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GEOCHEM-EZ: a chemical speciation program with greater power and flexibility

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Introduction

Chemical speciation programs, such as GEOCHEM (Sposito and Mattigod, 1980), GEOCHEM-PC (Parker et al., 1995), PHREEQC, MINEQL+, and MINTEQA2 have been excellent tools for scientists to use in designing appropriate solutions for their experiments. Programs of this type allow the user to estimate the interactions between metals and ligands and to calculate the free activities of the ions of interest. In doing so, the scientist can make a solution in which requisite conditions are satisfied and the design is intelligent. For many years we have used GEOCHEM-PC to formulate hydroponic solutions for plant growth, including those employing a variety of metal-chelate systems (Parker et al., 1995b) to control Fe (II), Fe (III), and Zn status. In addition, this program has been an important tool in creating test solutions for plant aluminum (Al) tolerance experiments. Thus, we are able to estimate Al^{3+} activities and to create solutions without significantly lowering available phosphate or sulfate. Many of the Al-containing nutrient solutions that are presently in use contain very high Al levels in order to achieve the desired root growth inhibition. These solutions may be redesigned with GEOCHEM-EZ to avoid these problems.

As helpful as GEOCHEM-PC has been to a number of scientists in their work, the consensus among users was that the program was not very user friendly and suffered from several functional weaknesses. There were no help files to guide those who were new to the program. The program was written in FORTRAN to be run in a DOS environment, so naming files was limited to eight characters or less. If there were any input errors, then the program did not indicate what they were, just that there were errors. Data entry involved parsing the salts added to the solution into the individual metals and ligands, calculating their respective concentrations, and then entering these concentrations as the –log [ ] into a DAT input file. Some calculations may have taken several iterations, which involved having to save the file, run the calculation, examine the output file, then make appropriate corrections, input the data again, save the file, and make additional calculations. In discussing these issues with the authors of GEOCHEM-PC we were encouraged to build upon and improve the existing program, so that it would work in a Windows XP or Vista environment and would have increased power and function.

Methods

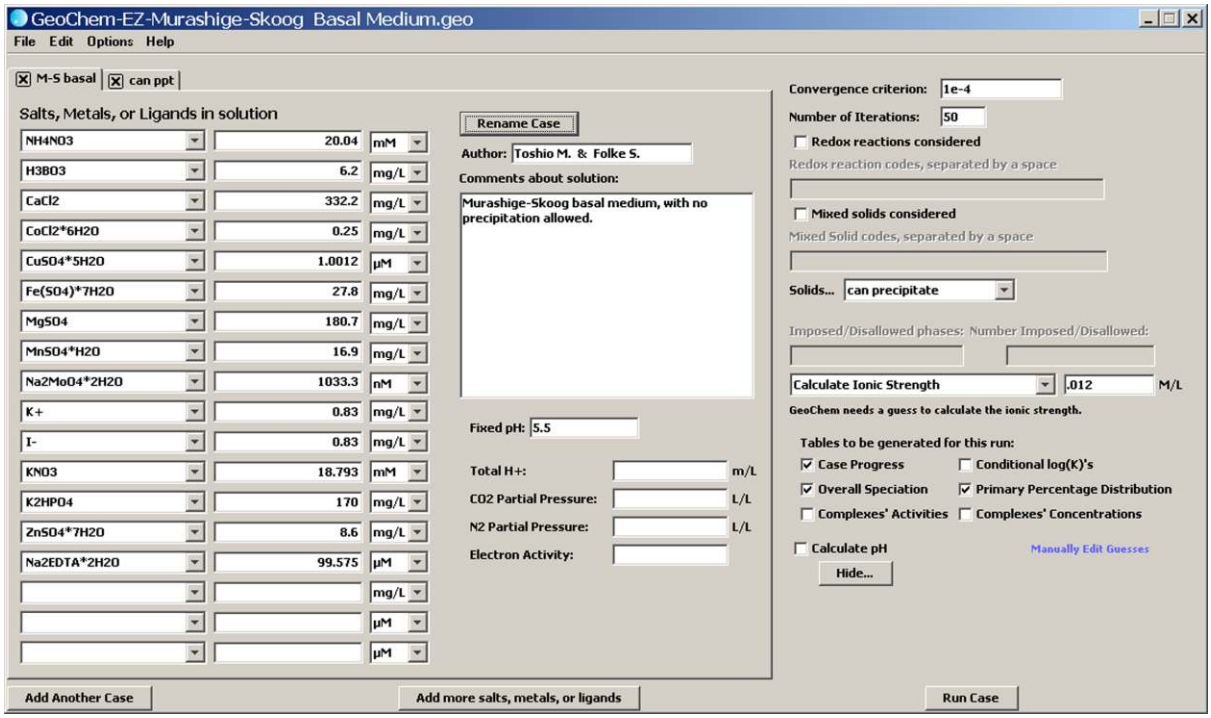
All code has been written and compiled using Java Standard Edition 6. All components of the Graphical User Interface (GUI) were created using the Netbeans 6.0's GUI editor. The active interface will be released as a precompiled, executable JAR file.

When we upgraded GEOCHEM-PC, we embedded it in a Java interface with an image display that was uncomplicated and clean. New and basic users can easily negotiate the interface for simple data entry. However, we have retained within the interface all of the more complex elements of GEOCHEM-PC, which allows for more advanced calculations. This program will run on any computer that supports a Windows XP, Vista, or Windows 7 environment. This includes Mac operating systems with Windows emulation programs. Help files were developed using Adobe Dreamweaver and scripted in HTML to be viewed through any conventional Web browser (e.g., Firefox, Internet Explorer). These Help files were built into the program, but can also be viewed outside of the program as a stand alone feature. The http://www.plantmineralnutrition.net/Geochem/geochem%20home.htm web site will be used to distribute the program (as free software), download help files, and to correspond with the authors if there are any technical questions regarding the program.

Results

Included in GEOCHEM-EZ are improvements which would be expected by modern users (customizable user-experience, extensive interactive and illustrated help files, hierarchical organization of options, logical output, real-time error checking), while maintaining complete backward compatibility to the GEOCHEM-PC format. A customizable database of common salts has been included, which eliminates the need to parse and to calculate the concentration of each metal or ligand. In addition, the user is no longer limited to enter concentration as nM, µM, or mM, but can now enter the concentrations as g/L or mg/L, provided the salts of interest are part of the salts database. These last two features will make data input more rapid and help in eliminating the most common user errors. The program does automatically check for errors in data entry, convergence, and case similarity. The user can instantly preview input and output files and make necessary corrections (e.g. charge balance the solution), something that formerly involved having to save these files and run the calculations a second or third time. Output files may be customized by filtering the output tables prior to saving the file. Within the Help menu we have included a Unit Converter which can convert any salt in the database from g/L or mg/L to molar concentrations or vice versa.

Shown below is the GEOCHEM-EZ interface. This example is for a basal Murashige –Skoog medium, with the salt, metal, and ligand concentrations entered in mg/L. Note that the entries are mostly salts (e.g., NH_4NO_3) that are contained within the salts database and are accessed via the drop down list on the left side. However, the user may still add individual metals or ligands, if that is preferred. This entry for the M-S medium represents a simple case (fixed pH, no redox reactions, solids can precipitate). Note that there are two tabs open (m-s basal, can ppt), representing two separate cases (calculations) that are being run simultaneously. Many cases can be run at the same time, another feature that makes solution analyses more rapid.



Discussion

Why should one use this program to design experimental solutions? Many scientists have modified standard nutrient solutions for hydroponics-based research or for specific experimental treatments without having analyzed these solutions to see whether any precipitation or solids may form because of the changes that they made to the solution composition. Geochem-EZ can help predict potential problems in experimental media. This program can also be used to design sensible chelate buffer systems or to calculate the concentration of a particular ion needed to provide a constant ionic activity. It is also a good way to know whether there is sufficient free activity of important nutrients in the solution of interest. Often there is the assumption that if the nutrient is part of the solution, then it is readily available to the plant. This is not necessarily true. Interaction with other ions, pH effects, complexation, and precipitation may occur, reducing the free activity of the ion of interest.

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