# Visual MINTEQ – a brief tutorial

Visual MINTEQ was developed from the DOS program MINTEQA2, which was originally coded by the U.S. Environmental Protection Agency (EPA). Since 2000, when Visual MINTEQ was first published on the web, it has departed considerably from the original MINTEQA2 code, and therefore it is today a program on its own right. The aim of the program is to simulate equilibria and speciation of inorganic solutes in natural waters. The development of Visual MINTEQ was supported by the Swedish Research Council (VR) and by the Foundation for Strategic Environmental Research (MISTRA). You are free to download it to your own PC from the following WWW address:

http://www2.lwr.kth.se/english/OurSoftware/vminteq/index.html

A help file, vminhelp.htm, can be accessed from the program by clicking *Help – Open help file.* Consult the help file for topics not covered by this brief tutorial.
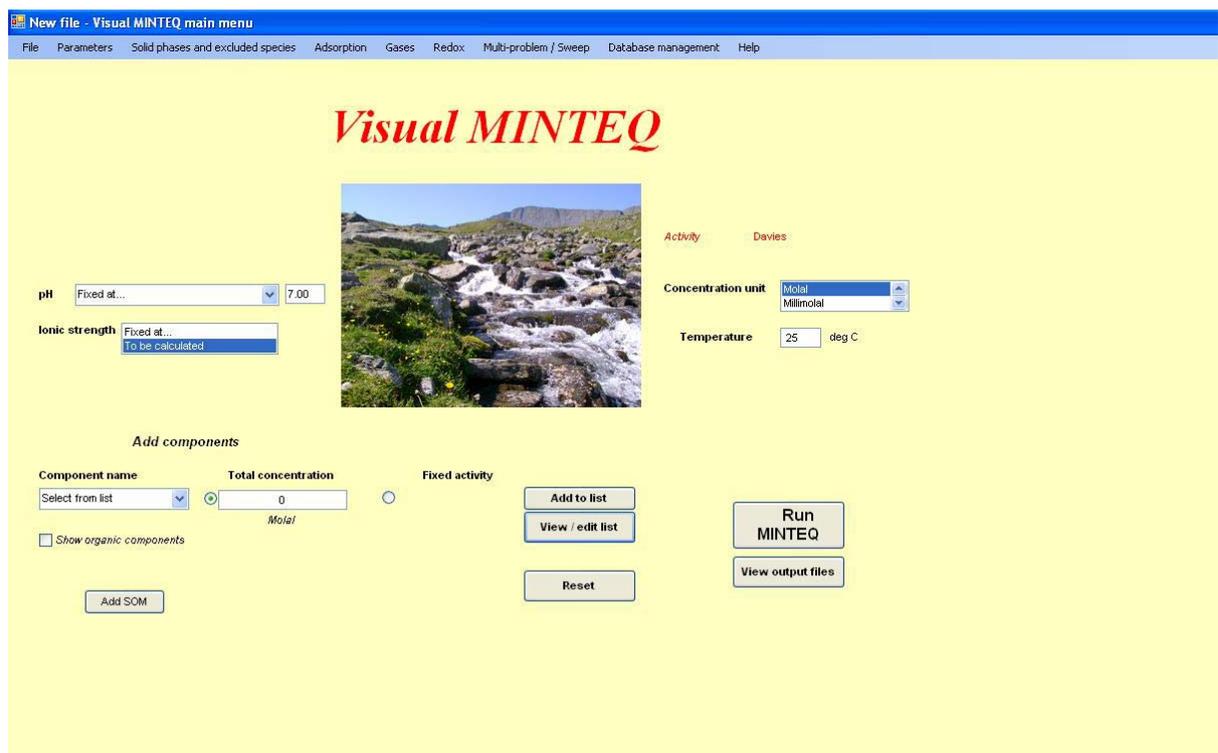
Define the problem

When you start working with MINTEQ, the first thing to do is to define the problem. If you have an old problem file with indata, you *File - Open* from the scroll-down menus. Otherwise, you will add the data of the problem yourself, starting from the *Main menu*, which is shown when the program is opened for the first time. On the *Main menu*, check the following:

- If the pH value is known, it is 'fixed' in the problem, so choose this option and enter the pH value. If the pH is to be calculated, you should generally choose 'Calculated from mass and charge balance' although you can also choose 'Calculated from mass balance' in some cases. For more details see the Visual MINTEQ user guide, accessible from the help file system.

- If the ionic strength is fixed or not (in the same manner as for the pH). In most cases, you let the ionic strength be determined by the program. If so leave it at the option 'to be calculated'.

- Choose the concentration units for the input data. Remember one important thing, however: Regardless of what concentration unit you choose, the results in the output will be shown in mol/l.

- If the water contains dissolved organic matter, there is a choice between three different models (Gaussian DOM, SHM and NICA-Donnan); you are advised to use SHM or NICA-Donnan because these are modern advanced models that are considered to be state-of-the-art, whereas the Gaussian DOM model was inherited from earlier MINTEQA2 programs. To use NICA-Donnan or SHM for aqueous speciation, you should **not** click "Add SOM"; instead choose DOC (NICA-Donnan) or DOC (SHM) from the list of components. For more detailed instructions, see the help file "vminhelp.htm" under the link "Humic complexation".

- The temperature. Chemical reactions are temperature-dependent. Visual MINTEQ corrects equilibrium constants for temperature by using the van't Hoff equation. Note that these corrections are done at runtime, which means that the log K entered into the program should always be valid for 25°C (in other words, you don't need to correct any constants yourself)

- Add the *components* of the problem, as well as their concentrations. This is done under the heading "Add components", where you feed in one component at a time, together with its total concentration. Don't forget to press the button *Add to list* after each new component! Alternatively, you can state a fixed activity of a component, but this option is used much less often. By pressing the button *View & Edit list* you can edit the concentrations of individual components or delete them from the problem.

Components in Visual MINTEQ

A component is the form of a chemical compound that Visual MINTEQ uses as a building block in chemical reactions. Some examples of components in MINTEQ are: H^+, Cl^-, Ca^{2+}, SO_4^{2-}, CO_3^{2-} and PO_4^{3-}. Many ions are not components, *e.g.* HCO_3^- and $H_2PO_4^-$. The reason is that they may be expressed from other components:

$HCO_3^- \rightleftharpoons H^+ + CO_3^{2-}$
$H_2PO_4^- \rightleftharpoons 2H^+ + PO_4^{3-}$

The choice of the component species is rather arbitrary, so it is possible to use HCO_3^- as a component rather than CO_3^{2-}. If so, CO_3^{2-} would be defined in the following way:

$CO_3^{2-} \rightleftharpoons HCO_3^- - H^+$

However, since all reactions are defined with a given component, it is heavy work to edit the databases should you wish to change a component, so this is normally not done.

When the concentration of, for example, PO_4^{3-} is stated in the Main Menu, it is important to note that you in fact state the total concentration of all PO_4 species (*e.g., TOTPO$_4$*). In the output lists of the results section however, the concentrations of the different PO_4 species will be shown separately, except on the page "Equilibrated mass distribution", in which the total concentration of phosphate will be given.

Remember that you should always define more components than fixed species in Visual MINTEQ. In some cases you may receive a message, which tells you this. In these situations, Visual MINTEQ will usually add a small concentration of one more component that does not influence the result.

By using the scroll-down menus, you can choose among a large number of alternatives, which modifies your input data in various ways. Here are some of the most common options (we suggest that you test these and other alternatives yourself).

- *Parameters - Inorganic carbon.* If you have a measurement of the carbonate alkalinity, state it here. There are four different units you can choose from.

- *Solid phases - Specify infinite solid phases.* If you know that you have equilibrium with respect to a certain solid phase, you define what phase it is and its equilibrium constant at 25°C (log K_s^0). You also supply the reaction enthalpy ΔH_r^0, which is used when the constant is corrected for temperature. If you accept the values suggested, you do not change anything here. Click *Add* to add the solid phase to your problem.

- *Solid phases - Specify possible solid phases.* The same as *Specify infinite solid phases* except that equilibrium is assumed to occur only if the concentrations of the species involved are found to be sufficiently large; this will cause precipitation of the phase. In the calculations, the program will equilibrate the solution with this phase absent, but if it finds that the speciated solution is oversaturated with respect to this phase, MINTEQ will recalculate the problem assuming that the water is in equilibrium with the phase.

- *Adsorption.* Here you can add parameters and constants for several different surface complexation models and empirical adsorption equations. Detailed instructions are found in the help file "vminhelp.htm" under the link "Adsorption problems".

- *Gases - Specify.* This page is useful particularly for stating fixed partial pressures of CO_2. If the "CO2" option is selected, the first line will show the atmospheric CO2 pressure. On the next line, you enter the value as a multiple of the atmospheric CO_2 pressure. Don't forget to press *Add* to add the gas to the problem.

- *Redox – Specify redox couples.* Before calculating the speciation of different redox-sensitive species, you need to start here and define the redox couples you are interested in. Once you have done this, Visual MINTEQ will suggest a pe value (electron activity). This value can be changed under *Parameters – Specify pe and Eh.* See also the help file under "Redox problems".

- *Multi-problem / Sweep*. This option enables you to run many different problems at the same time. There are four different options on the menu; the *Multi-problem generator* enables you to define a number of problems in the same file; the concentration of the components may be different. However, when you have a number of almost identical problems, you can choose the *Sweep* option. This option is particularly useful when you illustrate the pH-dependence of different processes; if so the pH is varied whereas all the other components remain constant. The *Titration* option enables you to simulate, e.g., acid-base titrations with a constant addition of acid or base. Further down the *Multi-problem / Sweep* menu, you can choose a number of components and species that are to be shown on a separate list of output results.

Important note for users in non-English-speaking countries

The program works best if you use **decimal points**, not decimal commas! Also, for some advanced functions to work properly, such as data import from Excel, it is advised that decimal points are selected as the default decimal type on your machine. This is done with the following procedure:

- From the Start menu in Windows, select the Control Panel.

- Choose Date, Time, Language or Regional Options (Win XP) or the equivalent option.

- Choose Change the format of numbers, dates, and times

- Under Number, change the decimal comma to a point.

Running Visual MINTEQ

When you are finished with defining your problem, you are advised to save your input data in a file, particularly if you would like to access them again later without repeating all the steps above. You do this through choosing *File - Save*. After this it's time to run the problem; press *Run*. This will start the calculation program, which appears as a black box on the screen. When the program has finished running, you close it by pressing OK in the box shown. After this, the results will be displayed.

Interpretation of results

The first page shown is the main *Output* page. In the upper part of the page, the equilibrium pH and ionic strength will be shown. If you had used a fixed value of pH and ionic strength, the value you had defined will of course be shown here. You will also be informed on the number of iterations required to reach a solution, and the calculated equivalent concentrations of anions and cations will be shown. The latter is useful to examine the apparent charge balance of the solution. If you had chosen one of the *Multi-problem / Sweep* options, a text box appears showing the number of the problem that the results apply to (you can switch to the other output results through

scrolling). In addition, you will see a button (*Selected sweep results*), which directs you to a page of selected results for all the problems you have run. You may also export the results to Excel.

The lower part of the *Output* page is dominated by a results list showing the concentration, activity and the logarithm of the activity for all species (ions, complexes etc.). From *Options* in the scroll-down menu, you can export these results to Excel.

When clicking the button *View Species Distribution* you are transferred to page showing the percentage (on a molar basis) of the total concentration of each component that is distributed on each species in solution. However, to appear in the list, the species should contribute to at least 0.01 % of the total concentration of the component.

If you choose *Display Saturation Indices* you will get a list showing whether the equilibrium solution is over- or undersaturated with respect to different solid phases. Please note that the constants for the solid phases have been recalculated if the temperature is different from 25°C. Also note a detail that can cause some confusion: the saturation index is always calculated by comparing with the database values in the program. Therefore, if you had changed the equilibrium constant when you defined the problem, the program will compare the ion activity product in solution with the database value of the constant.

Finally, on the page *Equilibrated Mass Distribution* the total concentration of each component will be shown, as dissolved, adsorbed and precipitated phases.

Problems that may arise

Because the program was developed with Visual Basic in a Windows Environment, you will normally have to use a PC with a Windows operating system (e.g., 2000, ME, XP, Windows 7). When installing version 3.0 of the program, administration rights are usually not required although the installer may ask for these. When installing a new version of the program, you are advised to uninstall any old versions – otherwise installation will not be complete. An exception is when you upgrade from a 2.xx version to version 3.0 – these versions are installed in different folders and thus they do not interfere with one another.

Good luck!