Electronic Scientific Notebook
888E

Software Validation for FITEQL 4.0

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Software Validation for FITEQL 4.0

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Objective: To test FITEQL 4.0 to make sure that the output of this updated model matches that of its previous form FITEQL 2.0. This will be achieved by running the same problems (from the FITEQL 2.0 validation) to see the degree of accuracy.

Training: In order to perform said mentioned validation one needs to be familiar with the FITEQL program and have a basic understanding of various aqueous systems and graphs and tools to interpret such systems. I personally read the instruction manuals and became acquainted with the program by performing examples from the books.

Hypothesis: Although FITEQL has been updated to version 4.0, most of the modifications have been done to produce a windows version and minimal changes have occurred to the standard version. I expect the results for version 4.0 to be exactly the same as they were for 2.0.

Approach: To use the same set of validation problems used in the validation of FITEQL 2.0 (which is under TOP_018 control) to see if the results are the same when run on the windows version of FITEQL 4.0. The FITEQL 4.0 program was compared to MINTEQA2, 4.03 and analytical data from Kohler et. al, 1999 for validation.

Mathematical and other model assumptions: The user is referred to the manual that accompany the program to determine theory and assumptions employed by the program. However it's currently not in electronic form, a hardcopy is included when ordering the program.

Input Files: The input files used will accompany the validation report (and the version 2.0 reports) or see below for file location.

File Location: D:\My Documents\fiteql\FITEQL4.0_validation
These files will be burned to cd and submitted with all other validation materials and possibly be purged from the D drive.

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6/28/07
Getting acquainted with the program I used the validation input file from the 2.0 validation to run through the various input screens in the Windows version pre-processor. I copied and pasted the input file into textpad and saved it as .for, the extension used in version 2.0. I then from the Dos prompt called up the conversion program and created a file with extension of .F40, which is the format and extension used by version 4. The

updated file was run without problems, and comparison of the output to that of version 2.0, they are the same with minor rounding errors. However the program did converge much faster and the weight sum of squares was smaller than that found in verion 2.0, but this didn't effect the output. I also ran the input file, provided from the FITEQL 2.0 validation, for MINTEQA2 in the latest version 4.03. Comparison of the two MINTEQA files from two versions 4.02 and 4.03, show no differences. Since the output format of FITEQL 2.0 to 4.0 has changed, the output file couldn't be compared using Microsoft Word. The output was manually checked and being the same, the original spreadsheet created for the FITEQL 2.0 validation was included along with the output files to summarize the output of both versions. This spreadsheet also has the calculations of Kd and sorption data for the validation test.
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There are 15 input test files that accompany the program that can be used as seed files when creating input files. I used these files to perform the installation check to compare the FITEQL 4.0 output against the output that accompanies the program. The output files were compared using Microsoft Word and put into a separate comparison folder within the FITEQL 4.0 validation folder. All 15 files produce the same output when compared with the given output. Since the installation files all work properly, the Kohler file test from the 2.0 validation that was run yesterday was kept as is because the program passed the installation test and produced the same validation output. All validation files, installation (input/output), validation (input/output-for both MINTEQA2 and FITEQL), and documentation are all included in the FITEQL 4.0 validation folder.
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