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A Comprehensive Application To Assist in Acid−Base Titration Self-Learning: An Approach for High School and Undergraduate Students

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Ⓢ *Supporting Information*

ABSTRACT: Currently, there are a number of educational applications that allow students to reinforce theoretical or numerical concepts through an interactive way. More precisely, in the field of the analytical chemistry, MATLAB has been widely used to write easy-to-implement code, facilitating complex performances and/or tedious calculations. The main objective of this research is to present an ad hoc open MATLAB code toolbox, named AChemTitri, aimed to construct acid−base titration curves in an interactive format. The software has been designed by the means of pop-up windows where students only need to be acquainted with a basic or elementary knowledge of MATLAB. With this application, students will be able to practice with comprehensive titration options such as the titration of strong, weak, or polyfunctional acids and bases and, for each titration, different concentration of each compound as well as the titration volume can be selected. As a result, the software plots the titration curve (pH vs volume) and the first and second derivative of this former curve as well, together with the numerical results. Thus, students will have the opportunity to calculate the final point and pH of the titration graphically and numerically. In addition, concentration diagrams are also displayed (log of the species participating in the titration vs pH); thus, it will be easy to follow how the acid−base titration is progressing. In conclusion, this application is a feasible way to improve the basic concepts of acid−base titration throughout the practice of numerical exercise assisted by computer calculation. The possibility of changing all the chemical parameters and the graphic visualization of results could ease the learning process of students facing the titration concepts for the first time.

KEYWORDS: *Analytical Chemistry, First-Year Undergraduate/General, Computer-Based Learning, Distance Learning/Self Instruction, Acids/Bases, Inquiry-Based/Discovery Learning*
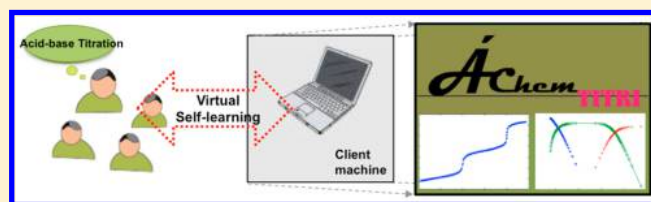
INTRODUCTION

Chemical equilibrium in general and acid−base equilibrium in particular play a major role in chemistry education. It is a fact that acid−base chemistry is and has been a common feature in general chemistry curriculum for a number of years. Also, titration curves have been traditionally the most common approach to understand acid−base equilibrium, both in theoretical and practical approaches. The teaching of titration curves has been lately a controversial topic among the teaching communities; however, so far, in 2014 it is contemplated in the curriculum in many universities and even in the last year of high school education.

Harris[1] and Hawkes[2] maintained an interesting correspondence, published in the *Journal of Chemical Education*, in the frame of "what textbooks should contain" and what chemistry teachers should teach. This conversation reflects well the two main positions of teachers with regard to titration curves. Among the teaching communities, there are defenders[1] and detractors[2] at

teaching calculation of titration curves to undergraduate students. Harris[1] supports the inclusion of acid−base titration curves in analytical chemistry textbooks, as well as its teaching in class. This author claims the value of learning the theory beyond titration curves, in spite of the fact that most chemists will not bring titrations curves into practice. He defends that studying titrations curves will make students learn chemical equilibrium. Titration curves are normally studied by breaking them into regions, i.e., initial point, before equivalence point, at the equivalence point, and after equivalence point, and the knowledge of proper chemical processes taking place in each region will provide students a better understanding of chemical equilibrium. For instance, it would be a wise way to understand how buffers work. He also states the usefulness of titration curves in the calculation of equilibrium constants.[3] Some authors defend

A

as well the usefulness of titration curves to aid in the selection of the right indicator.[1,4]

Harris stated that the performance of buffers can be understood through titration curves. Under this point of view, buffer capacity has to be understood like the variation of pH with the volume of titrant. Thus, a simple look at titration curves of polyprotic acid or base would allow students to locate the maximum buffer capacity of a given buffer. The intermediate form of a diprotic acid is sometimes considered las a buffer since it always has a pH $\approx (1/2)(pK_1 + pK_2)$; however, just by looking at its titration curve it would be easy to understand that it presents a minimum buffer capacity.[1]

On the other hand, Hawkes[2] is not in complete agreement with teaching titration curves calculation. He defends focusing teaching on more "needed knowledge". He states that confusion could be created in "sub-average" students, for instance, when relating buffers to titrations. He claims that calculating titration curves is a complicated way to understand buffers and is unneeded to choose the right indicator. In his opinion, equilibrium calculations have been in general overemphasized in the curriculum.[2,5] It has been reported by this author in his 10 peer-reviewed publications that the standard curriculum for introductory chemistry includes much that is valueless and even misleading and does not reflect the needs of students. He proposes a revision of the curriculum taking into account the real needs and interests of students and states that prestigious organizations such as The International Union of Pure and Applied Chemistry (IUPAC) or the American Chemical Society (ACS) should lead the change.[5]

The usefulness of computer-assisted experiments and the so-called virtual laboratories for acid−base teaching has been recently reported by Hernández-Espinoza and Astudillo-Saavedra.[6] Hernández and Czerwinska demonstrated applicability of applicability of an online module to teach key concepts within acid−base such as hydrolysis of salts, conjugate acids and bases, and strength of acids and bases.[7] Different examples of computer generated acid−base titration data and curves can be found in the related literature.[8,9] However, probably the most related background to our work, in the field of computer-generated acid base titration curves, is the one recently published by Smith et al.[10] enabling the generation of 3-D surfaces to visualize how pH behaves during titration and dilution procedures. Nevertheless, in this article, equimolar concentrations of the target species and titration agent are always considered, while with "chemistry", those variables can be freely varied, giving rise to a more open and general view of the influence with all the involved variables.

In this article, the application "AChemTitri" is presented as a tool aimed to assist students in the learning process of acid−base titration. The application is framed in MATLAB and it has been designed to be used by means of pop-up windows where the final user only needs to have basic or elementary knowledge of MATLAB. The benefits of using new technology tools to promote learning have been already proved. In fact, the current virtual courses using collaborative web tools such as aLF, Moodle, or WebCT are already used in most universities and educational institutions.[11] Beside these web tools, the implementation of user-friendly coding systems and interactive e-Learning or m-Learning applications allows instructors to develop ad hoc pieces of software or applications to reinforce the concepts that students have already learned from textbooks or lectures, especially in those subjects with sophisticated contents of mathematical calculations applied to chemical data.[12,13] The benefits of these e-learning methodologies include the means for creation of motivational environments significantly enhancing students' meaningful learning. Different reported studies[14,15] indicate that students achieve better comprehension, retain the information longer, and enjoy classes more effectively when e-learning methodologies are employed, empowering and enhancing their construction of a more cohesive understanding with the interconnected facets of a discipline.

"AChemTitri" has been conceived to be useful for students at different levels and with different degrees of knowledge in the study of acid−base equilibria and titration curves. When the main objective is to teach calculation and drawing of titration curves, "AChemTitri" can be used by the students as excellent feedback to their calculations and plots. On the other hand, the application can be also employed in a more holistic way since titration curves under different experimental conditions can be produced for the further study of the influence of the main variables. This second practice is intended for a more critical and practical interpretation of titration curves through the actual influence study of the involved variables, namely, the nature of the titrant and the problem to be titrated, initial volume of problem solution and relative concentrations of titrant agent and target species.

■ BACKGROUND

Educational Framework

Acid−base titration can be taught by using different approaches. In the most traditional procedures, teaching relies primarily on passive-student lectures with algorithmic-problem exams. Occasionally, scripted lab classes follow theoretical titration lectures, where students have the chance to practice their observational skills and make links between theory and practice.[16] In contrast, inquired-based learning (IBL) puts emphasis on the learner as an active agent in the process of knowledge acquisition. With the use of IBL,[17] students have the opportunity to practice how scientists do science, in this way acquiring a significant learning of the chemistry key concepts, as it is the acid−base titration. On the other hand, the use of computer technologies in science education has been extensively reviewed. For instance, Rutten et al.[18] mentioned in their review that the use of computational tools in the science classroom has the potential to generate higher learning outcomes,[19] since students have the chance to do authentically inquiry activities. Besides, with the use of computational tools in science teaching, students can explore hypothetical situations, interact with a simplified version of a process or system, change the time-scale of events, and practice task and solve problems in a realistic environment without stress.[18] Thus, motivated by this teaching methodology, in this research, we propose an acid−base titration computer application used in IBL methodology as acid−base titration lab simulator. Thus, to work with this application, each group of students will have a real-case titration experiment, where they will be asked to find the answer through the experimentation with the application. Typical examples could be the study effect of the experimental conditions, such as the initial volume of the acid/base to be titrated, chemical concentrations, and acid or base dissociation constant.

Software Description

To achieve the teaching aims established before, an innovative computer application was developed in MATLAB environment. The application, named "AChemTitri", has been designed to provide students with a powerful tool that will allow them to understand through the self-practice and experimentation with the main concepts of acid−base titration. AChemTitri is a group

Figure 1. This figure represents the main screen of the application AChemTitri (undergraduate view). This main screen is divided into three sections: in the first section ("Check before start"), the student will have access to practical information such as video tutorials or theoretical contents; the second section ("Titration curves") constitutes the main part of the application and is dedicated to the titration calculations; and, finally, in the third section ("Post-task survey"), an online survey is implemented to evaluate the usability of the software.

of MATLAB text-code files that are freely available from the authors upon request. The targets of this application are both senior high school students and undergraduate students in science. To switch from one mode to the other, users will need to select the proper option in the main menu (Figure 1). (Video tutorials on how to use AChemTitri are available as Supporting Information.)

In both cases, the application has three sections: check before start (section one), titration curves (section two), and post-task survey (section three). The first and third sections are common for both types of users. The first section ("Check before start") contains practical information about the application, like the user guide, theoretical contents, HTML-5 multimedia tutorial and online questionnaires, in order to assess whether the user is ready to use the application in order to have significant learning. The other common section ("Post-task survey") is dedicated to survey the overall experience with this application, where users are allowed to comment or submit feedback in order to improve future versions of this application. The "Titration curves" section contains the different scenarios where students might practice and learn about pH titration curves. High school students will be able to titrate strong acid/base with a strong base/acid or a weak acid/base with a strong base/acid. Undergraduate students will be additionally able to titrate polyfunctional acid/base with strong base/acid and also the undergraduate student view includes more sophisticated experiments related to the concentration/dilution influence in the titration curve (Figure 2).

To construct the titration curve, users first need to decide the type of solution to titrate (strong acid/base, weak acid/base or polyfuntional acid/base), its concentration (expressed as molar) and the initial solution volume. After making this first selection, students will have to select the concentration of the acid/base known solution. Once all variables are selected, the application shows the result of titration curve (pH vs known solution volume of titrant); in addition, students might have the possibility to plot the first and second derivative in order to get some graphical assistance for selecting the equivalence point (Figure 3).

In the case of polyfunctional acid/base in the results windows the concentration diagram is also plotted. This concentration diagram represents the evolution of the concentration in all chemical species involved in the titration. In addition, the numerical results of the equivalence point (strong or weak acid/base) or equivalence points (polyfunctional acid/base) and equivalence pH are also displayed in the results windows (Figure 4).

At this point, it is possible to change all experimental conditions, the identity of the weak or polyfunctional acid/base and the concentration of the known acid/base solution. Finally, the last option displayed in the undergraduate students view is the "acid/base advance studies". Here students will have the chance to experience how the titration curve is affected by the solution concentration. The users will be able to observe in the same plot up until five different concentration scenarios and therefore will have the possibility to study the different titration curves as well as the concentration diagrams (see detail in Figure 5).

Figure 2. Close-up view of pop-up windows that support students will have to carry out a titration of a weak acid (A) or a simultaneously comparison of different experimental conditions (B).
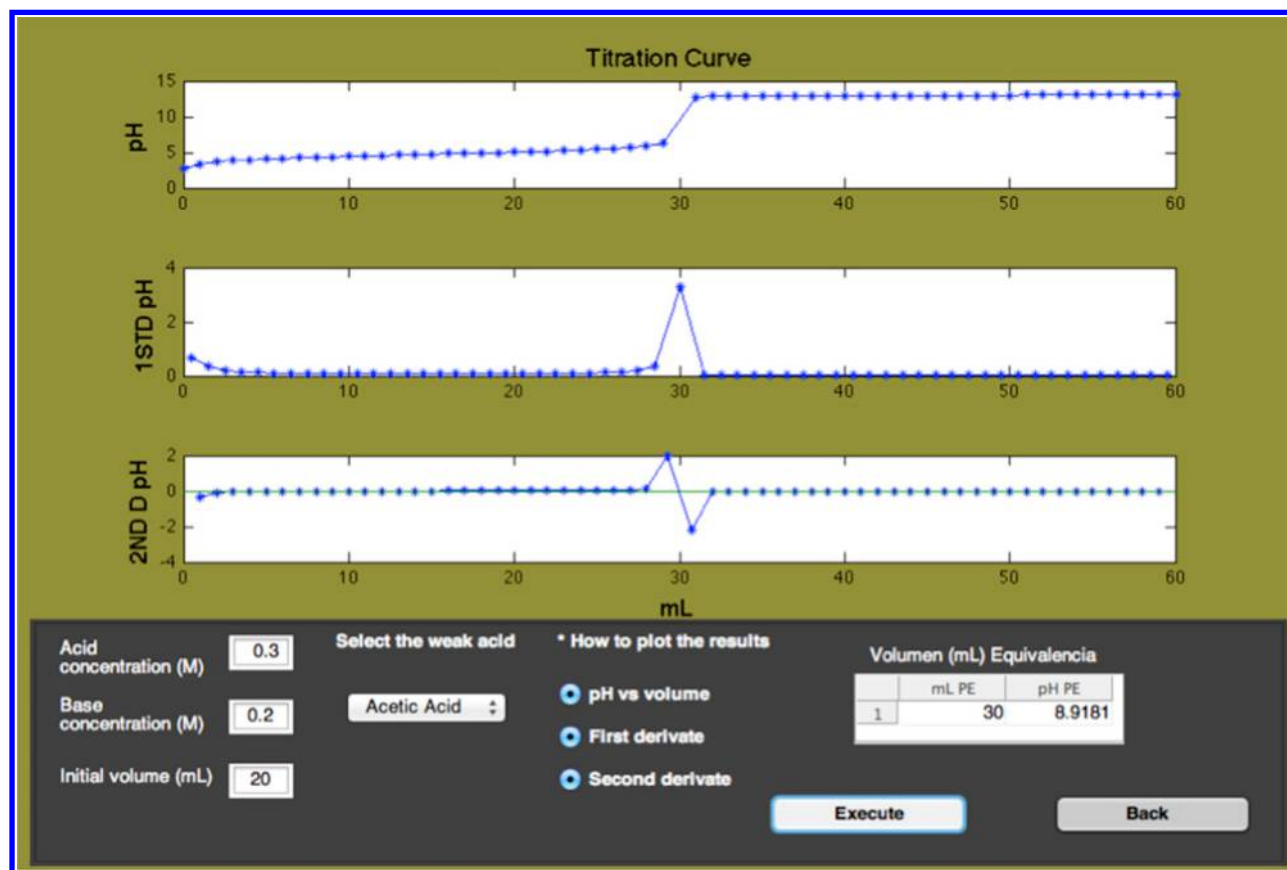

Figure 3. Example result windows for the titration of a weak acid (acetic acid). In the result windows, the graphical and numerical results are displayed. In this window, students will have the possibility to change all the experimental conditions and to evaluate the different results.

The Supporting Information of this manuscript includes a set four video instructions about how to use AchemTitri. The first video tutorial shows how to titrate a strong acid, in the second one how to titrate a weak acid, the third one is dedicated to polyfunctional acids, and finally, the last video explains how to use the advance studies options.

Acid−Base Theory

The acid−base theory constitutes one of the major concepts that students must learn during their science education training. All general chemistry syllabuses include the acid−base concept, not only in undergraduate courses but also in the last year of the high
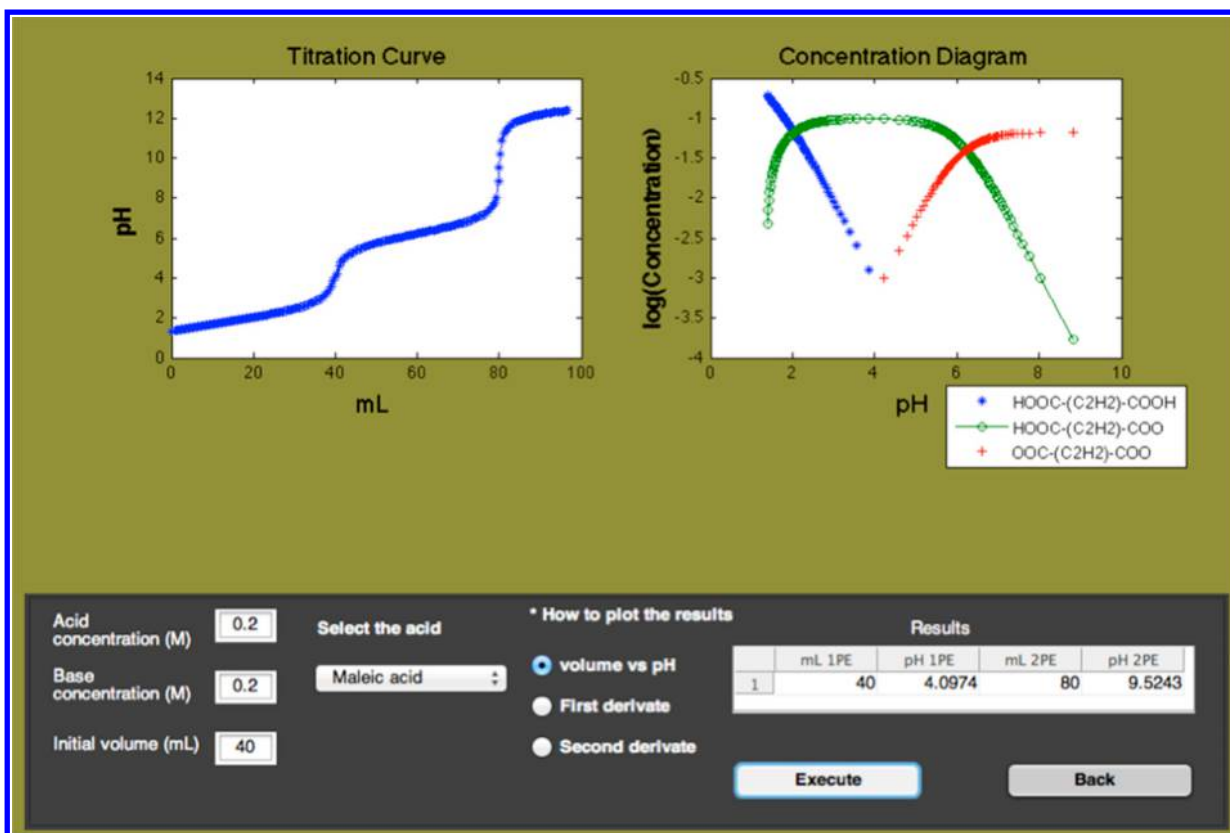
Figure 4. Example result windows for the titration of a polyfunctional acid (maleic acid). For this type of titration, the concentration diagram is also included to provide students with more information about the evolution of the different chemical species involved in the acid−base equilibrium.
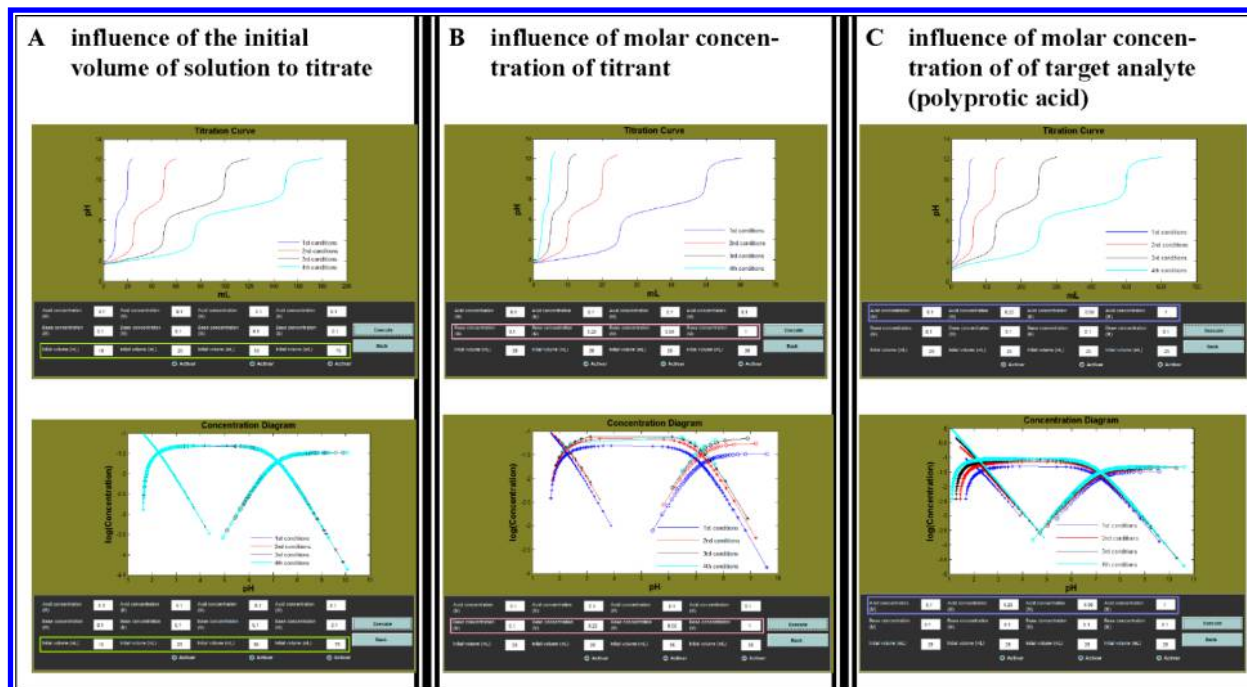

Figure 5. Images of the titration curves and concentration diagrams obtained with AChemTitri advance studies option. In column A, the influence of the initial volume of the solution to titrate is assessed (initial maleic acid solution). In column B, the influence of the molar concentration of the titrant (sodium hydroxide concentration) is shown. Finally, in column C, the influence of the molar concentration of the target analyte (maleic acid solution) is studied.

school education. Among the different theories, the Brønsted−Lowry acid−base model forms a practical and useful compromise between other approaches as the Arrhenius, Lewis and Usanovich concepts.[20] Thus, the application developed in this research used the Brønsted-Lowry acid−base concept as theoretical framework to provide students a computer tool for better understanding of

this concept, which causes many questions and takes a toll on students grade, as it was mentioned before.[21]

According to Brønsted−Lowry theory, an acid is defined as the substance able to donate a proton, and a base as the substance able to gain a proton.[22] Considering this definition, a Brønsted−Lowry acid behaves as an acid when there is another substance able to gain the lost proton from the acid (Brønsted−Lowry base).

As a consequence, when an acid substance loses a proton, it forms a conjugate base and, in the opposite way, when a base substance gains a proton, it forms a conjugate acid of a base. It is also important to consider that the strongest a Brønsted−Lowry acid is, the weaker the corresponding conjugate base and vice versa. In addition, the solvent nature is another factor to be considered, since they can act as a proton-donor or proton-acceptor, and as a consequence, they influence the acid−base behavior of the solute solved. According to this, a strong acid or base is that substance that undergoes a complete dissociation when reacting with other acid/base, and in contrast, for a weak acid/base, the dissociation reaction proceeds to only a small extent. The equilibria constant of this reaction constitutes a quantitative measure of the acid/base strength.

On the other hand, an acid−base titration could be defined, from an analytical point of view, as the action of counting the average number of analyte particles in solution through the reaction with a known number of standard particles.[23] Titration calculation, using conventional equivalence point detection, can only be applied accurately when the neutralization reaction proceeds to a large extent; therefore, it is not appropriate for the titration of very weak acids/bases. For this reason, the calculations compiled in AChemTitri application do not include very weak acids/bases. Tables 1 and 2 summarize some of the calculations coded in the software to determine the titration equivalent points as well as the concentration of the different species existing in the solution during the titration.

■ DISCUSSION

Description and Discussion of the Obtained Titration Curves

Case I: Titration of a Strong Acid with a Strong Base. Initial pH of the solution will correspond to a hydronium ion concentration, exactly equal to the molar concentration of the acid to be titrated, since it is completely ionized. The solution will present acid character until the equivalence point and basic character after that. The solution will be neutral at the equivalence point. The hydronium ion concentration at every moment before the equivalence point will correspond to the molar concentration of non-neutralized acid; in the same way, the hydroxide ion concentration after the equivalence point will be equal to the molar concentration of the titration agent in excess. Under equimolarity conditions, i.e., molar concentration of titrant equal to molar concentration of analyte, the equivalence point will be reached after adding a volume of titrant equal to the initial volume of analyte solution.

Graphically, the equivalence point corresponds to the inflection point of the titration curve in this kind of system. It is also possible to obtain the first and second derivative plots of the titration curve for a more easy localization of the equivalence point. The equivalence point will appear like a maximum and a cut with the x-axis in the first and second derivative plots, respectively. It is a fact that a maximum or a cut with abscises is much more easy to be unequivocally located in a plot than an inflection point.

Table 1. Chemical Reactions and List of Equations Used To Construct the Titration of Strong Acids in the Initial Point, before the Equivalence Point, in the Equivalence Point, and after the Equivalence Point

Titration Type	Initial Conditions	Before the Equivalence Point	Equivalence Point	After the Equivalence Point
Titration of a strong acid with a strong base	$HCl + H_2O \rightarrow H_3O^+ + Cl^-$ $[H_3O^+] = [C_{HCl}] = Ci$	$HCl + NaOH \rightarrow H_2O + NaCl$ $HCl + H_2O \rightarrow H_3O^+ + Cl^-$ $[H_3O^+] = \dfrac{C_{HCl} \times V_{iHCl} - C_{NaOH} \times V_{added}}{V_{HCl} + V_{added}}$	$HCl + NaOH \rightarrow H_2O + NaCl$ $[H_3O^+] = [OH^-]$	$NaOH + H_2O \rightarrow HO^- + Na^+$ $[OH^-] = \dfrac{C_{added} \times V_{added} - C_{HCl} \times V_{HCl}}{V_{iHl} + V_{added}}$
Titration of a weak acid with a strong base	$HOAc + H_2O \rightarrow OAc^- + H_3O^+$ $[H_3O^+] = \sqrt{K_a C_{HOAc}}$	$HOAc + NaOH \rightarrow NaOAc + H_2O$ $HOAC + H_2O \rightarrow OAc^- + H_3O^+ \; (K_a)$ $C_{HOAc} = \dfrac{C_{iHOAc} \times V_{iHOAc} - C_{NaOH} \times V_{added}}{V_{iHOAc} + V_{added}}$ $C_{NaOAc} = \dfrac{C_{iHOAc} \times V_{iHOAc}}{V_{iHOAc} + V_{added}}$ $K_a = \dfrac{C_{NaOAc} \times [H_3O^+]}{C_{HOAc}}$	$OAc^- + H_2O \rightarrow HOAc + OH^-$ $K_b = \dfrac{[HOAc] \times [OH^-]}{[OAc]}$ $[HOAc] = [OH^-]$ $K_b = \dfrac{[OH^-]^2}{(C_{iHOAc} \times V_{iHOAc})/(V_i + V_{added})}$	$NaOH + H_2O \rightarrow HO^- + Na^+$ $[OH^-] = \dfrac{C_{added} \times V_{added} - C_{HCl} \times V_{HCl}}{V_{HCl} + V_{added}}$

Table 2. Chemical Reactions and List of Equations Used To Construct the Titration of Polyfunctional Acids in the Different Stages of the Acid−Base Equilibrium

	Reaction 1: $H_2M + H_2O \rightarrow H_3O^+ + HM^-$ K_1	
	Reaction 2: $HM^- + H_2O \rightarrow H_3O^+ + M^{2-}$ K_2	
Initial Point	**Before First Equivalence Point**	**First Equivalence Point**
$[H_3O^+] = [HM^-]$ $[H_2M] + [HM^-] = C_{iH_2M}$ $K_1 = \dfrac{[H_3O^+]^2}{[H_2M]} = \dfrac{[H_3O^+]^2}{C_{iH_2M} - [H_3O^+]}$	$C_{NaHM} \approx [HM^-] = \dfrac{C_{NaOH} \times V_{added}}{V_{iH_2M} + V_{added}}$ $C_{H_2M} \approx [H_2M] = \dfrac{C_{iH_2M} \times V_{iH_2M} - C_{NaOH} \times V_{added}}{V_{iH2M} + V_{added}}$ $K_1 = \dfrac{[H_3O^+][HM^-]}{[H_2M]}$ $= \dfrac{[H_3O^+]^2 \times (C_{NaHM} + [H_3O^+])}{C_{H_2M} - [H_3O^+]}$	$[H_3O^+] = \sqrt{\dfrac{K_2 C_{NaHM}}{1 + \dfrac{C_{NaHM}}{K_1}}}$
Before Second Equivalence Point	**Second Equivalence Point**	**After Second Equivalence Point**
$C_{Na_2M} = \dfrac{C_{NaOH} \times V_{added} - C_{iH_2M} \times V_{iH_2M}}{V_{iH_2M} + V_{added}}$ $C_{NaHM} = \dfrac{C_{iH_2M} \times V_{iH_2M} - (V_{added} - V_{1stEP}) \times C_{NaOH}}{V_{iH_2M} + V_{added}}$ $K_2 = \dfrac{[H_3O^+] \times C_{Na_2M}}{C_{NaHM}}$	$M^{2-} + H_2O \rightarrow OH^- + HM^-$ $\dfrac{[OH^-] \times [HM^-]}{[M^{2-}]} = \dfrac{K_w}{K_2}$ $[OH^-] \approx [HM^-]$ $V_{2ndEP} = \dfrac{2 \times C_{iH_2M} \times V_{iH_2M}}{C_{NaOH}}$ $[M^{2-}] = \dfrac{(C_{NaOH} \times V_{2ndEP})/2}{V_{iH_2M} + V_{2ndEP}}$	$[OH^-] = \dfrac{(V_{added} - V_{2ndEP}) \times C_{NaOH}}{V_{iH_2M} + V_{added}}$

To discuss the effect of the concentration of analyte and titration agent on this type of titration curves, it is necessary to consider equimolarity, in order to make things easier to understand. Then it will be observed that the more diluted they become, the less pronounced the pH change around the equivalence point will be.

Case II: Titration of a Strong Base with a Strong Acid. In the titration of a strong base with a strong acid, initial pH will corresponds to a hydroxide concentration equal to the molar concentration of the base to be titrated. The solution will remain strongly alkaline close to the equivalence point, neutral at the equivalence point and acid beyond it. Again, like in Case I, pH is calculated along the whole titration through hydroxide and hydronium ion concentrations, which are equal o molar concentrations of base and acid, respectively.

The effect of concentration will be exactly the same as in Case I: the intensity of the pH jump around the equivalence point will increase with the concentrations of analyte and titrant.

Case III: Titration of a Weak Acid with a Strong Base. Calculations in this case are not that straightforward as in Cases I and II, since it is necessary to take into account the presence of the acid itself, its conjugated base and the possible mixtures of both species. The pH of those mixture solutions will depend on the relative position of two competitive equilibria: the ionization of the acid and the hydrolysis of the conjugated base. Thus, pH depends, on the one hand, on the relative values of their ionization (K_a) and hydrolysis (K_b) constants and, on the other hand, the ratio between the concentrations of weak acid and its conjugate base. These solutions containing a weak acid and its conjugated base are known as *buffer solutions* and their main feature is that they present a remarkable resistance to changes in pH as a result of either dilution or small additions of acids or bases.[22] Maximum buffer capacity is reached at equal

concentrations of weak acid−conjugated base, but it also depends on their total concentration. pH calculations in these kind of systems have to be done considering different regions: before starting the titration, the solution contains a weak acid and the extent of its dissociation is given by its dissociation constant (Table 1); when adding increasing volumes of titrant, before reaching the equivalence point, different buffers are generated, which pH depends on K_a and the ratio between the concentrations of weak acid and conjugated base. We should mention that when 50% of the acid is neutralized, pH is equal to pK_a; at the equivalence point the only sample present in solution will be the conjugated base and pH will be calculated through its hydrolysis constant, K_b (Table 1); after the equivalence point, the pH will be determined by the excess molar concentration of strong base used as titrant. The shape of this curve in the region beyond the equivalence point becomes identical to that for a strong acid (Case I).

To discuss the effect of concentration, it is necessary to consider again analyte and titrant solutions of the same strengths. The initial pH value will increase and the pH at the equivalence point will decrease with the dilution. For intermediate titrant volumes, pH will not be very affected by the dilution due to the presence of buffers, since it is a fact that pH of buffered solutions is largely independent of dilution.

With respect to the effect of the dissociation constant of the acid on the shape of the titration curves, the pH jump around the equivalence point will become smaller as the acid becomes weaker. This is due to less quantitative completion of the reaction between analyte and titrant. This fact, together with the effect of the concentration, makes more limited the choice of indicator for the titration of weak acids with respect to strong ones.

Case IV: Titration of a Weak Base with a Strong Acid. Deduction of the titration curve for a weak base titrated with a

Table 3. Comparative Survey Results Concerning Student's Satisfaction with AChemTitri

Questionnaire Usability Topics	Respondents (N = 50) Selecting a Given Satisfaction Ranking by Topic, %					
	Very Unsatisfied	Unsatisfied	Neutral	Satisfied	Very Satisfied	Not Applicable
Q1. Application setup and configuration	0	0	0	14.3	57.1	28.6
Q2. Tutorials tools	0	0	0	20.2	78.0	1.8
Q3. The way to work with the application (user-friendly and self-explanatory)	0	0	0	21.4	71.5	7.1
Q4. Calculations and application performance	0	0	0	21.4	71.4	7.2
Q5. Quality of figures (titration curves)	0	0	7.1	14.3	71.5	7.1

strong acid is analogous to Case III. Again, it is indicated to break the curve into regions to perform calculations: initial pH will be obviously alkaline and will depends on the base concentration and its hydrolysis constant (Table 1); different buffers will be generated after increasing volumes addition of titrant up to the equivalence point; the conjugated acid of the analyte will be the only sample in solution in the equivalence point and thus pH will depend on its concentration and dissociation constant (K_a); the excess of added titrant after the equivalence point will determine the pH in that region.

The effect of concentration and hydrolysis constant of the base will be analogous to that in Case III. That is, initial pH will decrease, the pH at the equivalence point will increase with the dilution and the magnitude of the pH decrease around the equivalence point will decrease with the hydrolysis constant of the analyte.

Case V: Titration of a Polyprotic Acid with a Strong Base, Advanced Studies. Multiple end points can be observed in this kind of titration, as long as the acidic groups of the analyte differ sufficiently in strength. In general, two individual equivalence points of practical value will be observed for an acid with two protons when the ratio between the two dissociation constants (K_{a1}/K_{a2}) is[22] at least 10^4. The main assumption or approximation that is done in such cases consists in neglecting the second dissociation in the early part of the curve. The same approximation also implies that shortly beyond the first equivalence point, the first equilibrium can be also not taken into account at any extension. For higher values of the ratio K_{a1}/K_{a2}, the introduced error by considering these assumptions is minimized. From the educational point of view, it is advisable to consider the cases of acid with huge differences among successive ionizations, but in the same way, it would be also interesting to compare with acids with not that big of a difference in successive K_a values to make the student aware of the limitations of the approximations and the subsequent limitations in the choice of a suitable indicator.

Once the above referred approximations are assumed, the development of the titration curve is not that different from the corresponding curve of a weak acid in each of the possible dissociations of the polyprotic one of interest.

"AChemTitri" gives also students the possibility of studying the effect of three experimental variables: initial volume of solution to be titrated, molar concentration of the target analyte and molar concentration of titrant. Figure 5 shows the obtained titration curves when studying the effect of each one of these variables.

Case VI: Titration of a Polyfunctional Base with a Strong Acid as Advanced Studies. The calculation of the titration curve for a polyfunctional base follows the same principles as those stated in Case V.

In this case, also, the effect of the same variables can be studied.

In all the presented cases, "AChemTitri" provides also composition diagrams as a function of pH in order to make it easy to the student to understand compositional changes taking place in the presented titrations.

Assessment of Application Usability

Knowing the limitations of computer software supports to evaluate the capability and functionality of the application design. The evaluation procedure should include a complete assessment of how well the programs functions on users' computer hardware and this capability and functionality must be tested on all possible equipment.[24] Then, the review of usability requirement is related to the evaluation of software components to see if they conform to the evaluation guide for engineering software. Likewise, the application interface included with these features is a significant component that could impact the capability and functionality of software and the efficiency of users. Before permitting public online access, the proposed application was verified by authors to perform all its tasks correctly after all application capabilities has been tested. Then, to test the usability of the AChemTitri application, an online survey was conducted among different type of users (professors, professionals, undergraduate students, graduate students and high-school students). The survey was consisted in three blocks of questions: in the first one, basic information about the user was asked; the second block was dedicated to collect information about the usability of application; and finally, the third part of the survey was intended to find how satisfied were the students after using AChemTitri.

A total of 50 participants completed the online survey: among them, 39% were professors, 11% were graduate students, 33% were undergraduate students, 5.5% were high school students and the remaining 11% were professionals not related with the education field. The results of this survey, expressed as percentage, are summarized in Table 3.

In general, users did not experience trouble with setting up the application in their computers (over 70% of the participants were either satisfied or very satisfied with the installation process). Regarding the video tutorial implemented in the software, all participants found them very useful to learn how to use the application and to exploit all the potentialities from it. In addition, almost all the participants found the application user-friendly and self-explanatory. With regard of the calculations processes, students were in general satisfied or very satisfied. Finally, around 7% of the participants were neutral about the quality of graphical results, while 85% of the participants were satisfied or very satisfied. On the other hand, users were also surveyed about which function of the application would be the most useful from them. The results show that the majority of the participants will use the application to compare different experimental conditions (73%). In addition, an important number of user point out that the main applicability will be the titration of polyfunctional acids or bases (67%). Finally, 27% and 20% of users selected the titration of strong acids or bases, as the

most useful function. This percentage could be explained by the small representation of high school students in this survey.

Finally, in the last part of the survey, participants were asked how likely they were to recommend the application to other students or professors. The results show that 81% of the participants will definitely recommend the application and 19% will probably recommend the application to other peers.

CONCLUSIONS

A new computer application, to construct acid−base titration curves, has been designed to assist students from the last courses of high school education and undergraduate students, in the studies of acid−base titration. The application, named AChemTitri, has been written under the MATLAB environment, and combines graphical with numerical calculations, to ensure a better understanding of titration concepts. Moreover, with this application, students will be able to practice basic titration concepts, such as titration of strong acid/base with a strong base/acid, as well as the titration of more complex systems such as weak and polyfunctional acids/bases. Besides the titration curves, concentration diagrams are also shown, in the case of polyfunctional acids and bases. With these diagrams, students will evaluate the evolution of the different chemical species involved in the acid−base equilibrium. To check the capability of the proposed computer application, a survey was performed among different type of users (professor, undergraduate and high school students, and other professionals) resulting in over 80% of the participants recommending the use of this application. Should the reader be interested in testing and using the application or the code presented in this work, please contact the authors by e-mail to get files.

ASSOCIATED CONTENT

Ⓢ Supporting Information

We present four video tutorials about how to use AChemTitri. The first video tutorial shows how to titrate a strong acid, in the second one how to titrate a weak acid, the third one is dedicated to polyfunctional acids, and finally, the last video explains how to use the advance studies options. This material is available via the Internet at http://pubs.acs.org.

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Notes

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REFERENCES

(1) Harris, D. C. In Partial Defense of Calculating Titration Curves. *J. Chem. Educ.* **2008**, *85* (4), 498.

(2) Hawkes, S. J. Discussion: Should Students Calculate Titration Curves? *J. Chem. Educ.* **2008**, *85* (4), 498.

(3) Kraft, A. The Determination of the pK_a of Multiprotic, Weak Acids by Analyzing Potentiometric Acid−Base Titration Data with Difference Plots. *J. Chem. Educ.* **2003**, *80* (5), 554.

(4) Kooser, A. S.; Jenkins, J. L.; Welch, L. E. Acid−Base Indicators: A New Look at an Old Topic. *J. Chem. Educ.* **2001**, *78* (11), 1504.

(5) Hawkes, S. J. Introductory Chemistry Needs a Revolution. ACS and IUPAC and AAAS and ICUC Should Lead It. *J. Chem. Educ.* **2005**, *82* (11), 1615.

(6) Hernández Espinoza, D.; Astudillo Saavedra, L. Titulaciones Ácido−Base con el Empleo de Software. *Educ. Quim.* **2014**, *25*, 42.

(7) Hernandez, M. A.; Czerwinska, J. A Web-Based Interactive Module To Teach Acid-Base Principles of Drug Action. *J. Chem. Educ.* **2008**, *85*, 1704−1704.

(8) Papadopoulos, N.; Limniou, M. pH Titration Simulator. *J. Chem. Educ.* **2003**, *80*, 709.

(9) de Levie, R. A General Simulator for Acid−Base Titrations. *J. Chem. Educ.* **1999**, *76*, 987.

(10) Smith, G. C.; Hossain, M. M.; MacCarthy, P. 3-D Surface Visualization of pH Titration "Topos": Equivalence Point Cliffs, Dilution Ramps, and Buffer Plateaus. *J. Chem. Educ.* **2014**, *91* (2), 225.

(11) Heck, B. S.; Poindexter, S. E.; Garcia, R. C. Integrating the Web into Traditional Teaching Methods. In *Proceedings of the American Control Conference*, Chicago, Illinois, 2000; IEEE: Piscataway, NJ, 2000; pp 3444−3448.

(12) González Gómez, D.; Gallego Picó, A.; Muñoz de la Peña, A.; Jeong, J. S. Implementation of a Computer-Aided Learning Toolbox for Establishing an Instrumental Analysis Calibration and the Quality Parameters of an Analytical Chemistry Method. *Chem. Educ.* **2013**, *18*, 136−143.

(13) Muñoz de la Peña, A.; González-Gómez, D.; Muñoz de la Peña, D.; Gómez-Estern, F.; Sánchez Sequedo, M. Automatic Web-Based Grading System: Application in an Advanced Instrumental Analysis Chemistry Laboratory. *J. Chem. Educ.* **2013**, *90* (3), 308−314.

(14) Regueras, L. M.; Verdu, E.; Munoz, M. F.; Perez, M. A.; de Castro, J. P.; Verdu, M. J. Effects of Competitive E-Learning Tools on Higher Education Students: A Case Study. *IEEE Trans. Educ.* **2009**, *52* (2), 279−285.

(15) Lubliner, D. J. Integrated Learning Environments: From eBooks to e^{2}Books: From e-Learning 3.0 to e-Knowledge and Beyond. In *Enhancing Learning with Online Resources, Social Networking, and Digital Libraries*; Belford, R. E.; Moore, J. W.; Pence, H. E., Eds.; ACS Symposium Series 1060; Oxford University Press: New York, 2010.

(16) Supasorn, S. Enhancing Undergraduates' Conceptual Understanding of Organic Acid-base-neutral Extraction Using Inquiry-Based Experiments. *Procedia Soc. Behav. Sci.* **2012**, *46* (0), 4643−4650.

(17) Cummins, R. H.; Green, W. J.; Elliott, C. "Prompted" Inquiry-Based Learning in the Introductory Chemistry Laboratory. *J. Chem. Educ.* **2004**, *81* (2), 239.

(18) Rutten, N.; van Joolingen, W. R.; van der Veen, J. T. The Learning Effects of Computer Simulations in Science Education. *Comput. Educ.* **2012**, *58* (1), 136−153.

(19) Akpan, J. P. Issues Associated with Inserting Computer Simulations into Biology Instruction: A Review of the Literature. *Electron. J. Sci. Educ.* **2001**, *5* (3); http://ejse.southwestern.edu/article/view/7656/5423 (accessed Jan 2015).

(20) Kauffman, G. B. The Brønsted−Lowry Acid−Base Concept. *J. Chem. Educ.* **1988**, *65* (1), 28.

(21) Adcock, J. L. Teaching Brønsted−Lowry Acid−Base Theory in a Direct Comprehensive Way. *J. Chem. Educ.* **2001**, *78* (11), 1495.

(22) Skoog, D. A.; West, D. M.; Holler, J. F. *Fundamentals of Analytical Chemistry*, 6th ed.; Sounder College Publishing: New York, 1992; p 976.

(23) Azevedo, M. C. C.; Cavaleiro, A. M. V. The Acid−Base Titration of a Very Weak Acid: Boric Acid. *J. Chem. Educ.* **2012**, *89* (6), 767−770.

(24) Jeong, J. S.; Hernández-Blanco, J.; García-Moruno, L. Approaches to Validating a Mutual Participatory Web-Planning Interface in Rural Extremadura (Spain). *Land Use Polym.* **2014**, *39* (0), 211−223.