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

MINEQL+ Version 4.5 User Guide

System Requirements

- PC (running Windows 3.1 or later, ie NT, 95, 98, 2000, Me, XP, Windows 7, etc.)
- At least 4 MB of RAM
- At least 2.5 MB of hardisk space

Installation

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

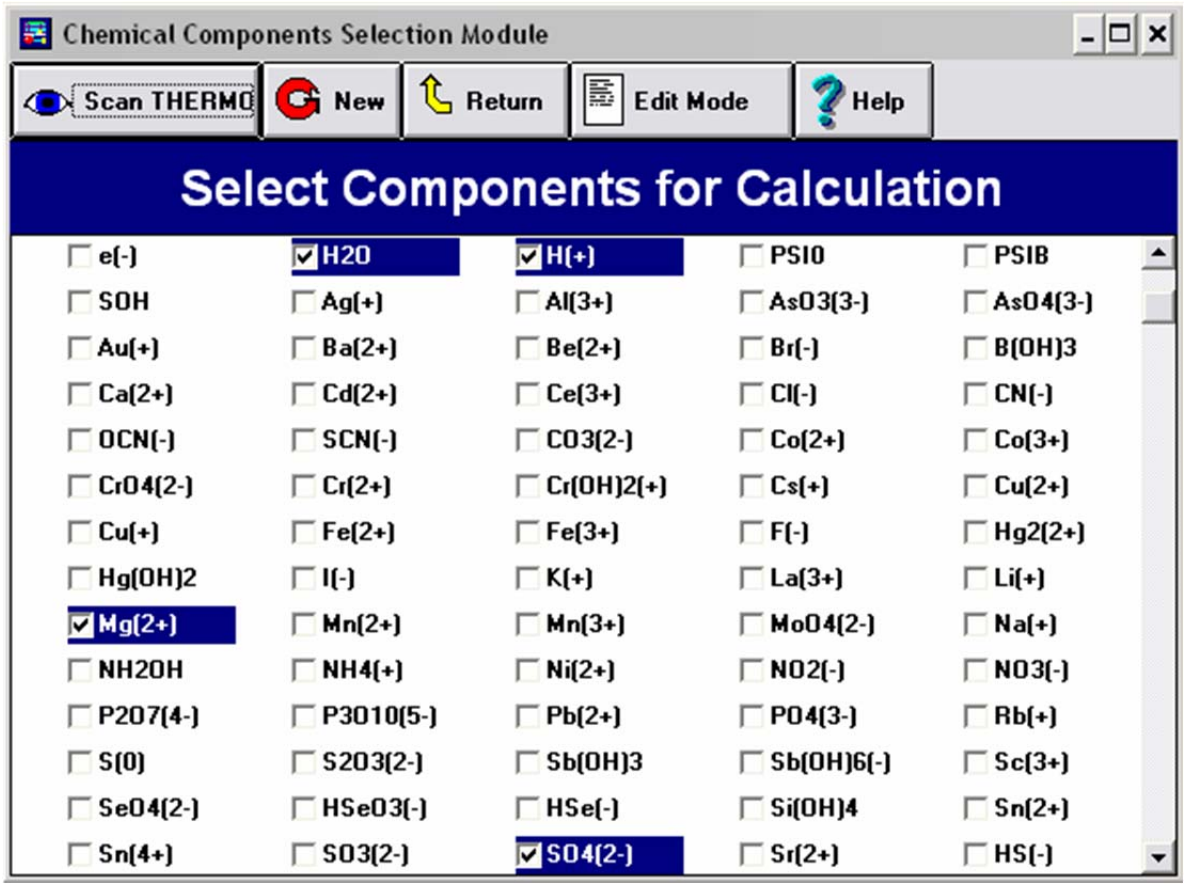
Launch **MINEQL+** Program

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

Tutorial

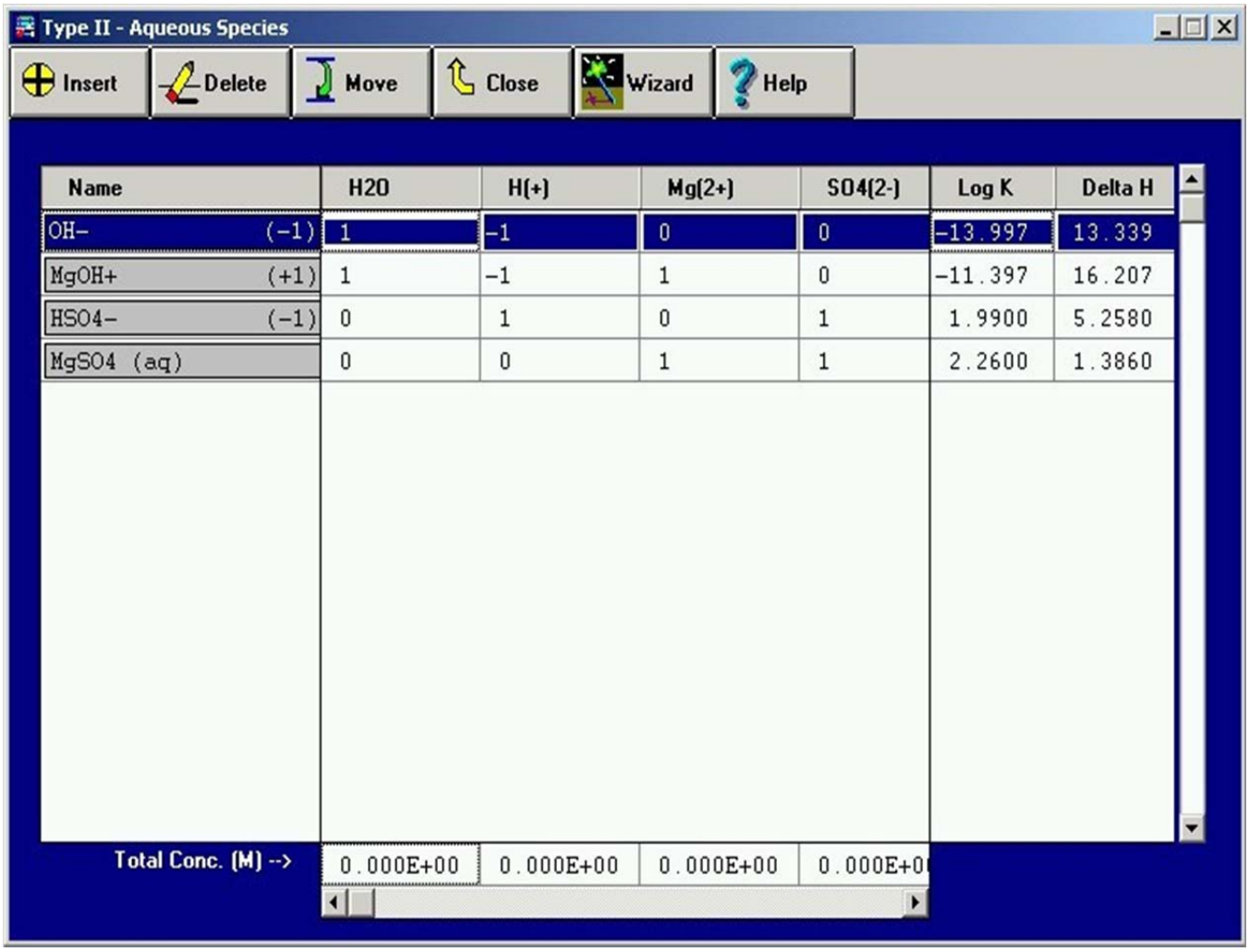
Please note that this is only intended to be a basic instructional guide to set up simple ionic equilibrium problems. Please consult the **HELP** wizard for more details. This guide will consider $MgSO_4$ at pH 8.2 at 25°C as an example. Launch **MINEQL+** by going to **Start | Programs | MINEQL+ | MINEQL+**

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, H_2O and H^+ are highlighted by default)



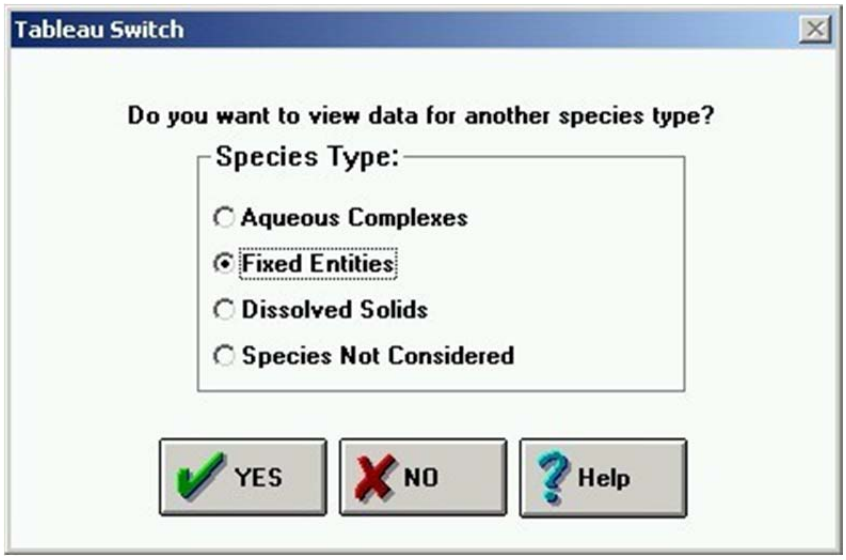
After selecting all the components, click **Scan THERMO**.

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.

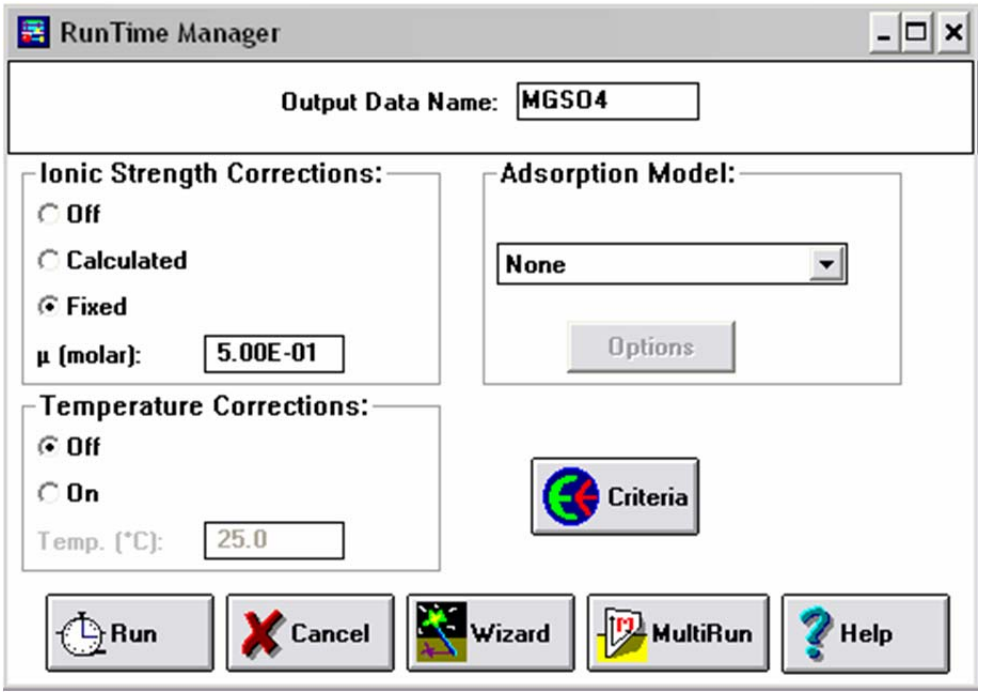


For this example, no change is made. Click **Close**.

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**.

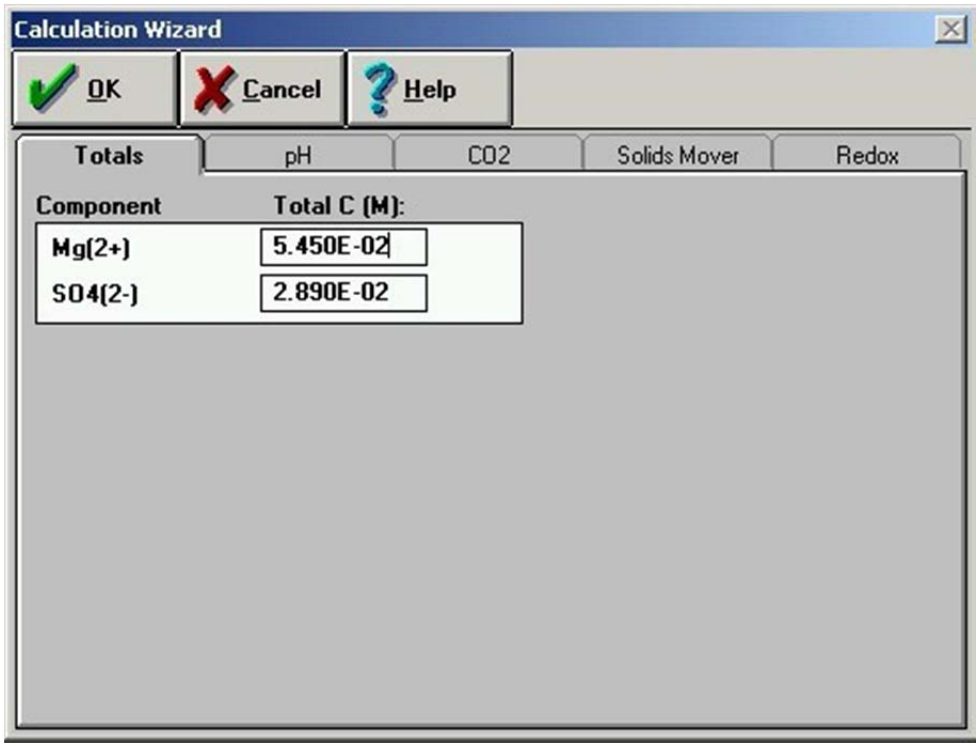


Run Time Manager allows the user to specify a fixed temperature (default = 25°C) and ionic strength (≤ 0.50) or let **MINEQL+** calculate ionic strength using the concentrations of the species entered by the user and thermodynamic data (K values) which are built in the program.

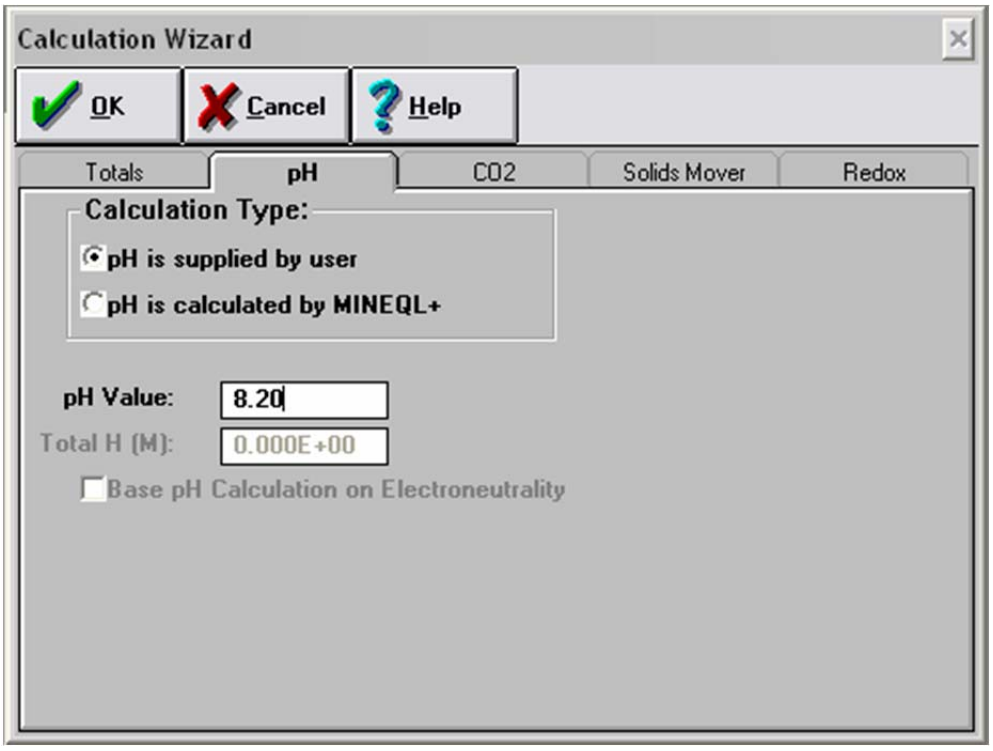


For our $MgSO_4$ example, fix the ionic strength at 0.500 molar and temperature at 25°C. Enter an Output Data Name, then click the **Wizard** button.

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 $MgSO_4$ example, enter 0.0545 M for Mg^{2+} and 0.0289 M for SO_4^{2-}.

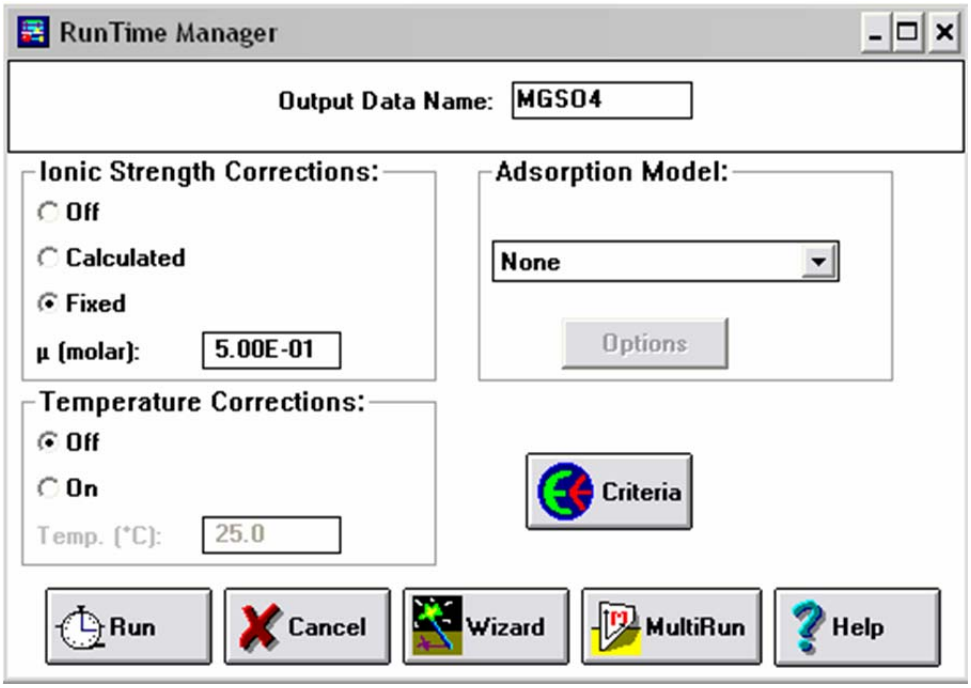


Click on the **pH** tab to supply a fixed pH value or allow the **MINEQL+** program to calculate pH base on the components entered by the user. For our example, fix the pH at 8.20.

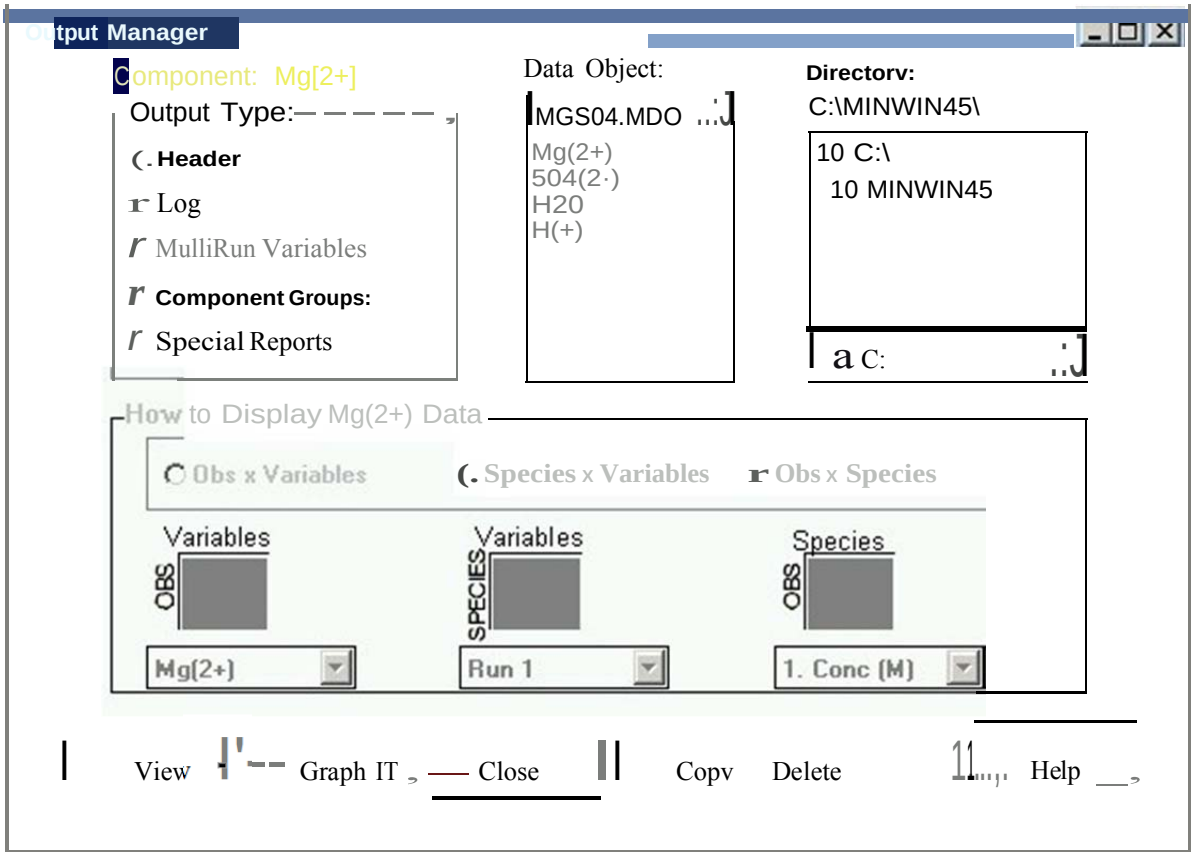


Click on the **CO_2, Solids Mover** and **Redox** tabs if necessary. For our example, we will not concern ourselves with them at this time.

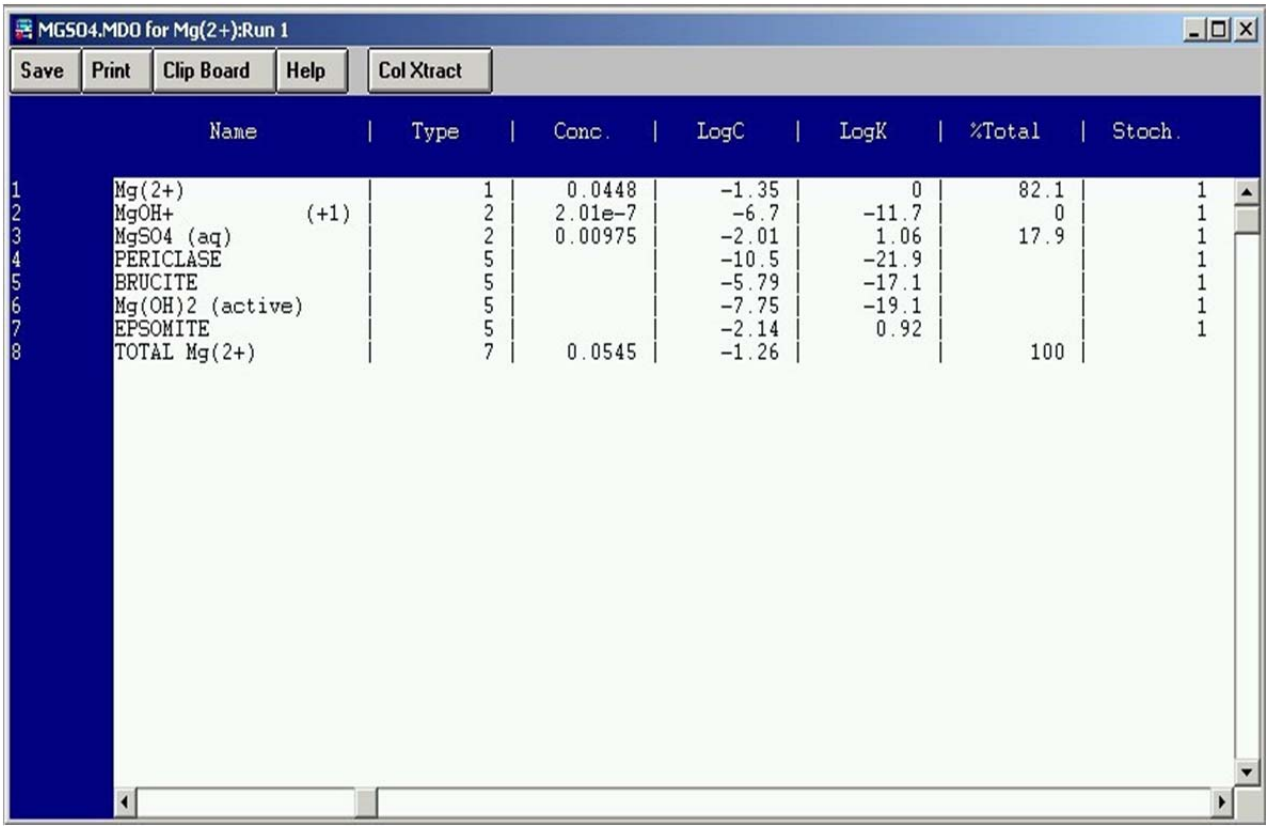
Click **OK** to go back to **Run Time Manager**. Click **RUN**.



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.

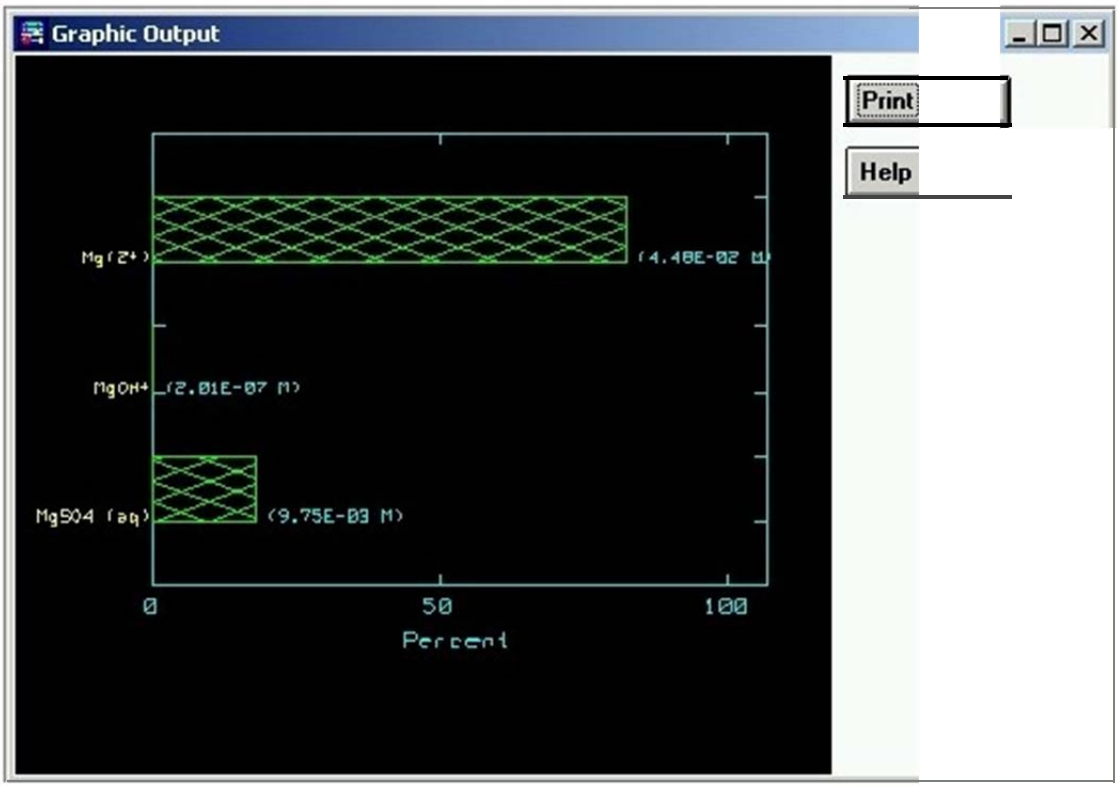


A table of all Mg^{2+} species should appear containing concentration of each species and their respective percentages.

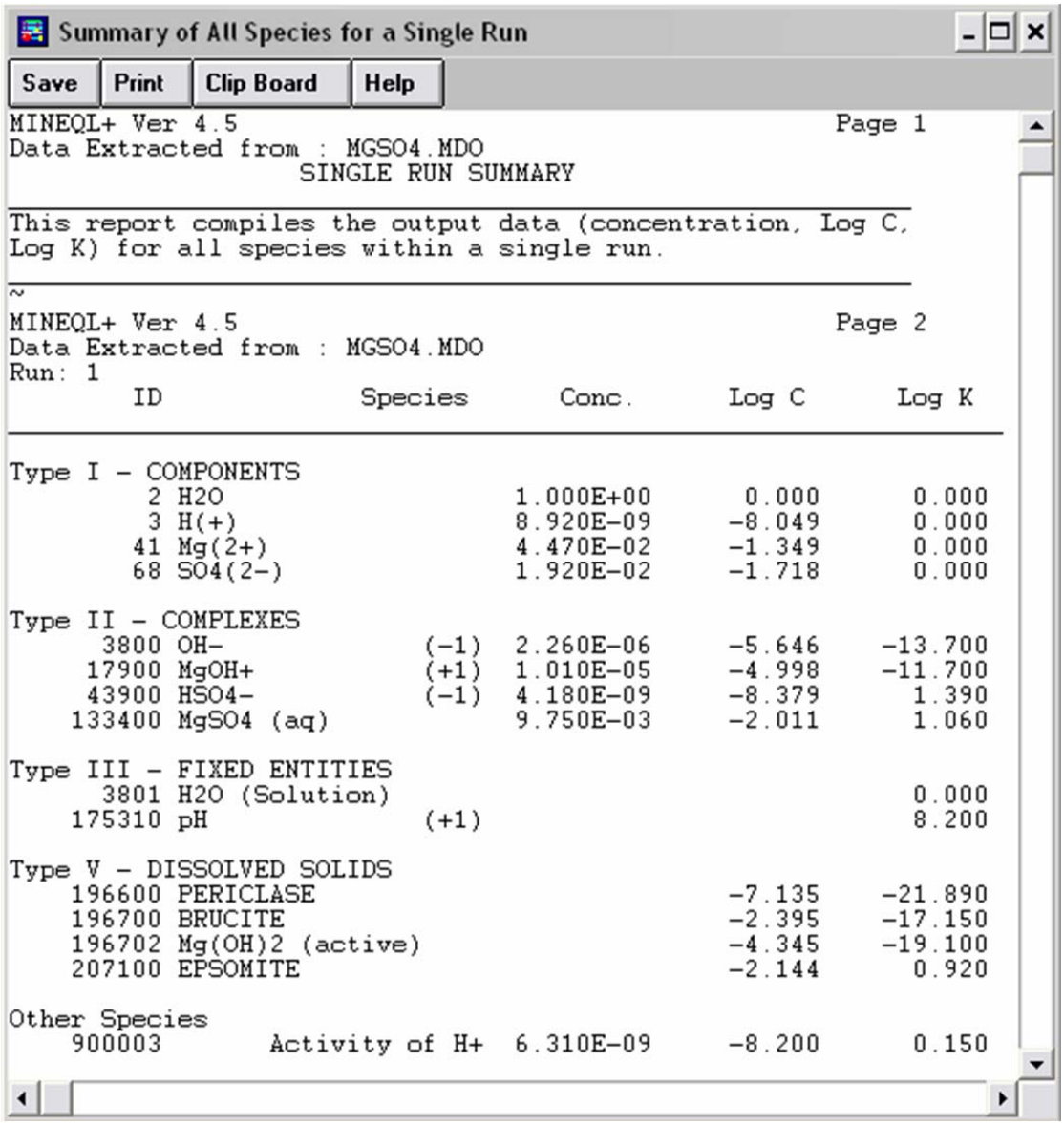


	Name	Type	Conc.	LogC	LogK	%Total	Stoch.
1	Mg(2+)	1	0.0448	-1.35	0	82.1	1
2	MgOH+ (+1)	2	2.01e-7	-6.7	-11.7	0	1
3	MgSO4 (aq)	2	0.00975	-2.01	1.06	17.9	1
4	PERICLASE	5		-10.5	-21.9		1
5	BRUCITE	5		-5.79	-17.1		1
6	Mg(OH)2 (active)	5		-7.75	-19.1		1
7	EPSOMITE	5		-2.14	0.92		1
8	TOTAL Mg(2+)	7	0.0545	-1.26		100	

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**.



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
Run: 1

ID	Species		Conc.	Log C	Log K
Type I - COMPONENTS					
2	H2O		1.000E+00	0.000	0.000
3	H(+)		8.920E-09	-8.049	0.000
41	Mg(2+)		4.470E-02	-1.349	0.000
68	SO4(2-)		1.920E-02	-1.718	0.000
Type II - COMPLEXES					
3800	OH-	(-1)	2.260E-06	-5.646	-13.700
17900	MgOH+	(+1)	1.010E-05	-4.998	-11.700
43900	HSO4-	(-1)	4.180E-09	-8.379	1.390
133400	MgSO4 (aq)		9.750E-03	-2.011	1.060
Type III - FIXED ENTITIES					
3801	H2O (Solution)				0.000
175310	pH	(+1)			8.200
Type V - DISSOLVED SOLIDS					
196600	PERICLASE			-7.135	-21.890
196700	BRUCITE			-2.395	-17.150
196702	Mg(OH)2 (active)			-4.345	-19.100
207100	EPSOMITE			-2.144	0.920
Other Species					
900003	Activity 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.