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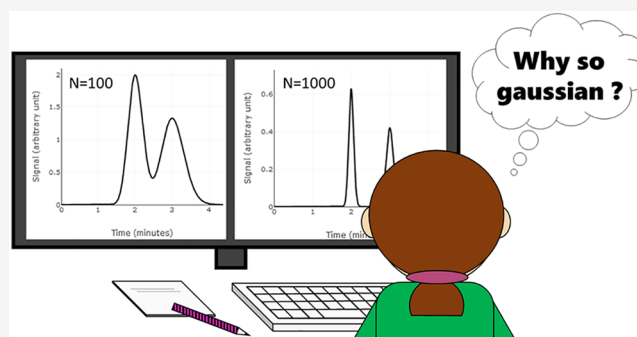
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Interactive Web Application as a Teaching Tool to Introduce Basics of Chromatography and the Plate Theory

Lars Petter Jordheim, Anne Denuzière, Christelle Machon, and Wael Zeinyeh*

ABSTRACT: The understanding of the basic principles of chromatography is of high importance for chemistry, pharmacy, and biology students. In this paper, we present a free web application which can be used as a teaching tool to introduce chromatography to undergraduate students, using one of the simplest chromatography models: the plate theory.



KEYWORDS: First-Year Undergraduate/General, Analytical Chemistry, Computer-Based Learning, Internet/Web-Based Learning, Chromatography, HPLC

■ INTRODUCTION

Computer-based teaching tools continue to gain popularity among chemistry students and teachers, especially after most universities moved toward distance learning during the COVID-19 pandemic. Within our team, we have already developed and published a pedagogical web application concerning Fourier transformation in NMR spectroscopy in this *Journal*.¹ Here, we present another web application intended for the introduction of the principles of chromatography based on the plate theory.

Chromatography occupies an important place in the teaching of analytical chemistry, whether for future chemists, or for pharmacy and biology students. In order to introduce chromatography, most courses and manuals in analytical chemistry use the plate theory as a starting point. This theory was first applied to chromatography by Martin and Synge, the inventors of liquid/liquid chromatography,² and was the first theory used to explain chromatographic separation and to predict the shape of chromatogram peaks. Despite its approximations, and the development of more sophisticated models, the plate theory continues to be widely used as a theoretical introduction to chromatography, and notions derived from this theory, such as the number of theoretical plates of a column, are still commonly used in chemical analysis laboratories.

Several scientific publications have proposed software or Excel spreadsheets as tools to assist chemists in their use of chromatography. Some of these publications present simulation software destined to help advanced students, as well as skilled chemists, to optimize chromatographic separations.^{3,4}

Consequently, we do not believe that these software applications are suitable for an introductory course to undergraduate students.

Among the applications intended for pedagogy, two caught our attention. The Excel spreadsheet developed by Kadjo et al.⁵ offers a demonstration of chromatographic separation using an automated plate-theory-based approach. It also allows modeling more complex profiles, as gradient elution, or nonlinear isotherms. Another interesting approach is the applet developed by C.E. Efstathiou⁶ which simulates compound separation and chromatogram progress at the column output. Nevertheless, we believe that neither of these two applications fully meets our goals. Both applications lack several features that we consider essential in order to use the software as a teaching tool. These features are listed in the next section.

■ SOFTWARE

We describe here a web application (Figure 1) developed within our team which satisfies the following specifications:

- It is free and open-source and does not require proprietary software (like Microsoft Excel which might

Plate number	Compound 1		Compound 2	
	Stationary phase	Mobile phase	Stationary phase	Mobile phase
14	≈ 0	≈ 0	6.91	1.73
15	0.02	0.02	4.82	1.20
16	0.05	0.05	3.05	0.76
17	0.12	0.12	1.76	0.44
18	0.24	0.24	0.93	0.23
19	0.47	0.47	0.45	0.11
20	0.85	0.85	0.20	0.05

Auto-scroll the table

Push mobile phase Reset

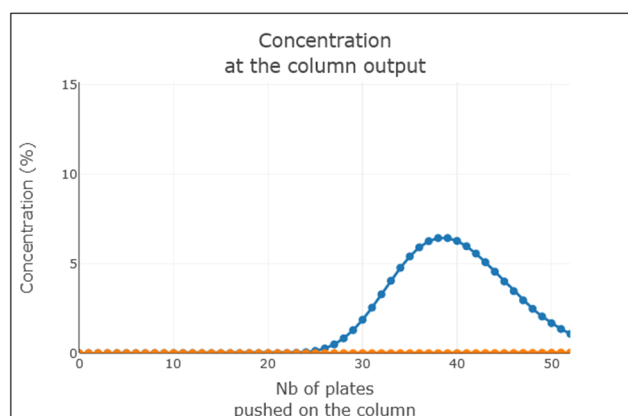
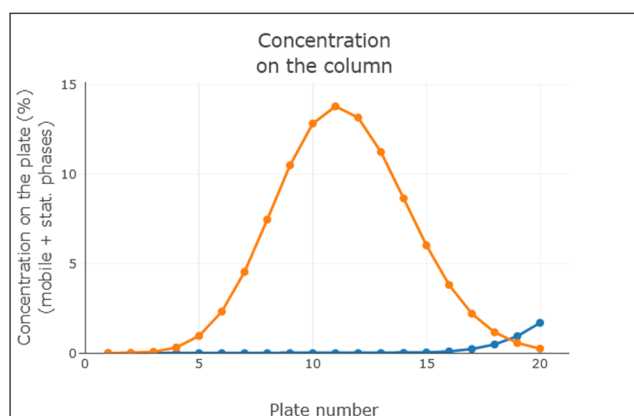


Figure 1. Screen capture of the web application running on the Mozilla Firefox browser. Shown are the equilibration table explaining the distribution of analyte concentrations between stationary and mobile phases during chromatography, and its graphical representation.

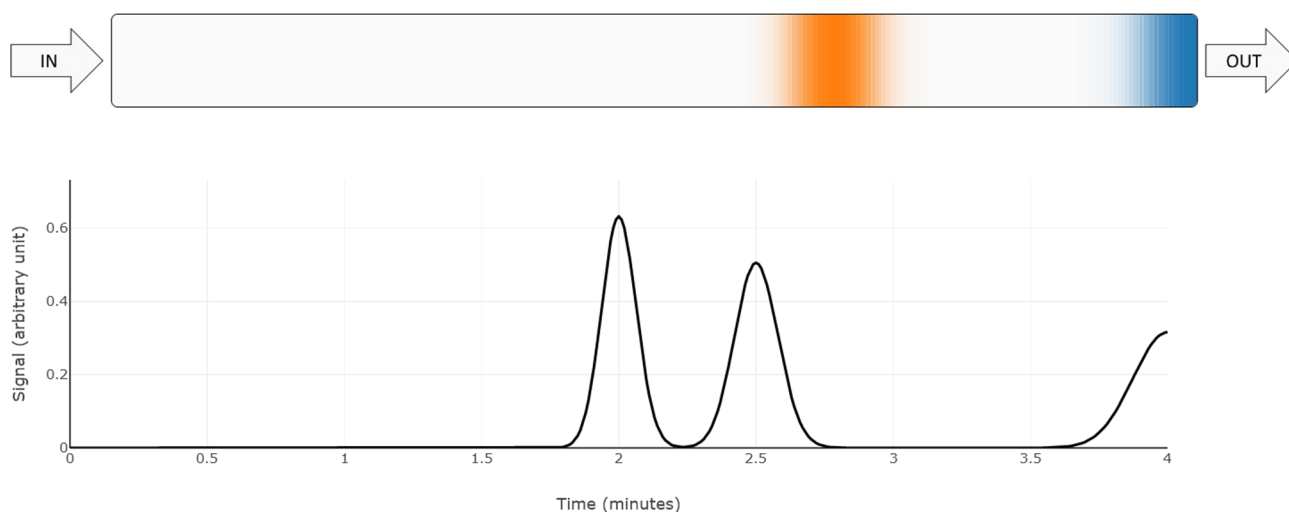


Figure 2. Example of a chromatogram generated by the application with four studied compounds. Two compounds have already left the column, and a third one (in blue) is leaving.

- not be accessible to all students) or any other installation.
- It is adapted to personal computers, as well as tablets and mobile phones, which allows its use during the course by teachers and students.
- It allows a step-by-step demonstration of the plate theory through an equilibration table which is easily commanded by the student by clicking a button.
- It offers a chromatogram simulation, with readily measurable peak parameters (retention time and peak

width) thanks to graduated time and signal axes (Figure 2).

- Most of the parameters can be changed by the student, like the number of compounds, the partition coefficients, the number of theoretical plates, the column volume, and the mobile phase flow rate.

The code is written in JavaScript and is available on Github.⁷ Details of the calculations used in the software are provided (Supporting Information, Part B). French and English versions of the application are already available, but other versions can be created by translating the texts in the available source code. The web application was tested with most modern internet browsers on computers and mobile devices⁸ and can be run from the following address: <https://sites.google.com/view/chimie-analytique-pharma-lyon/web-apps>.

■ EDUCATIONAL BENEFIT

The software is intended for students following introduction courses in chromatography. We believe that the limits of the plate theory make it unsuited for advanced analytical chemistry students for which the van Deemter equation, or other more sophisticated models, would allow more precise answers.

Our initial teaching experience with the software was obtained with second year pharmacy students without any practical knowledge about chromatography. It was first presented briefly during a lecture on liquid chromatography introducing various theories including the plate theory. Then, we integrated it in an exercise about qualitative parameters of liquid chromatography (Supporting Information, Part A) that was used in online teaching with groups of students (10 times 20–25 students). Students managed to easily implement data in the correct parts of the software on the basis of the provided text. Students answered a questionnaire after using the software, and the survey showed that they were satisfied with it overall (Supporting Information, Part C). From the teachers' point of view, we believe the understanding of theoretical aspects of chromatography (distribution of analytes between phases, notion of plates, how a chromatogram is obtained and drawn) was better assimilated by students and more easily explained by teachers when using this tool as compared to our experience from previous years. Moreover, students were more independent during the following laboratory work concerning the management of the sample injections and the end of each analysis. For instance, we noticed that students less frequently made the mistake of injecting a sample in the HPLC instrument before all compounds from the previous injection had left the column.

■ CONCLUSION

This application has been shown to be usable by chromatography-naïve students, and we believe there is an added value of implementing it in problem-solving such as for the proposed exercise. The possibility to change the number of compounds together with their relative polarity, as well as the characteristics of the chromatographic column, allows students to evaluate the impact of these parameters on the retention, distribution, and separation during an experiment of liquid chromatography.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at <https://pubs.acs.org/doi/10.1021/acs.jchemed.1c00314>.

Example of exercise used with the application, details of calculations used in the application, and a survey of students' opinion (PDF, DOCX)

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Notes

The authors declare no competing financial interest.

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(7) <https://github.com/waelzeinyeh/PlateTheory> (accessed Mar 2021).

(8) Please note that the application will not run on Internet Explorer, which is outdated and no longer supported by Microsoft Corp.