species Not Considered
11 TO 14 CO. • CARD S CALDER CONTROL OF A CARD AND S CA

Run Time Manager allows the user to specify a fixed temperature (default = 25° C) and ionic strength (≤ 0.50) or let **MINEQL**+ calculate ionic strength using the concentrations of the species entered by the user and thermodynamic data (K values) which are built in the program.

📇 RunTime Manager	_ 🗆 ×						
Output Data Name: MGSO4							
lonic Strength Corrections:	Adsorption Model:						
C Calculated	None						
© Fixed	0-5						
μ (molar): <u>5.00E-01</u>							
Off							
O On	Criteria						
Temp. (*C): 25.0							
🕒 Run 🔀 Cancel	Wizard WultiRun ?Help						

For our MgSO₄ example, fix the ionic strength at 0.500 molar and temperature at 25° C. Enter an Output Data Name, then click the **Wizard** button.

After clicking **Wizard**, the **Calculation Wizard** should appear. This module allows the user to enter the total dissolved concentration of each component chosen. For our MgSO₄ example, enter 0.0545 M for Mg²⁺ and 0.0289 M for SO₄²⁻.

Calculation Wizard								
у <u>о</u> к	X <u>C</u> ancel	Help						
Totals	рн	C02	Solids Mover	Redox				
Component	Total C (M):						
Mg(2+)	5.450E-02							
SO4(2-)	2.890E-02							

Click on the **pH** tab to supply a fixed pH value or allow the **MINEQL**+ program to calculate pH base on the components entered by the user. For our example, fix the pH at 8.20.



Click on the CO_2 , Solids Mover and Redox tabs if necessary. For our example, we will not concern ourselves with them at this time.

Click OK to go back to Run Time Manager. Click RUN.

🗮 RunTime Manager	_ 🗆 ×					
Output Data Name: MGSO4						
lonic Strength Corrections:	Adsorption Model:					
COff						
C Calculated	None					
⊙ Fixed						
μ (molar): 5.00E-01	Options					
Temperature Corrections:						
© Off						
C On	Criteria					
Temp. (*C): 25.0						
🕒 Run 🔀 Cancel	Wizard - MultiRun ? Help					

Output Manager should appear. Choose the Output Type and click Component that you wish to view. For example, select Component Groups and Mg(2+) and choose View.

Component: Mg[2+] Output Type:	Data Object: MGS04.MDOJ Mg(2+) 504(2·) H20 H(+)	Directorv: C:\MINWIN45\ 10 C:\ 10 MINWIN45
Component Groups:	Species x Variables	ac:
Variables	Variables Nun 1	Species 8 1. Conc (M)
View Graph IT ,	Close Copv 1	Delete

A table of all Mg^{2+} species should appear containing concentration of each species and their respective percentages.

📇 MGS	504.MDO	for Mg(2+):Rur	11							_ 🗆 ×
Save	Print	Clip Board	Help	Col Xtract						
		Name		Type		Conc.	LogC	LogK	%Total	Stoch.
1 2 3 4 5 6 7 8	Mg Mg PEI BRU Mg EPS TO	(2+) DH+ SO4 (aq) RICLASE JCITE (OH)2 (acti SOMITE FAL Mg(2+)	(+1) ve)		1 2 2 5 5 5 5 5 7 7	0.0448 2.01e-7 0.00975 0.0545	-1.35 -6.7 -2.01 -10.5 -5.79 -7.75 -2.14 -1.26	0 -11.7 1.06 -21.9 -17.1 -19.1 0.92	82.1 0 17.9	
	•									•

In addition to the table output format, the results can also be displayed as Bar Graphs by clicking the **GRAPH IT**, then the **PLOT** botton.



A more comprehensive display can be found in table format by clicking **Special Reports** under **Output Type** and select **Summary of All Species for a Single Run**.

📴 Sun	nmary	of All Species f		- 🗆 🗙					
Save	Print	Clip Board	Help						
MINEQL+ Ver 4.5 Page 1 Data Extracted from : MGSO4.MDO SINGLE RUN SUMMARY									
This report compiles the output data (concentration, Log C, Log K) for all species within a single run.									
MINEQL+ Ver 4.5 Page 2 Data Extracted from : MGSO4.MDO									
Kull. I	ID		Species	Conc.	Log C	Log K			
Type I	- CO 2 3 41 68	MPONENTS H2O H(+) Mg(2+) SO4(2-)		1.000E+00 8.920E-09 4.470E-02 1.920E-02	0.000 -8.049 -1.349 -1.718	0.000 0.000 0.000 0.000 0.000			
Type I 1 4 13	I — C 3800 7900 3900 3400	OMPLEXES OH- MgOH+ HSO4- MgSO4 (aq)	(-1) (+1) (-1)	2.260E-06 1.010E-05 4.180E-09 9.750E-03	-5.646 -4.998 -8.379 -2.011	-13.700 -11.700 1.390 1.060			
Type I 17	II — 3801 5310	FIXED ENTIT] H2O (Solutic pH	IES on) (+1)			0.000 8.200			
Type V 19 19 19 20	- DI 6600 6700 6702 7100	SSOLVED SOL] PERICLASE BRUCITE Mg(OH)2 (act EPSOMITE	IDS :ive)		-7.135 -2.395 -4.345 -2.144	-21.890 -17.150 -19.100 0.920			
Other 90	Speci 0003	es Activi	ty of H+	6.310E-09	-8.200	0.150			
•						•			

You now have taught yourself how to set up an ionic equilibrium problem in **MINEQL**+. Please explore all the convenient functions that **MINEQL**+ has to offer and enjoy. To get more information about **MINEQL**+, please go to their website **WWW.MINEQL.COM**

Reference

Schecher, William D and McAvoy, Drew C. *MINEQL*+ A Chemical Equilibrium Modeling System Version 4.5 for Windows User's Manual. 2nd Ed. Environmental Research Software: Hallowell, ME 2001.