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Computers in Chemistry

Spreadsheet Assisted Learning in Quantitative Analysis

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In principle, learning about learners allows faculty to create a structure in which novice learners may

We have used the text *Quantitative Chemical Analysis* by Daniel C. Harris [1] for ten years, and we adopted the 4th edition in the Fall of 1995. This edition contains a major change in that it uses spreadsheets for student exercises within the chapters and in the problem sets. Using these spreadsheet exercises requires the development of some computer expertise in students who do not generally start the class with any computer experience. Also, the exercises often require significant time to complete, time that could be devoted to other types of study, problem-solving, or laboratory experiments. For these reasons, the efficacy of using spreadsheet exercises to

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help students better understand the course concepts needs to be evaluated. Here we present some preliminary results that indicate that the exercises are beneficial, the primary benefit being that they allow students to generate and manipulate graphs (pictures) of the relationships they encounter, which helps them achieve a better understanding of those concepts.

The text *Quantitative Chemical Analysis* by Daniel C. Harris [1] is used for the five-hour quantitative analysis course at MTSU. The 4th edition contains a major change-the inclusion of spreadsheets for student exercises, which are first introduced in the statistics chapter and continued throughout the equilibrium chapters. A spreadsheet can be a powerful tool for the analysis of mathematical relationships, but we wanted to evaluate their efficacy for helping students understand complicated concepts in light of the added learning and time commitment they may require. This course already requires a significant time commitment by students that includes lecture, laboratory briefings, lengthy laboratory analyses, and report preparation, as well as the traditional homework assignments. Furthermore, beginning students tend to have either a passive involvement with computer exercises [2, 3] or they tend to go overboard in their computational zeal. We wanted to ensure that the computer was used as a learning tool and did not itself become the focus of the exercises.

It may be that in other chemistry departments, the use of spreadsheets is taught as early as freshman chemistry [2], or that entering freshmen possess significant computer skills. In our quantitative analysis classes, however, there are many first-time computer users. The tradition at MTSU is for students to first encounter spreadsheets in the Physical Chemistry course.

Ten to twenty percent of our students are non-traditional, often returning to the University after, for example, a military assignment. Additionally, approximately 80% of the quantitative analysis students work half- to full-time while attending school. These students need help and encouragement in approaching these spreadsheet exercises and need to be shown that the time spent is worth their while. To this end we provided handouts containing the basics of computer use and skeleton spreadsheets that save time by reducing the amount of data that needs to be entered. Test questions that stressed topics that were supported by spreadsheet exercises were asked, but they were not in themselves computer related questions.

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Included in the results is a summary of the examination averages contrasting spreadsheet users and non-users. Although this is a preliminary account, we believe it will be of assistance to teachers and students in other quantitative analysis classes containing a large number of non-traditional students.

Background

Microsoft Works® version 3.0 is available for use by both students and faculty though a departmental site license. This allows participants access to a spreadsheet program without cost. In order to fully appreciate many of the graphs that are generated in the exercises, a high resolution video display (EGA or better) was used.

Before using the spreadsheet exercises in the Fall 1995 Quantitative Analysis class, the student co-author (John Marsh) completed those exercises contained in the portions of the text we cover in the course. This student had successfully completed the quantitative analysis course in the previous semester, when concepts were presented without the assistance of spreadsheet exercises. He rated the exercises according to their efficiency at demonstrating the concepts without requiring excessive time or computer knowledge to complete. His evaluation is presented in Table 1.

During the Fall semester, the students were *not required* to complete the spreadsheets; rather, they were given an incentive to do so. They were made aware that the spreadsheet exercises supported examination questions. Each major examination (60 points total) contained a 5-point question about a topic similar to one covered in a spreadsheet exercise from the textbook or on a handout. On each examination the students were asked if they had completed the suggested spreadsheet exercise, and how much time the exercise had required.

During the Spring semester, the spreadsheet exercises were *mandatory*: Students were required to complete a set of four computer exercises described in the handouts presented in Appendix I. To receive credit the students were required to submit computer disks containing files of the completed exercises along with printed graphs. Two changes were made in the presentation of the spreadsheet exercises to better prepare students to immediately begin using the spreadsheets. First, features of spreadsheets not covered in the text were introduced to the class by way of the handouts. Blanks were left in the handouts so that the assignments could be

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individualized; that is, each student had a different set of data to manipulate. Second, spreadsheet templates were developed for the students to use. This helped minimize the time required to set up the data.

The following spreadsheets, used in the exercises, may be downloaded here. They can be viewed with MS Works 3.0 or MS-Excel™.

Spreadsheet 1: Gaussian Curves for Variable Standard Deviations. (sheet1.wks 10 Kbytes)

Spreadsheet 2: Effects of Higher Order Complex Formation on Total Dissolved Silver at Equilibrium. (sheet2.wks 12 Kbytes)

Spreadsheet 3: Fractional Composition of a Diprotic Acid Solution. (sheet3.wks 11 Kbytes)

Spreadsheet 4: Titration of Three Halide Solutions with Silver Nitrate Solution. (sheet4.wks 20 Kbytes)

Figures 1, 2, 3, and 4 show how the spreadsheet data looks on the computer screen when graphed from each properly completed spreadsheet. The test questions related to the exercises are given in Appendix II.

Grading the completed spreadsheets and graphs required about 5–10 min per student per exercise. The most efficient method was to set a deadline for the work to be turned in and to spend an afternoon grading the exercises.

A caution is in order for those who choose to have students turn in files on computer disks. At least one student disk contained a computer virus (*Monkey B Virus* or the *Stoned Empire Monkey Virus*). A faculty computer contracted the virus, transferred it to subsequently graded student disks, and through them to most of the computers in the laboratory. To disinfect all the computers required several afternoons of a student assistant’s time. This impelled us to purchase and install on all the faculty and laboratory computers, a good antivirus shield.

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TABLE 1. Evaluation of Spreadsheet Exercises

Exer[a]	Topic Covered by Spreadsheet	hrs[b]	Rank[b]	Notes[b]
4.7	Gaussian Curve	1.5	1	
4.8	Gaussian Curves for Variable S.D.	0.5	2	4.7 req.
4.23	Least Squares Calculation	2.00	3	very hard
5.21	Manual Repetitive Approximation	1.0	2	simple
5.22	Automatic Iteration	0.5	1	simple
5.32	Effects of Complexes on Equil. Conc.	2.0	1	moderate
	Fig 7-10. Titration of I^- with Ag^+	1.0	1	moderate
	Fig 7-11. Titration of Cl^-, I^- with Ag^+	1.0	1	moderate
7.29	Titration of Three Halides with Ag^+	2.0	3	hard
7.30	Titration of Halides w/Ag^+, % Separation	2.0	1	hard
7.31	Titration of Halides w/Ag^+, Mass Bal. Eqs.	2.0	3	very hard
8.12	Effect of Charge on Activity Coefficient	0.75	1	
8.17	Calculation of Solubility by Iteration	0.25	3	
8.18	Calc. of Solubility by Iteration, Part 2	1.5	2	hard
10.16	pH of a Weak Acid Solution	4.0		didn't work[c]
10.24	pH of a Weak Base Solution			didn't work[c]
10.41	pH of a Weak Base Solution			didn't work[c]
11.11	pH of an Amphiprotic Salt Solution	2.0	3	hard
11.32	Fraction. Comp. of a Diprotic Acid Soln.	0.5	1	easy
11.33	Fraction. Comp. of a Triprotic Acid Soln.	0.5	2	easy
11.34	Fraction. Comp. of a Tetraprotic Acid Soln	0.5	2	easy
12.58	Weak Acid Titration	2.0	3	hard
12.59	Weak Acid Titration	0.75	3	moderate
12.60	Weak Base Titration	0.75	3	hard

[a]Exercises are numbered as in reference 1.
[b]John Marsh's estimate of the time required, the benefit (1 = most useful, 3 = least useful), and comments.
[c]The spreadsheet required algorithms beyond the capacity of MS Works.

Results

Table 1 contains the student co-author's evaluation of the textbook spreadsheet exercises. The least-squares spreadsheet, though important, was judged too difficult for beginners. We focused our attention on four other exercises from the list, those which

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TABLE 2. Analysis of Using Spreadsheet Exercise in the Fall-1995 Class (Spreadsheet exercises voluntary)

Exam		Class			Spreadsheet Users			Non-users			
#	Exer	n	sp avg[a]	avg[b] ±s.d.	n	sp avg[a]	avg[b]	time,[c] hrs	n	sp avg[a]	avg[b]
I	4.8	34	3.1	39.7±9.5	2	5	41.3	2	32	2.9	39.5
II	5.32	32	1.8	39.5±8.9	2	3.8	45.6	2.5	30	1.7	39.0
III	11.32	30	0.4	27.3±10.3	0	---	---	---	30	0.4	27.3
IV	7.29	30	1.1	28.5±10.5	0	---	---	---	30	1.1	28.5

[a]Average on spreadsheet related test question.
[b]Examination average.
[c]Time required to complete spreadsheet.

seemed best suited in their utility to help the students clarify difficult concepts. Only two students in the Fall-1995 class reported having completed the spreadsheet exercises prior to the tests. Those two students scored higher on spreadsheet supported test questions than those who had not completed the spreadsheets (Table 2). This improvement might not be an actual benefit of completing the spreadsheet exercise, but might instead be due to the non-random nature of the sample (spreadsheet users were self-selected in the Fall class). To examine this hypothesis, the examination averages (avg) and the averages on the spreadsheet-related questions (sp avg) were computed for the entire class, for the spreadsheet users alone, and for the non-spreadsheet users. The students in the Spring 1996 class were required to complete the four exercises, still, some did not. Table 3 shows the results for the Spring-1996 Quantitative Analysis class and provides for a comparison of the performance of the two classes.

Discussion and Conclusions

Quantitative analysis, because of its in depth investigation of complex equilibria, can be an excellent application for spreadsheets. The question, however, is how to best use them in a class already requiring a heavy time commitment of its students. We have found that providing partially completed spreadsheet files and making their completion and the construction of the graphs mandatory provides students with the greatest benefit.

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TABLE 3. Analysis of Using Spreadsheet Exercise in the Spring-1995 Class (Spreadsheet exercises required)

Exam		Class			Spreadsheet Users			Non-users			
#	Exer	n	sp avg[a]	avg[b] ±s.d.	n	sp avg[a]	avg[b]	time,[c] hrs	n	sp avg[a]	avg[b]
I	4.8	23	3.26	39.5±14.0	20	3.35	40.8	1.5	3	2.66	37.3
II	5.32	23	2.3	31.1±12.7	18	2.8	33.4	1.5	5	0.4	22.9
III	11.32	16	2.8	25.0±8.3	15	3.0	24.8	1.0	1	0.0	28.0
IV	7.29	19	2.16	33.1±13.1	16	2.6	33.6	1.0	3	0.0	19.7

[a]Average on spreadsheet related test question.
[b]Examination average.
[c]Time required to complete spreadsheet.

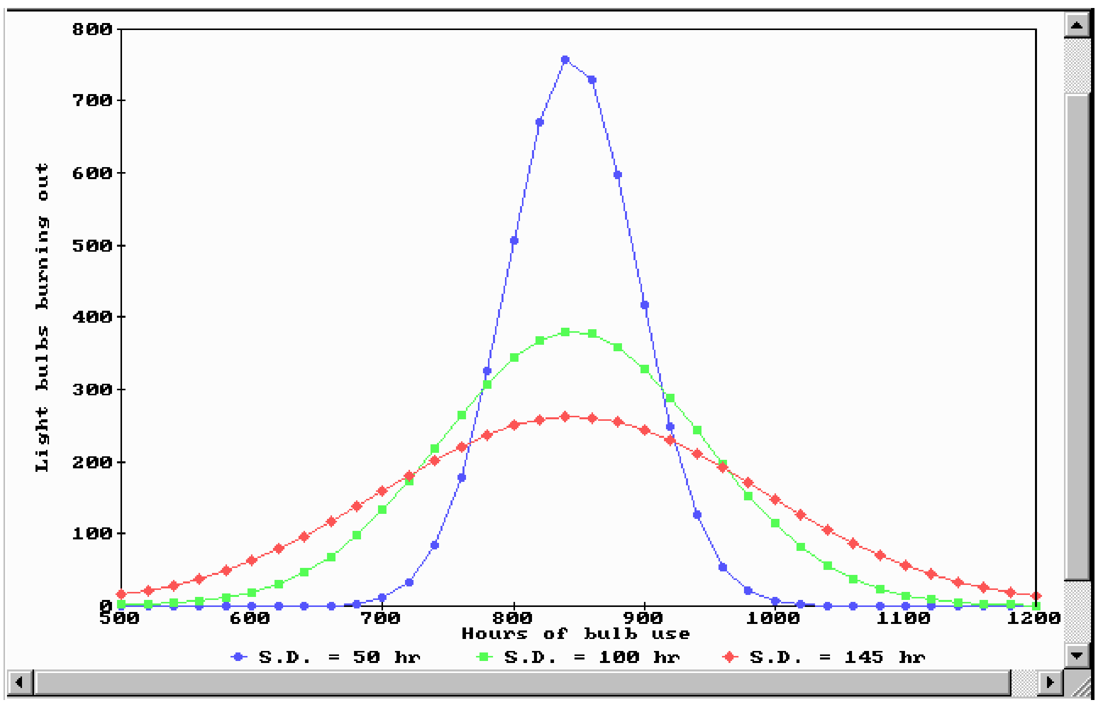

FIGURE 1. GAUSSIAN DISTRIBUTIONS OF LIGHTBULBS (LIFETIMES SHOW DIFFERENT STANDARD DEVIATIONS); PLOTTED FROM SPREADSHEET 1.

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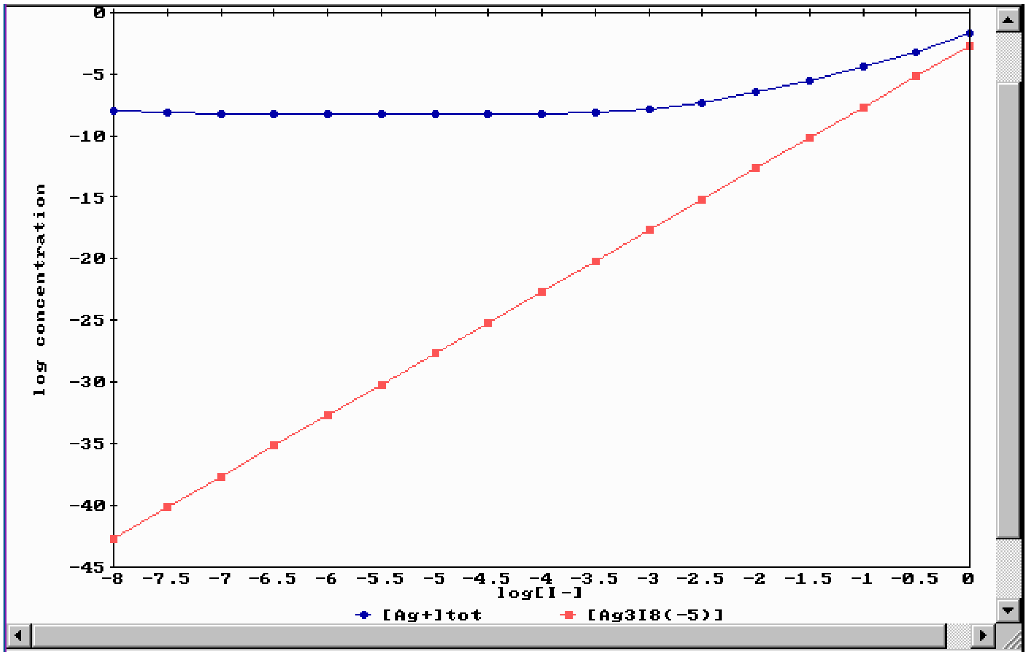

FIGURE 2. TITRATION OF A AG$^+$ SOLUTION WITH I$^-$ SOLUTION (SHOWS EFFECT OF FORMATION OF HIGHER ORDER IODIDE COMPLEXES ON TOTAL DISSOLVED AG$^+$ CONC.); PLOTTED FROM SPREADSHEET 2.

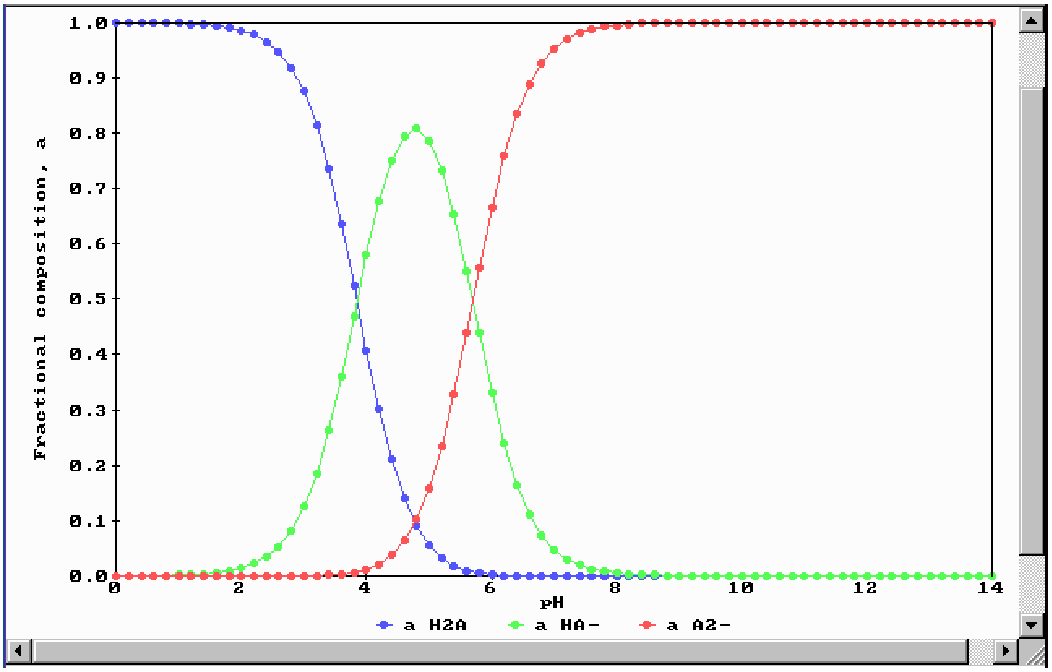

FIGURE 3. FRACTIONAL COMPOSITION DIAGRAM FOR MALONIC ACID (PK_{A1} = 2.847; PK_{A2} = 5.696); PLOTTED FROM SPREADSHEET 3.

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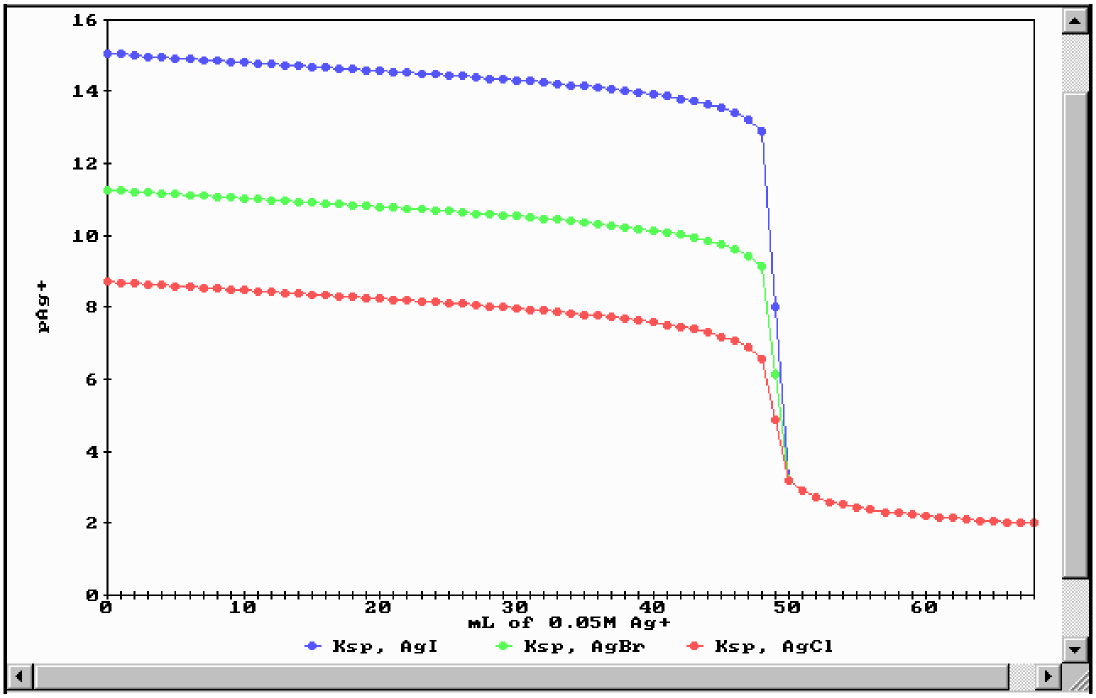

FIGURE 4. TITRATIONS OF 25 ML OF 0.1 M HALIDE SOLUTIONS WITH 0.05 M AG^+ SOLUTIONS (SHOWS EFFECT OF K_{SP} ON AG^+ CONC. AT ENDPOINT); PLOTTED FROM SPREADSHEET 4.

For those students who completed them, the spreadsheet exercises helped to illustrate many of the mathematical relationships presented in Quantitative Analysis. The primary benefit was that the exercises allowed students to generate and manipulate graphs of the relationships, thus, clarifiying them with pictures. Students who completed the exercises reported a greater feeling of involvement in their learning experience and a better comprehension of the problems presented than they received from just looking at graphs reproduced in a textbook. This was supported by the spreadsheeters' improved performances on the test questions that were based on spreadsheet analyses. This occurred in both classes, the one that *recommended* and provided incentive for their use (Fall 1995) and the one that *required* their use (Spring 1996). Although the Fall 1995 data is of limited use because only two students decided to use the spreadsheet exercises, it does provide a method of comparing a non-spreadsheet using class to a class required to complete the exercise. The question, of course, arises as to whether the students in the Fall class (only two) who chose to complete the spreadsheet exercises were simply students who spend more time studying for tests in general, and who would have achieved above average scores regardless of whether or not they had used

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spreadsheets. Other students in the Fall class admitted looking for problems in the chapter, like those presented in the spreadsheet exercises, in lieu of working the spreadsheet exercises themselves. Students appear willing to study a topic if they are certain it will be covered on an examination. The averages from the Spring-1996 class, however, suggest that students who ordinarily might not elect to use the spreadsheets still profit from having the spreadsheet problems assigned. Even though students in that class were required to use spreadsheets, some did not. The data in Table 3 suggests that these students, besides scoring below the class average on the test questions supported by spreadsheets, also scored lower on the entire exam. This result could be construed to demonstrate that these students not only failed to take advantage of the spreadsheet exercises, but also may not have devoted much effort to the course as a whole.

An analysis of the Spring semester student evaluations showed that the students were about two-to-one in favor of retaining the mandatory spreadsheet assignments. Two criticisms from the detractors were: (1) an uncertainty as to what it was they should be learning from the spreadsheets and (2) the possibility of paying little attention to the information in the spreadsheet and just following the instructions on the handout to get it completed. Many in the class were first-time computer users and non-typists. Several students admitted that they had been apprehensive at first about the amount of work that learning to use a spreadsheet would require, but when they found out it was possible, they began to enjoy using the computer. They supported the provision of partially completed spreadsheets because they could focus on learning the concept and setting up the proper formulas, rather than needing that time for constructing the entire spreadsheet. Many students were optimistic that the class had prepared them for later use of spreadsheets in their chemistry courses, and several said that the computer experience better prepared them for employment.

ACKNOWLEDGEMENT

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