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Print version

CEE 680: Water Chemistry

Lecture #19

MINEQL: Intro & Tutorial

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MINEQL today

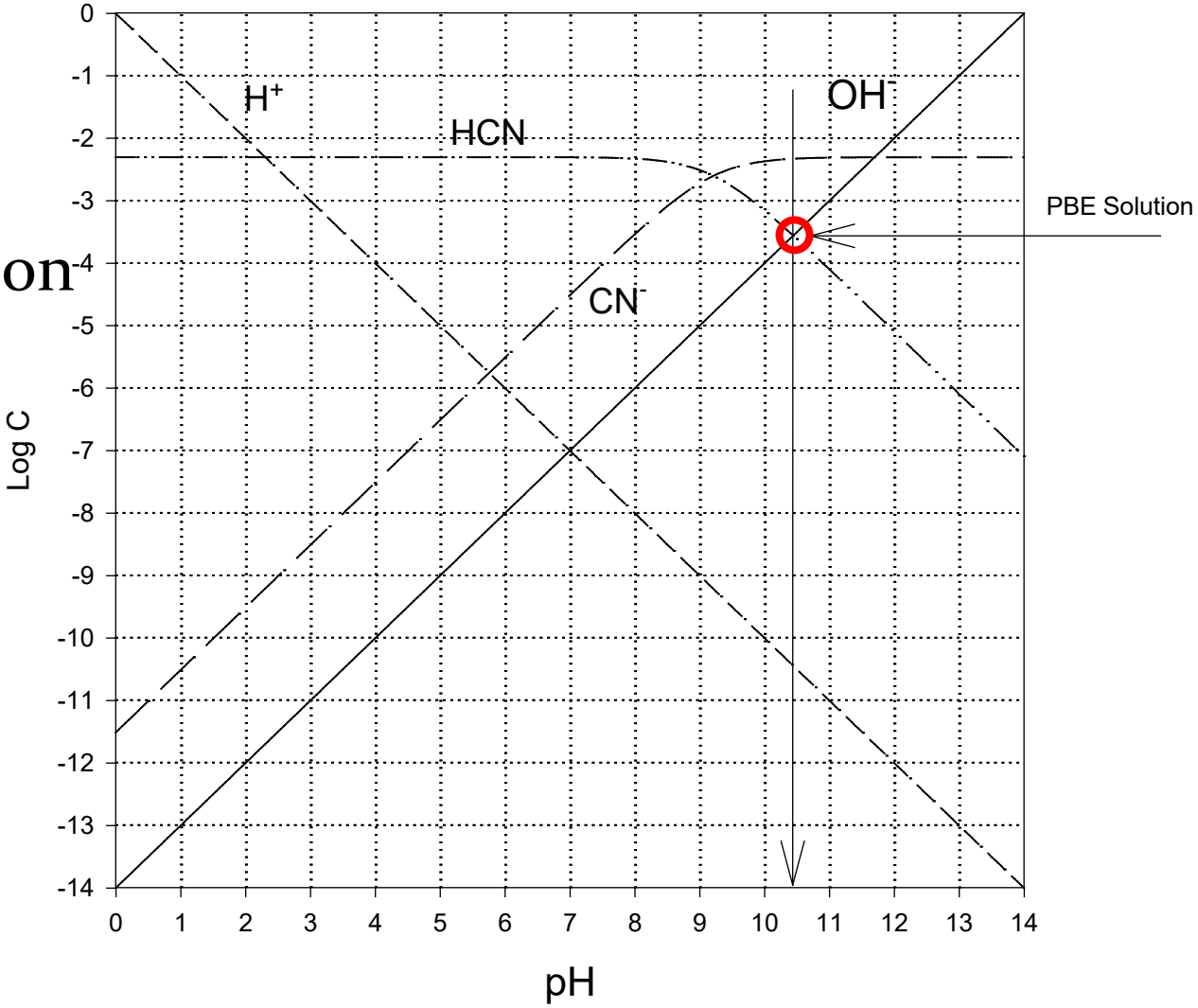
- MINEQL is available from Environmental Research Software:
  - https://www.mineql.com/
- Two options
  - Old DOS version (3.01) was available free of charge
  - A recent Windows version (4.6) has been available
    - I've acquired this version for our class use
  - Newest version (5.0) is now available
    - But we don't have a copy of this one yet ($635)

MINEQL species

- **Type-I Species**: soluble species that comprise the basic components of the solution and its solutes. These must be a collection of independent species. Species that are merely combinations of previously specified Type-I species should not be included.
- **Type-II Species**: aqueous complexes that form from the Type-I species.
- **Type-III Species**: solids or other substances with fixed activity (e.g., precipitates that never completely dissolve, atmospheric gases, pH in a pH-controlled environment)
- **Type-IV Species**: precipitates that could become completely dissolved and therefore go from an activity of one to zero
- **Type-V Species**: substances that could precipitate, but do not yet exist as a precipitate
- **Type-VI Species**: substances that are not considered in the calculations

Example Problem

- $5x10^{-3}$ M NaCN
  - pK_a=9.21
- Graphical solution



Example Problem

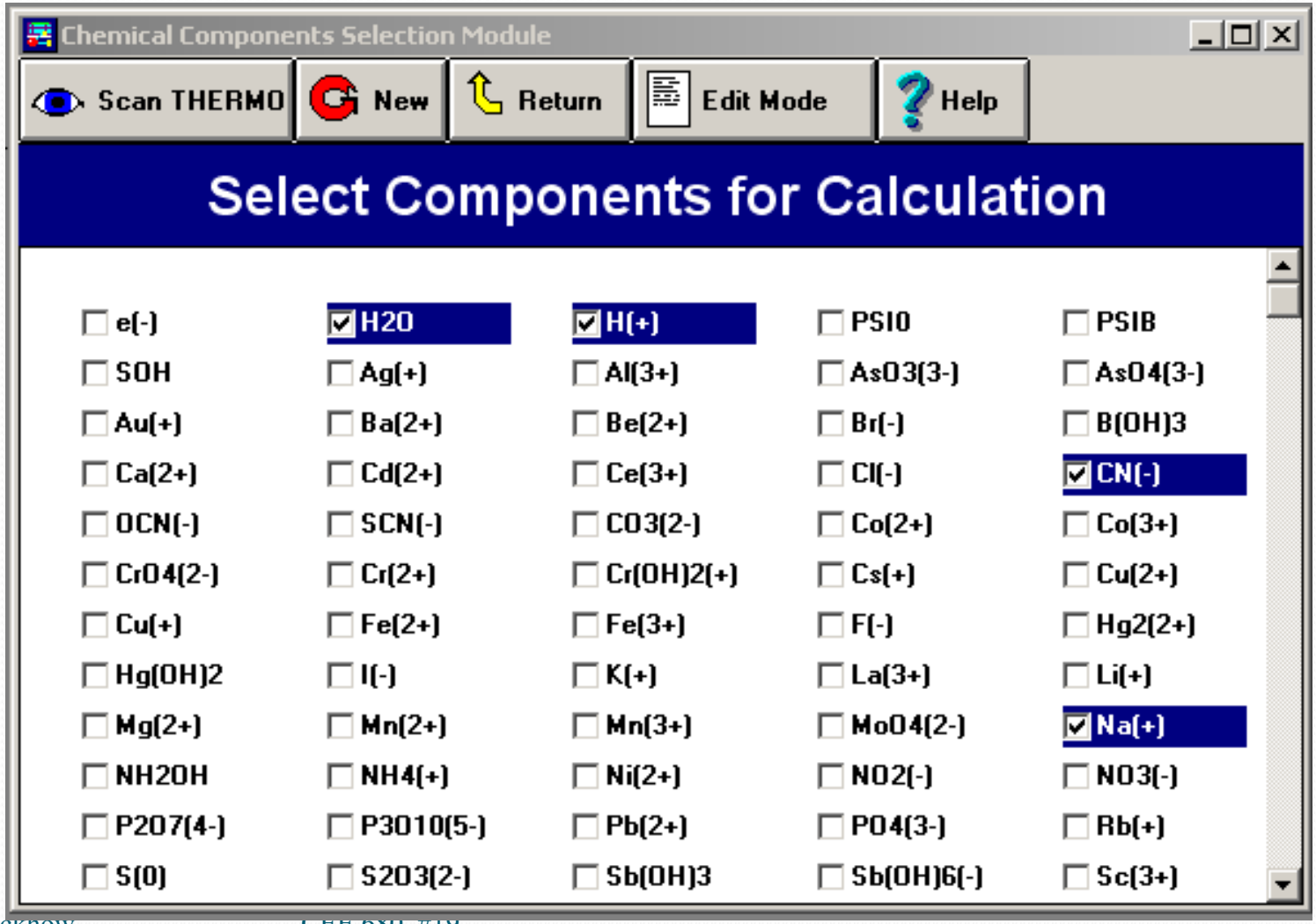
- Exact solution

Species	Conc (M)	pC
H^+	3.613×10^{-11}	10.4421
CN^-	4.724×10^{-3}	2.3257
HCN	2.768×10^{-4}	3.5579
OH^-	2.768×10^{-4}	3.5579

Example 1a (V 4.6)

- Determine the complete species composition from the addition of $5x10^{-3}$ moles of NaCN to 1 liter of water.
  - When you launch MINEQL, it should go right to the "select components" screen
    - If it doesn't, you can get there by selecting: Model>Select components
  - This screen contains the Type-I components, which can be selected by clicking on the check-boxes. The components, H_2O and H(+) and already selected for you.
    - For this problem, you should then add CN(-) and Na(+).
    - Note that OH(-) is not a selection, because it can be obtained by taking an H(+) away from H_2O so that it is not a independent substance. The same is true for HCN (it can be obtained by combining CN(-) and H(+).)

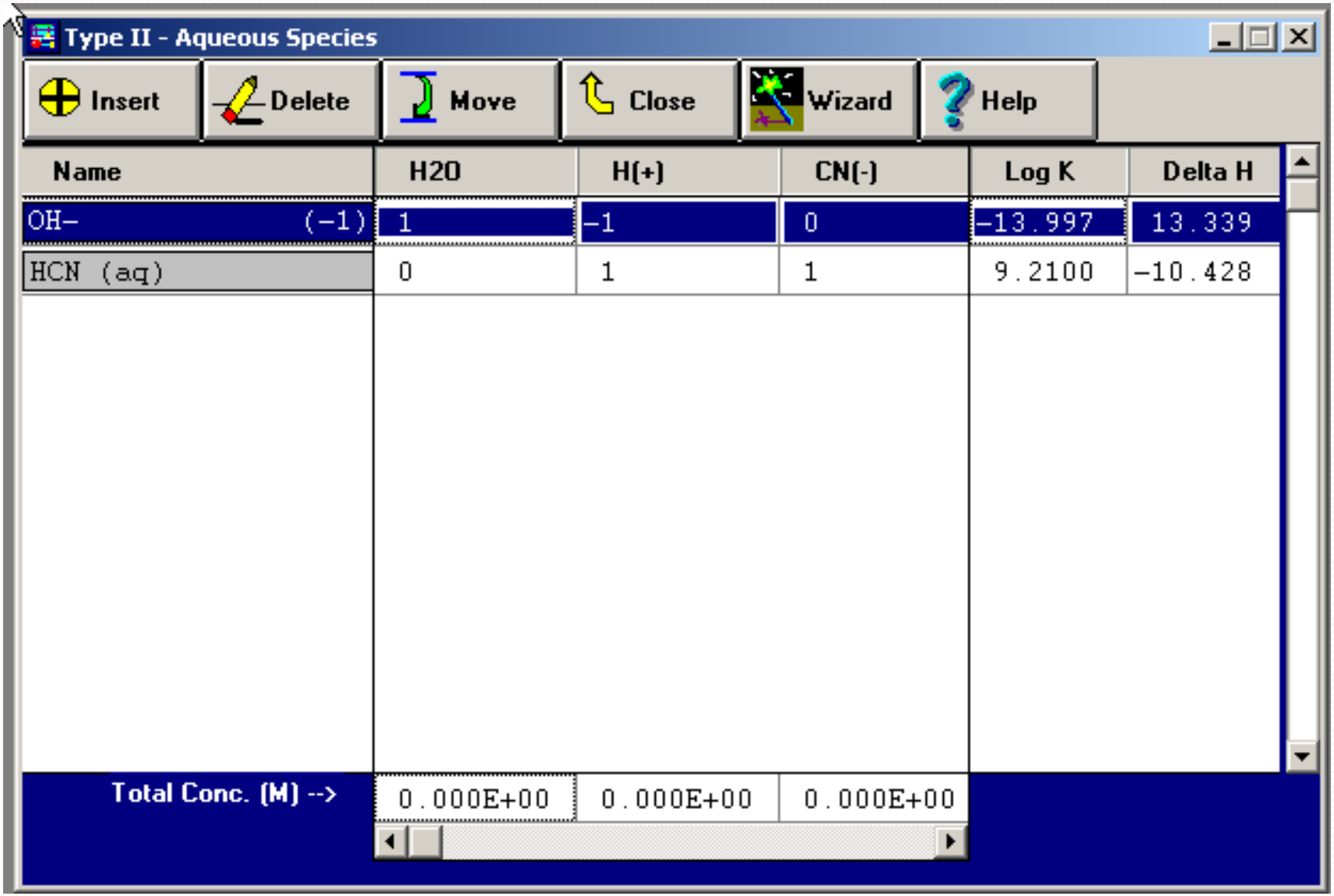
Select Components

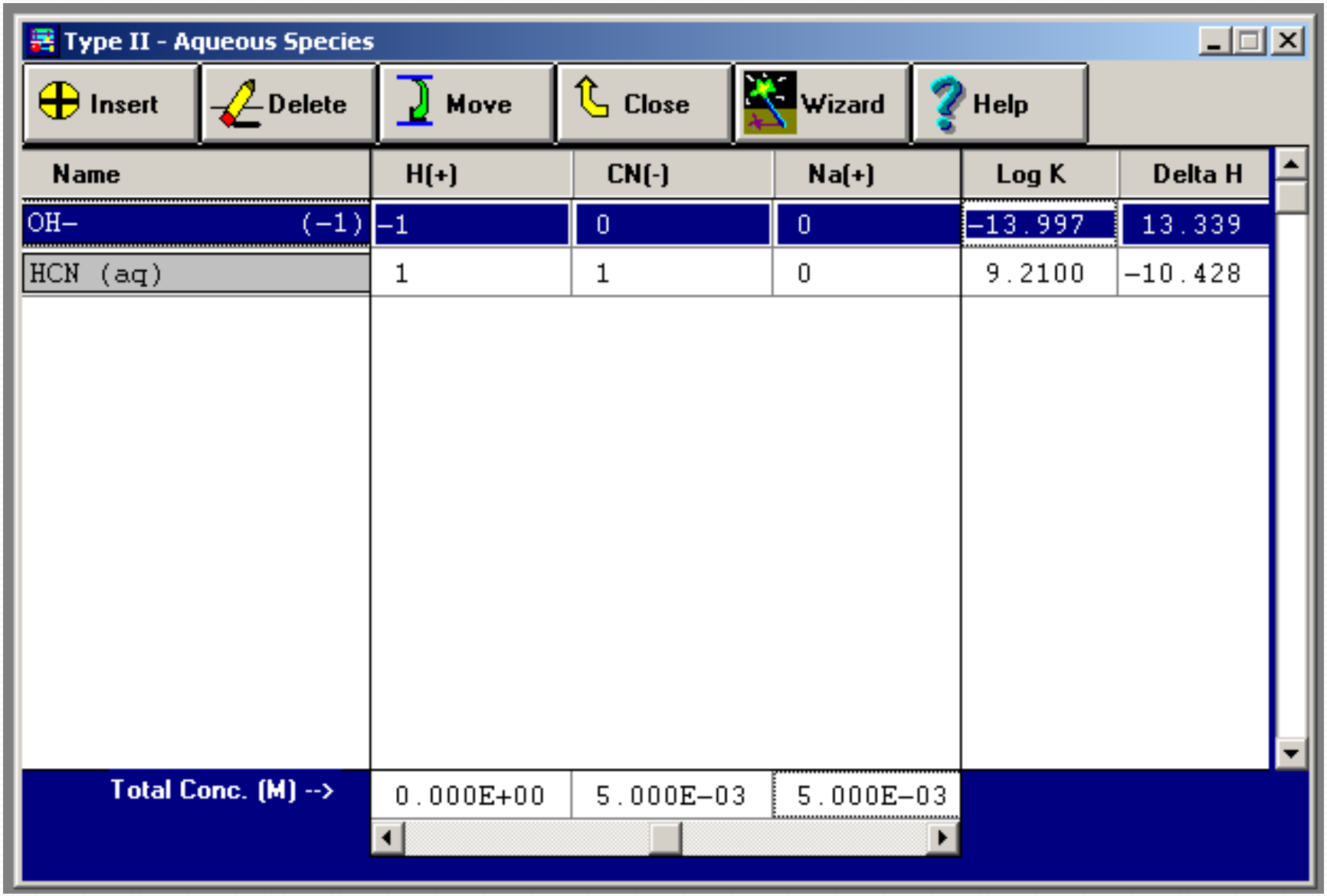


Example 1b (V 4.6)

- To move on to the Type-II species and the thermodynamic database, hit the "Scan Thermo" button
  - This will show the additional species that will form, along with equilibrium constants needed to calculate their concentrations.
  - This screen is also the place where you tell MINEQL how much of each component you're adding
  - Now move the cursor over to the total concentration line. Keep H_2O and H(+) at zero, but type in 5E-3 for the concentration of CN(-) and the same for Na(+).
- Hit the close button to move on to the next screen
- Select the "Fixed Solids" (i.e., Type-III species). Place the cursor on the pH line and hit the "move" button. Select "move to "species not considered (or included). These are "Type-VI" species. This is necessary, because we don't want to force the pH to stay at any particular level. In fact, one of the purposes of this problem is to determine what the final pH will be.
- You can also do this with the "Wizard"
  - Check the button, asking MINEQL to calculate pH

} This is probably easier


Type II - Aqueous Species
Insert
Delete
Move
Close
Wizard
Help
Name
H2O
H(+)
CN(-)
Log K
Delta H
OH- (-1)
1
-1
0
-13.997
13.339
HCN (aq)
0
1
1
9.2100
-10.428
Total Conc. (M) -->
0.000E+00
0.000E+00
0.000E+00


Type II - Aqueous Species
Insert
Delete
Move
Close
Wizard
Help
Name
H(+)
CN(-)
Na(+)
Log K
Delta H
OH- (-1)
-1
0
0
-13.997
13.339
HCN (aq)
1
1
0
9.2100
-10.428
Total Conc. (M) -->
0.000E+00
5.000E-03
5.000E-03

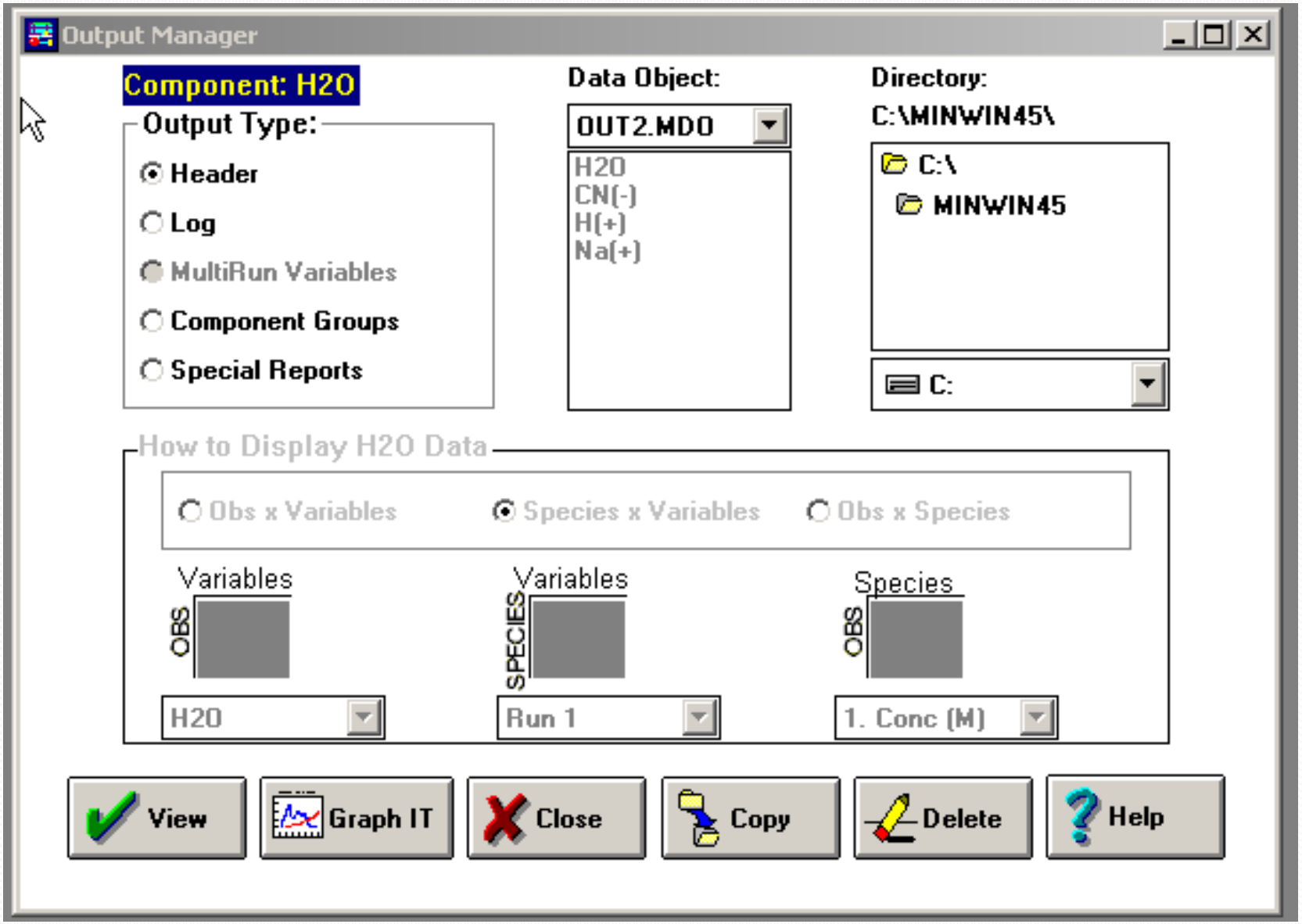
Example 1c (V 4.6)

- Hit “close” and then “no” to arrive at the “run time manager”
  - Type in an output data name
  - Keep “ionic strength corrections”, “temperature corrections” and “adsorption model” off
  - Hit the “Run” button

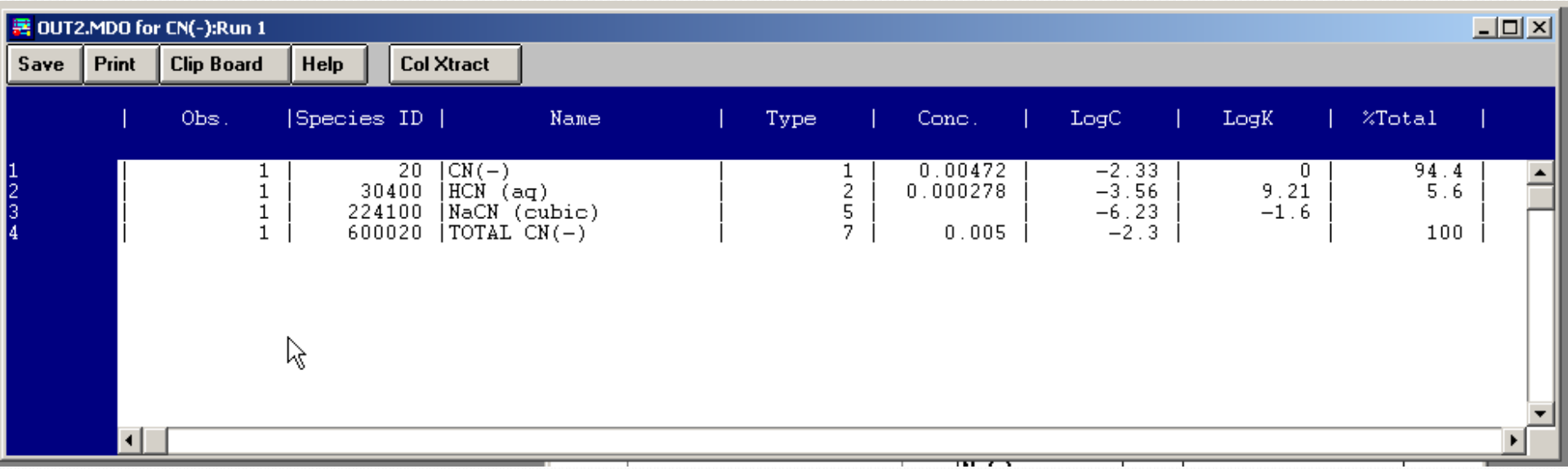
- Select “output manager” to view model results
  - Header gives input data
  - Component Groups has concentrations in a convenient tabular form

Example 1d (V 4.6)

- After the run is complete (should only take a second or two), select "output manager". Under "MINEQL object" select your output file name. Under "member" select "S1.H(+)". Then under "row type" select "species" and under "display criteria" choose "run1". This will display the concentrations of all species containing an exchangeable proton (i.e., H+). Copy down the relevant information. Ignore the line labeled "pH". Repeat this process, but this time choose "S1.CN(-)" under the "member" category. This time you will see data on all species that contain the cyanide group (i.e., CN).

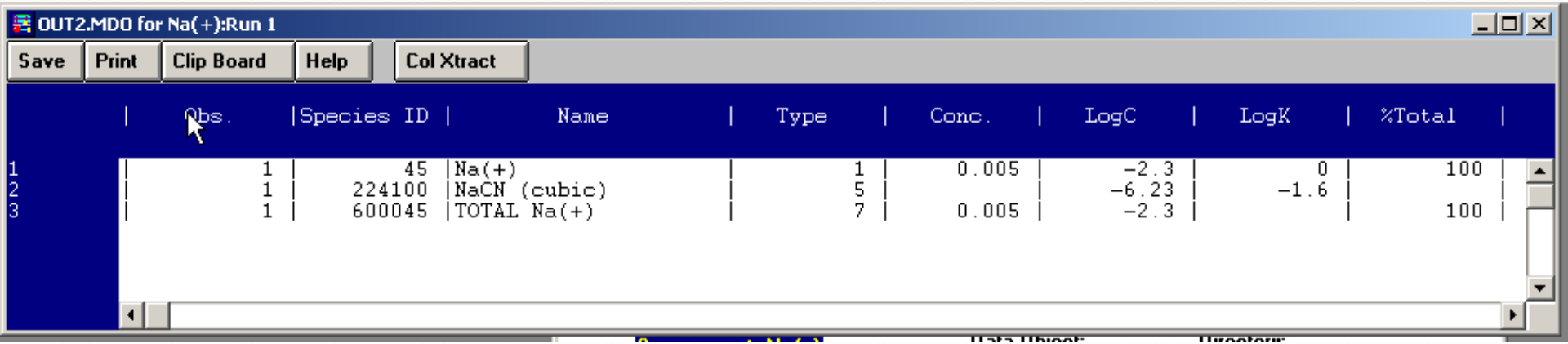

Output Manager
Component: H2O
Output Type:
Header
Log
MultiRun Variables
Component Groups
Special Reports
Data Object:
OUT2.MDO
H2O
CN(-)
H(+)
Na(+)
Directory:
C:\MINWIN45\
C:\
MINWIN45
C:
How to Display H2O Data
Obs x Variables
Species x Variables
Obs x Species
Variables
OBS
Variables
SPECIES
Species
OBS
H2O
Run 1
1. Conc (M)
View
Graph IT
Close
Copy
Delete
Help

- Output Type: Component Groups
  - Data Object: CN(-)



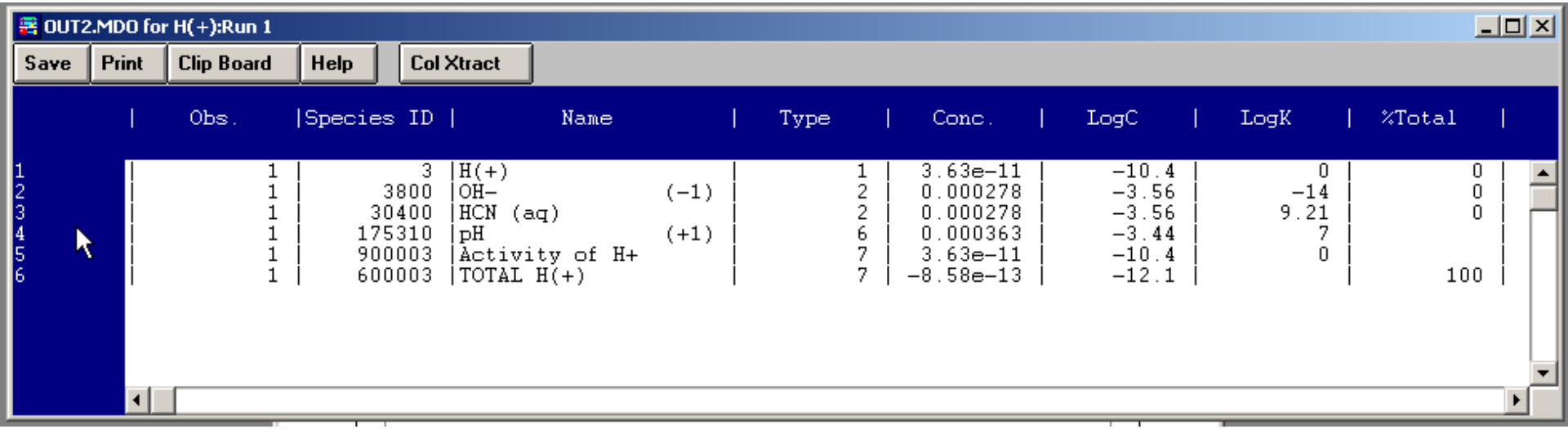
	Obs.	Species ID	Name	Type	Conc.	LogC	LogK	%Total
1	1	20	CN(-)	1	0.00472	-2.33	0	94.4
2	1	30400	HCN (aq)	2	0.000278	-3.56	9.21	5.6
3	1	224100	NaCN (cubic)	5		-6.23	-1.6	
4	1	600020	TOTAL CN(-)	7	0.005	-2.3		100

- Output Type: Component Groups
  - Data Object: Na(+)



	Obs.	Species ID	Name	Type	Conc.	LogC	LogK	%Total
1	1	45	Na(+)	1	0.005	-2.3	0	100
2	1	224100	NaCN (cubic)	5		-6.23	-1.6	
3	1	600045	TOTAL Na(+)	7	0.005	-2.3		100

- Output Type: Component Groups
  - Data Object: H(+)



	Obs.	Species ID	Name		Type	Conc.	LogC	LogK	%Total
1	1	3	H(+)		1	3.63e-11	-10.4	0	0
2	1	3800	OH-	(-1)	2	0.000278	-3.56	-14	0
3	1	30400	HCN (aq)		2	0.000278	-3.56	9.21	0
4	1	175310	pH	(+1)	6	0.000363	-3.44	7	
5	1	900003	Activity of H+		7	3.63e-11	-10.4	0	
6	1	600003	TOTAL H(+)		7	-8.58e-13	-12.1		100

Input data summary

- Output type: Header

OUT2.MDO HEADER

Save | Print | Clip Board | Help

```
   Oct 05, 2006  19:58
   MINEQL+ Header file for out2.mdo


          $$$  INPUT DATA  $$$
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
OPTIONS:  IADS= 0 IONIT= 0 IONPH= 0 IPHFX= 0 IPHA=  0
            IPHB= 0 ITITL= 0 IPCP=0 ICND=0
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
                ELECTRONEUTRALITY NOT GUARANTEED
               TEMPERATURE  =  25.0 CELSIUS
                IONIC STRENGTH CORRECTIONS OFF
                NO SURFACE MODEL USED
                      EPS =  1.0E-04
   ID          X     LOGX          T      COMPONENTS
    2   1.00D-20  -20.00   1.000E-18     H2O
    3   1.00D-07   -7.00   1.000E-18     H(+)
   20   5.01D-05   -4.30   5.000E-03     CN(-)
   45   5.01D-05   -4.30   5.000E-03     Na(+)

   ID     NAME                 LOGK      DELH      SPECIES:       TYPE I - COMPONENTS
      2 H2O                      .000       .000     H2O          1.0
      3 H(+)                     .000       .000     H(+)         1.0
     20 CN(-)                    .000       .000     CN(-)        1.0
     45 Na(+)                    .000       .000     Na(+)        1.0

   ID     NAME                 LOGK      DELH      SPECIES:       TYPE II - COMPLEXES
   3800 OH-              (-1) -13.997     13.339     H2O          1.0   H(+)       -1.0
  30400 HCN (aq)                9.210    -10.428     H(+)         1.0   CN(-)       1.0

   ID     NAME                 LOGK      DELH      SPECIES:       TYPE III - FIXED SOLIDS
   3801 H2O (Solution)          .000       .000     H2O          1.0

   ID     NAME                 LOGK      DELH      SPECIES:       TYPE V - DISSOLVED SOLIDS
 224100 NaCN (cubic)           -1.601      -.232     CN(-)        1.0   Na(+)       1.0

   ID     NAME                 LOGK      DELH      SPECIES:       TYPE VI - SPECIES NOT CONSIDERED
 175310 pH             (+1)    7.000       .000     H(+)         1.0
```

Example 1a (V 3.01)

- Determine the complete species composition from the addition of $5x10^{-3}$ moles of NaCN to 1 liter of water.
  - Go to the "Data/Run" menu and choose "components". Select the Type-I components by highlighting the desired species and hitting "return". The components you should select are: H_2O (almost always a selection), H(+), CN(-) and Na(+). Note that OH(-) is not a selection, because it can be obtained by taking an H(+) away from H_2O so that it is not a independent substance. The same is true for HCN (it can be obtained by combining CN(-) and H(+).)

Example 1b (V 3.01)

- While still in the Type-I components mode, hit F2. This selects from the thermodynamic database the equilibrium constants you will need and presents them in a table entitled "Type-II Chemical Complexes". Now hit F2 three times to bring the cursor to the total concentration line. Keep H2O and H(+) at zero, but type in 5E-3 for the concentration of CN(-) and the same for Na(+).
- Escape from the "Complexes" table and select "Fixed Solids" (i.e., Type-III species). Highlight the pH line and hit "F3" which is the "move" key. Choose to move pH to "Type-VI" species. This is necessary, because we don't want to force the pH to stay at any particular level. In fact, one of the purposes of this problem is to determine what the final pH will be.

Example 1c (V 3.01)

- Escape from “Fixed Solids” and select “Run”. Keep “μ corrections” (ionic strength corrections) off, and keep the temperature at 25°C. Shift over to the “file output” line and select a name for the file where the results of your run will be stored. Then select “run”.

Example 1d (V 3.01)

- After the run is complete (should only take a second or two), select "output manager". Under "MINEQL object" select your output file name. Under "member" select "S1.H(+)". Then under "row type" select "species" and under "display criteria" choose "run1". This will display the concentrations of all species containing an exchangeable proton (i.e., H+). Copy down the relevant information. Ignore the line labeled "pH". Repeat this process, but this time choose "S1.CN(-)" under the "member" category. This time you will see data on all species that contain the cyanide group (i.e., CN).

Review old exams

- Refer to web site: Exam #1
  - Many since 2007
  - Fall 2007 and solution
  - Fall 2006 and solution

- To next lecture