A Computer-based, Interactive, Multimedia Software System for Teaching and Independent Student Learning of Liquid Chromatography

Michelle A. Spaziani, Justin T. Fermann, and William J. Vining*

Department of Chemistry, University of Massachusetts Amherst, Amherst, MA 01003-4510, vining@chem.umass.edu

Abstract: This paper describes the design and development of an interactive, simulation-based education software system for the exploration of key concepts in liquid chromatography. Evaluation results of student use of the software will be presented.

Software modules have been designed to supplement, but not replace, classroom and laboratory learning about liquid chromatography, providing students with theory, visual aids, and interactive simulations. Combined with animations and narration, the modules complement the foundation on which chromatography is taught in a general, analytical, or organic chemistry setting. Furthermore, this software allows the student to interact with the illustrated chemistry lessons, which is especially important in instances where the concepts taught transcend typical classroom material.

This work serves to connect what one observes experimentally in a chromatography experiment to changing parameters such as capacity factor, number of theoretical plates, height equivalent of a theoretical plate, column length, resolution, retention time, and selectivity factor. Simulated separations are portrayed in an animated fashion as a chromatogram developing over time as a function of one or more of these variables. Finally, the software has real sample, mobile phase, column type, flow rate, and detection type options allowing the selection and simulation of solving a realistic chromatography problem. Hypothetical unknown mixtures can be separated and the sample components identified after simulating the separation of known samples.

Introduction

As part of a process of effective curriculum development, innovation, and implementation, this paper describes the design of an interactive, multimedia-based education software system for the exploration of key concepts in liquid chromatography, entitled *Chemland Interactive Analytical Chemistry: Liquid Chromatography*. This work is part of a broader effort to provide engaging software helpful at all levels of chemical education and covering all topical areas throughout the undergraduate curriculum.

Developed for the student, the software serves to improve the quality of chemical education as it encourages students to think like chemists, it promotes critical thinking by offering discovery-based instruction, and illustrates theory on a molecular or near-molecular scale. In addition, the combination of tutorial, student-tool, and simulation formats allows for the connection of chromatographic experimental observations to theory, and provides students with access to realistic applications of liquid chromatography via simulations. It has been shown [1, 2] that there is a greater degree of understanding and retention of material when there is significant interaction between student and software.

This software covers fundamental aspects of chromatography theory, including topics such as capacity factor, number of theoretical plates (N), height equivalent of a theoretical plate (H), column length (L), resolution, retention time, and selectivity factor. Simulated separations are portrayed in animated fashion as a chromatogram developing over time as a function of one or more variables. The program contains real sample, mobile phase, column-type, flow-rate, and detection-type options that allow the selection and simulation of realistic chromatography experiments. Hypothetical unknown mixtures can also be separated and the sample components identified after simulating the separation of known samples. Although best suited for analytical and organic chemistry courses, our software is germane to other subdisciplines and to general chemistry.

The recent explosion in the production of computer-assisted instruction (CAI) [3–7] warrants this work a timely development. A cursory literature search of the past two decades shows the prominent influence of CAI not only in chemistry, but also in biology, physics, nursing, and medicine. *Chemland Interactive Analytical Chemistry: Liquid Chromatography* is intended to be an especially interactive and multimedia-based software program; it is intended to support linking of molecular, laboratory, and symbolic (e.g., a chemical equation) levels of understanding to better relate experimental observations to imagined molecular structures and chemical events. Similar to the original *Chemland* [6], it is intended for independent use (a stand-alone package) or as a teaching tool to be used in class.

At the University of Massachusetts Amherst, CAI is becoming widely incorporated into a number of courses. Since the University is one of many institutions that does not have the personnel to provide truly individual attention to all students, the adoption of this learning tool into the curriculum has proven to be an excellent addition that makes individualized self-paced instruction available to more students.

Clearly, a CAI-based program must be tested for it to be considered effective and subsequently useful. Evaluations also assist educators regarding the purchasing of a product or the classroom implementation of a program. Formative

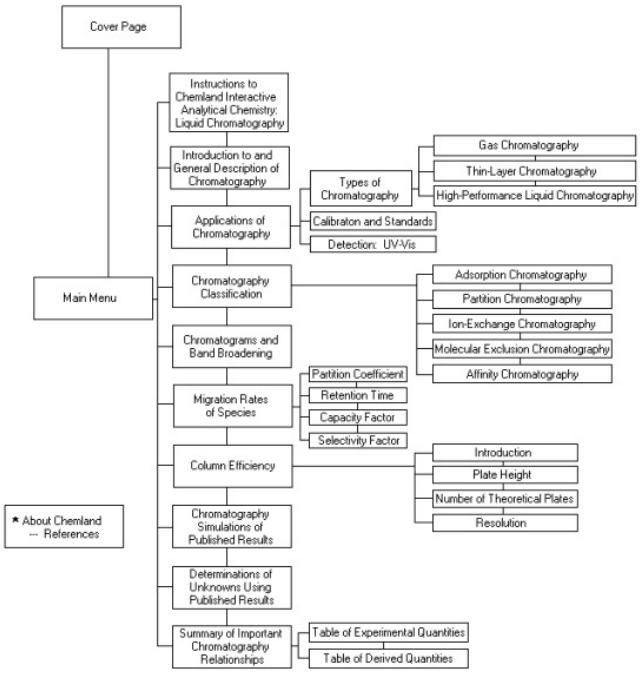

Figure 1. Map of software screen links.

Table 1. Simulations and Animations Available in Chemland Interactive Analytical Chemistry: Liquid Chromatography

Simulations	Animations
Introduction to and general description of chromatography	Applications of chromatography
Partition coefficient	Types of chromatography: gc
Retention time	Types of chromatography: tlc
Selectivity factor	Adsorption chromatography
Plate height	Affinity chromatography
Number of theoretical plates	Ion-exchange chromatography
Resolution	Molecular exclusion chromatography
Chromatography simulations of published results	Partition chromatography
Determinations of unknowns using published results	Chromatograms and band broadening

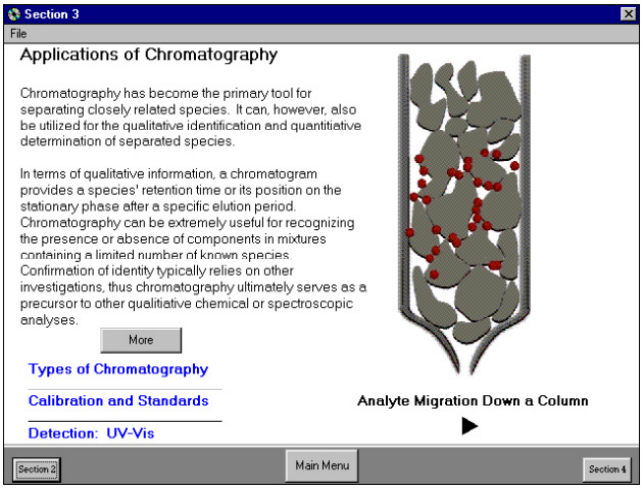

Figure 2. An animation of analytes migrating down a column in *Applications to* Chromatography (Section 3).

evaluations by faculty and students have been utilized to guide the project; the results of summative evaluations of student use will be discussed here. Both qualitative and quantitative measures have been employed in the evaluation process.

Software Design and Description

Chemland Interactive Analytical Chemistry: Liquid Chromatography is composed of 13 main interactive modules of text, animations, narration, and simulations. The entire program is implemented in the 32-bit version of Microsoft Visual Basic 4.0; the animations were created using MetaCreations Infini-D, Adobe Photoshop, and Adobe After Effects, and converted to Apple's QuickTime format. The software runs under Microsoft Windows 95, 98, and NT, and is packaged on CD-ROM. World Wide Web users may download the 9-MB software installation file from the author's research group's web page: http://soulcatcher.chem.umass.edu (supporting file 46wv3897.zip). Major computer requirements include: a 486 DX processor or above, 20 MB of free hard drive space, at least 8 MB RAM, and if installing from disc, a CD-ROM drive. The software runs best using a high-color-resolution video card. A sound card is not required but highly recommended.

Our general approach to designing this software was to present a unified view of a chromatography concept that made effective use of the animation and simulation tools available to a computer program. We have attempted to use these more interactive and visual presentations to support more standard text and mathematical treatments. The order of presentation and mathematical treatments presented here are not novel.

The software contains 10 sections consisting of a total of 31 "screens." The sections are designed to introduce the student to some part of chromatography theory or to the use of chromatography. Within each section, screens may be accompanied by a simulation or an animation to highlight the concept or theory. A map of the main screen links is shown in Figure 1; a list of features is presented in Table 1.

The *Main Menu* provides structure to the software and serves as the main link to all ten sections. Navigating through the software in a logical and sequential order, the student moves from the *Main Menu* to *Instructions*, and subsequently to Section 2. Important definitions and the basics of chromatography are presented in the *Introduction to and General Description of Chromatography*. A simulation of a separation with concentration variables for two species is also available, which allows the student to view a column chromatography simulation and the resulting chromatogram early on. We believe it important for the student to be able to interact with a simulation early in their use of the software, and chose to allow them to vary the concentration of each eluting species. This serves to familiarize them with use of the interactive portions of the software while considering a factor understandable to students at all levels.

Applications to Chromatography details the quantitative and qualitative uses of chromatography. An animation of analyte migration down a column (Figure 2) accompanies the text. Descriptions, animations, and block diagrams of three common types of chromatography (gas chromatography, high-performance liquid chromatography, and thin-layer chromatography) are also accessible from this screen, as are

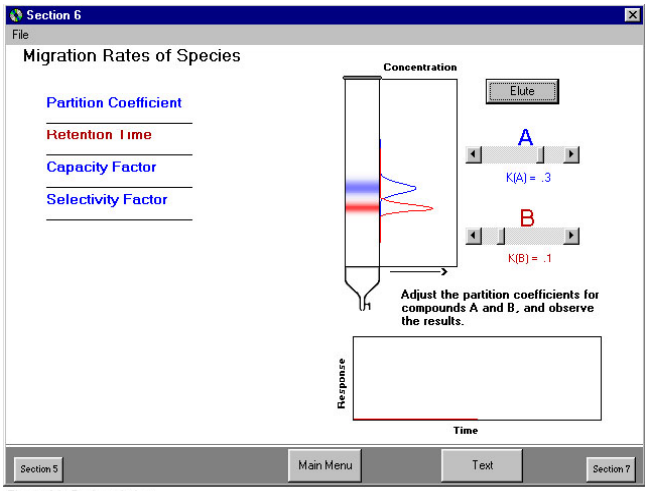

Figure 3A: During elution.

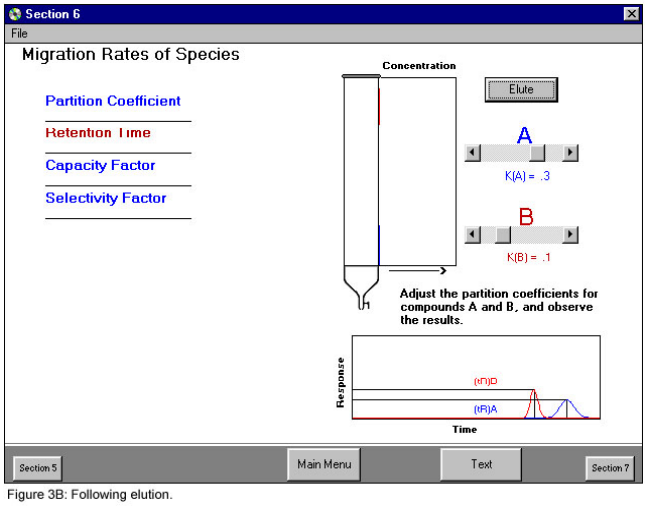

Figure 3B: Following elution.

Figure 3. A simulation from *Resolution* (Section 6). Students vary partition coefficients for two species, A and B, to observe differences in resolution. (a) Analyte migration down the column, during elution. (b) Chromatogram with retention times, following complete elution.

brief introductions to calibration and standards and UV-vis detection.

Chromatography Classification illustrates adsorption, partition, ion-exchange, molecular exclusion, and affinity chromatography; a narrated animation accompanies the text for each class, giving a molecular scale interpretation by which each separation takes place. A description of band broadening and a chromatogram are available in *Chromatograms and Band Broadening*. Gaussian, overloading-the-column, and tailing peak shapes are shown, along with a Gaussian peak animation.

Migration Rates of Species presents four major parameters generally used when discussing rates: partition coefficient, retention time, capacity factor, and selectivity factor. Simulations highlighting the effects of partition coefficient, retention time, and selectivity factor are available where the variables are the concentrations of two species, A and B. Figure 3 illustrates how this works. Students set the partition coefficient for the compounds, A and B, and press *Elute*. Figure 3A shows the result of the elution procedure part way through. The red and blue constituent species separate and broaden as they move down the column. At the same time, a chromatogram is drawn in the chart in the lower right of the screen. The results of the elution experiment are viewed in the chromatogram displayed in Figure 3B.

An introduction to plate theory and the relationship between plate height, number of theoretical plates, and column length is presented in a section on *Column Efficiency*. This precedes simulations for plate height, the number of theoretical plates, and resolution.

The *Chromatography Simulations of Published Results* section allows students to simulate real chromatography experiments based on literature data [9–13]. Students can choose pairs of compounds from three categories—nucleic acid components, amino acids, and tyroxines—and vary the mobile phase, column type, flow rate, and detection type. The partition coefficients for both species, A and B, and the selectivity factor are calculated and shown for the chosen set of experimental conditions. A chromatogram results from which students can observe the differences in response as a function of changing one or more of these variables.

Determinations of Unknowns Using Published Results corresponds to the simulations section. In this section, however, students explore the conditions for separating eight known compounds to enable them to identify components in unknown mixtures. Four mobile-phase choices are available; arbitrary retention times are given on the resulting chromatogram.

Finally, a summary of mathematical relationships is shown in the *Summary of Important Chromatography Relationships*. Derived quantities and experimental quantities are presented.

Evaluation Results

Both quantitative and qualitative measures have been employed for preliminary testing of our work. Our primary evaluation objective included evaluating students in terms of their understanding of the material presented in the software. Their attitude toward using the software set has also been assessed. An initial test of the software was performed by a second-semester general chemistry class (taught by one of the authors). The class used the software during one 50-minute class period. The students were led through specific sections and generally worked in pairs. This class performed well on a content-based quiz and liked the software, but our overall analysis of this group was flawed by providing inadequate time for students to use the software and answer quiz questions. Data from a second group, Population B, are therefore presented here. There was no control group in this testing. The results, however, will serve as a point of comparison with similar future assessments of student populations.

Population B consisted of students attending a six-week, second-semester general chemistry summer class (not taught by the authors). These students received a mini-lecture (approximately 30 minutes) on chromatography and then performed the first of two parts of a paper chromatography laboratory experiment prior to using and evaluating the software. These students had access to the software outside of class. Forty-nine students (n = 49) completed the evaluation assignment. Of these students, 7% were freshmen, 18% were sophomores, 43% were juniors, and 21% were seniors. Eleven percent did not indicate their present level of college education. Summer class sections have traditionally had more

Table 2. Population B: Results of the CKQ 112-1

CKQ 112-1 Question Number	Percentage of Students Responding Incorrectly (%)
1	6.4
2	31.9
3	10.6
4	46.8
5	55.3
6	27.7
7	34.0
8	12.8
9	57.4
10	14.9

Table 3. Population B: Results of the ATSP

Statement	Average Rating (SD)
The instructions and objectives are clear in *Chemland Interactive Analytical Chemistry: Liquid Chromatography*.	$2._7$ ($1._4$)
The animations and visual aids are useful in describing chromatography experiments and understanding the theory.	$2._0$ ($1._2$)
The simulations are useful in describing chromatography experiments and in understanding the theory.	$1._9$ ($1._2$)
This is a good learning device.	$2._1$ ($1._3$)
The simulations have prepared me for experimental studies in the laboratory.	$3._1$ ($1._5$)
This is a highly interactive software program.	$2._7$ ($1._4$)

upper-class students enrolled than the more traditional fall and spring semester sections.

The quiz given to Population B (CKQ 112-1) is presented in the Supporting Material (46wv1897.pdf). The quiz consists of ten multiple-choice questions, each worth one point. Questions were developed directly from the text, animation, movies, and simulations in specific sections of *Chemland Interactive Analytical Chemistry: Liquid Chromatography*, and did not relate to the material students learned in laboratory.

Forty-seven students completed the evaluation process. The class mean for Population B is $7._1$ with a sample n–1 weighted standard deviation of $1._7$. The percentages of students responding incorrectly to each question are presented in Table 2.

Overall, students from both populations scored well on the content knowledge quiz, scoring about as well or slightly better on this section of the course as on other lecture-based assessments. Clearly, Questions 4, 5, and 9 gave the students the most difficulty. Questions 4 and 5 required critical thinking. In addition, Question 4 required more than one answer to be selected, and poor performance on this question could be due to student carelessness. Question 9 was difficult and rather tricky, requiring students to perform multiple experiments to determine the answer. Thus most students answered it partly or entirely incorrectly.

An in-house-developed questionnaire to examine students' attitude toward a simulation program (ATSP) followed the review of the software and the completion of the CKQ. The ATSP consists of six questions and uses a seven-point scale; the results are presented in Table 3.

Overall, data from the ATSP questionnaire show that students had positive reactions to the software. The animations, visual aids, and simulations were well-liked, and most students indicated that the program was a good learning device. From these results, it is also obvious that some students felt the instructions and objectives were not as clear and the modules not as *highly* interactive as they could be. On a scale of 1 to 7, where a score of 1 indicates agreement with the statement and a score of 7 indicates disagreement with the statement, students reported that the animations and visual aids are useful in describing chromatography experiments and in understanding the theory ($2._0$); the simulations are useful in describing chromatography experiments and in understanding the theory ($1._9$); the software is a good learning device ($2._1$). The weakest aspect of the software's performance came in students' confidence that the simulations have prepared them for experimental studies in the laboratory ($3._1$). This is not surprising given that the software is intended to support *interpretation* of experimental results and trends, and is not aimed at teaching students as to how to obtain those results (which is more properly introduced in the laboratory).

Conclusion

The design and development of a complete, unified, interactive, and simulating computer-based education system for the exploration of key concepts in liquid chromatography has been described. Student and faculty evaluations indicate that this work is accurate, effective, and useful in chemistry classroom and laboratory settings. Software education systems such as this are intended to pave the way for easy implementation of innovative methods in academia. By and large, our intention is to continue developing computer-assisted, interactive, multimedia-based instruction for analytical chemistry classrooms, laboratories, and independent student learning. Current work aims at expanding upon existing programs, while designing new software for the many areas in chemistry for which interactive, multimedia-based computer software should be developed. It is worth noting that students' attitudes about how software of this type should be used agree with those of the authors; simulations are useful in supporting conceptual understanding, but not as a replacement for laboratory work.

It is our intent to facilitate introduction of these materials into the curriculum; a detailed set of Instructor's Notes is available in the Supporting Material (46wv2897.pdf). The Instructor's Notes contain installation instructions, suggestions for use of the software both in and outside of class, and a set of 17 potential quiz questions with an accompanying answer key.

Information

For more information on chemical education-based research at the University of Massachusetts Amherst, please refer to the World Wide Web page for the Chemistry Higher Education Workgroup (C.H.E.W.): http://soulcatcher.chem.umass.edu. Most software projects produced by C.H.E.W. are available free of charge and may be downloaded from this site.

Acknowledgment. The authors thank the University of Massachusetts Amherst for research funding, and M.A.S.

acknowledges financial support from the Department of Chemistry and Graduate School in the form of travel grants. In addition, we are grateful to Eric S. Wojtaszek for creating the animation sequences and to Kathy Tobiassen for narrations used in the program. Lastly, we acknowledge our evaluators for their time and interest.

References

1. Treadway, W. J., Jr. *J. Chem. Educ.* **1996,** *73*, 196–198.
2. Moore, C.; Smith, S.; Avner, R. A. *J. Chem. Educ.* **1980,** *57*, 19–198.
3. O'Haver, T. C. *Anal. Chem.* **1991,** *63*, 521A–534A.
4. Pontin, J. A.; Aricó, E.; Filoho, J. P.; Tiedemann, P. W.; Isuyama, R.; Fettis, G. C. *J. Chem. Educ.* **1993,** *70*, 223–226.
5. Bragin, V. M. *J. Chem. Educ.* **1996,** *73*, 747–748.
6. Smith, S.; Stovall, I. *J. Chem. Educ.* **1996,** *73*, 911–915.
7. Tasker, R. F.; Chia, W.; Bucat, R. B.; Sleet, R. *Chem. Aust.* **1996,** *63*, 395–397.
8. *CRC Handbook of Chromatography: General Data and Principles*, Vol. 1; Zweig, G.; Sherma, J., Eds.; CRC Press: Boca Raton, FL, 1972; pp 179, 181, 182, 249.
9. DeBersaques, J. *J. Chromatogr.* **1967**, *31*, 222–223.
10. Zadrazil, S.; Sormova, Z.; Sorum, F. *Coll. Czech. Chem. Commun.* **1961**, *26*, 2643–2650.
11. Woof, J. B.; Pierce, J. S. *J. Chromatogr.* **1967**, *28*, 94–103.
12. Blasi, F.; DeMasi, R. V. *J. Chromatogr.* **1967**, *28*, 33–36.
13. Eaker, D.; Porath, J. *Sep. Sci.* **1967**, *2*, 507–550.