

Implementation of a universal algorithm for pH calculation into spreadsheet and its use in teaching in analytical chemistry

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Introduction

Most of the analytical procedures proceed in aqueous solution and hence acid-base equilibria are a very important part of reaction systems. Teaching acid–base equilibrium systems constitutes a part of analytical chemistry in most chemistry teaching programs. In one aspect, they represent a part of general chemistry teaching and from the other hand they represent, as applied, a part of analytical chemistry. The second aspect, although mainly "analytical", is often paradoxically neglected. It is caused by the necessity of mathematical description, which is relatively awkward for students and requires lot of time. Thus, the teaching of chemical equilibrium in solutions in analytical chemistry mostly represents teaching of the chemical equilibrium calculation itself and teaching of the application in analytical chemistry is insufficient. Students first have to obtain calculation abilities as relates determination of the system composition and after that they can deal with the logic of system composition for particular analytical application. Teaching of equilibrium description is also important for development of the abilities of students in chemistry in general.

The simplified solutions and solutions "by eye" without complicated calculations (1, 2) are sometimes considered as good means which requires less calculation which give by short way more information about chemistry and mutual relation of compound properties, especially if the results are in good agreement with reality (3). They are, in fact, rather demonstration of good chemical knowledge of the teacher, but for students a priori information necessary for the choice of simplification represents serious encyclopedic problem. The calculations of such systems are in textbooks often divided according partial properties (acid-base, strong-weak, monoprotic-polyprotic... etc.) and the calculations are then simplified, although the complete procedure is only one. The general procedure can be transformed into unified solution using programmable means of calculation and equilibrium can be solved without risk of wrong choice of simplifications.

For example, simple simulator of acid-base titration based on solution of sole system is described in (4) and more general simulator is in (5). We also earlier described convenient general algorithm (6). Our first application was directed for 8-bit calculators with Basic. Nowadays, the spreadsheet represents great convenience and standardization of calculation on PC. This reduces the risk of declination from chemistry teaching to teaching of calculations in chemistry courses when PC's enter this process (7). The consequence is that, there is more chance to work with the relations between compounds and their properties and less with the calculations.

Algorithm of pH calculation and its implementation to the spreadsheet

The algorithm is described entirely in (6). It is intended to be universal for pH calculation of any mixtures of protolytes in aqueous solution and it requires as input only essential properties of compounds which constitute the system. It requires only the basic description of the chemical system.

Description of the chemical system

Each component of the system can be considered as the base or its protonated form (acid), each component having defined its overall concentration, an appropriate equilibrium constant and the charge of the maximum protonated form. Then the solution of a salt represent the mixture of two components – one acid and one base with stoichiometric (equal if monoprotic) concentrations. This can be better understood from the following examples.

Description of ammonium acetate at concentration c_0

	Acid	Base	total concentration	charge of the max protonated form
Protolyte 1		Ac^-	c_0	0
Protolyte 2	NH_4^+		c_0	1

Description of disodium hydrogenphosphate at the concentration of c_0 is almost the same, with exception of the total concentration of Na^+ (protolyte 2) that is $2 \cdot c_0$.

Description of ammonium-sodium hydrogenphosphate at concentration c_0

	Acid	Base	total concentration	charge of the max. protonated form
Protolyte 1		PO_4^{3-}	c_0	0
Protolyte 2	Na^+		c_0	1
Protolyte 3	NH_4^+		c_0	1

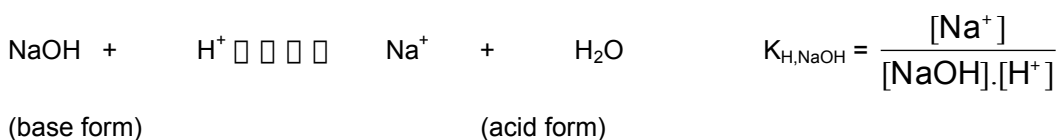
The values of the protonation constants for common acids (as H_3PO_4 , NH_4^+) are obvious as published in (8), but the values for acids associated with strong hydroxides should be derived from the known stability constants of hydroxocomplexes. The known values for some hydroxocomplexes (8) are listed in Table 1.



Table 1 Stability constants of some hydroxocomplexes

Ion	K^+	Na^+	Li^+	Ba^{2+}	Sr^{2+}	Ca^{2+}	Mg^{2+}
$\log \beta_1$	-0,5	-0,2	0,36	0,6	0,8	1,3	2,6

These constants can be transformed as follows:



thus

$$K_{H,NaOH} = \frac{[Na^+].[OH^-]}{[NaOH].[H^+].[OH^-]} = \frac{1}{\beta_{1,NaOH} \cdot K_w}$$

or

$$\log K_{H,NaOH} = -\log \beta_1 + pK_w \quad \text{and} \quad \log K_{H_1,MOH} = pK_{a1}$$

For diprotic strong bases is the situation similar as that for diprotic acids, for example sulfuric acid – the first step being stronger than second one, but in the case of the bases, there is a lack of literature data. From the known values of β_1 can be derived as above the value $\log K_{H_2,MOH} = pK_{a1}$.

Unfortunately, the constants β_2 in these cases have not been published and so an estimation can only be made. From the statistics of the stepwise hydroxocomplex stability constants we can estimate a relation of $\log K_{2,MOH} \approx \log \beta_1 - 0,6$. These values can be rewritten as above to the form of protonation constants of the bases and the appropriate dissociation constants of the conjugated acids are then given by $\log K_{H_1,MOH} = pK_{a2}$.

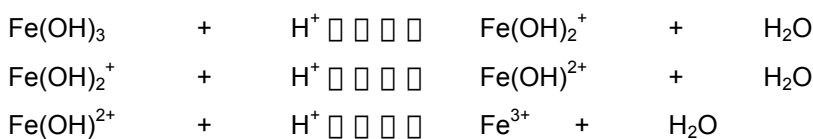
The results of such calculations are listed in Table 2.

Table 2 The values of equilibrium constants derived from stability constants of hydroxocomplexes

Ion	K ⁺	Na ⁺	Li ⁺	
$\log K_{H_1,MOH} = pK_{a1}$	14,50	14,20	13,64	
Ion	Ba ²⁺	Sr ²⁺	Ca ²⁺	Mg ²⁺
$\log K_{H_2,MOH} = pK_{a1}$	13,40	13,20	12,70	11,40
Ion	Ba ²⁺	Sr ²⁺	Ca ²⁺	Mg ²⁺
$\log K_{H_1,MOH} = pK_{a2}$	14,0*	13,8*	13,3*	12,0*

*estimated values

Analogically for Fe(OH)₃:



The most protonated acid form is then Fe³⁺.

thus

$$pK_{a1} = -\log \beta_1 + pK_w$$

$$pK_{a2} = -\log \beta_2 + \log \beta_1 + pK_w$$

$$pK_{a3} = -\log \beta_3 + \log \beta_2 + pK_w$$

The known stability constant of hydroxocomplexes of Fe³⁺ are: $\log \beta_1 = 11,8$, $\log \beta_2 = 22,3$, $\log \beta_3 = 30$, so the pK_a values for most protonated acid form Fe³⁺ are $pK_{a1} = 2,2$; $pK_{a2} = 3,5$; $pK_{a3} = 6,3$.

Mathematical description and solution

In general, the solution of any equilibrium problem consists of the following steps:

1. chemical description of the system – choice of relevant components and chemical relations (chemical equations).
2. expression of the appropriate equilibrium constants
3. formulation of mass and charge balance equations
4. algebraic solution of the equation system

A polynomial equation describing a general mathematical solution for any mixture of protolytes can be derived in this way (6). The iterative solution can be written in any programming language such as Basic or Pascal. We implemented the algorithm as user function into the EXCEL book. The input and output is realized as a convenient EXCEL sheet(s). This form is user friendly and needs only the basic knowledge about this spreadsheet, which can now be considered as a standard for lots of technical calculations and so it is familiar to students.

Description of the implementation

Implementation as the means for pH calculation (file name pH-mix.xls)

There are two always visible sheets named “Input-Output” (Fig. 1) and “Distribution” (Fig. 2) and the module where the algorithm is implemented as the user function. This module is directly visible in EXCEL 5, in newest version of the EXCEL the VBA editor have to be used for its visualization.

	A	B	C	D	E	F	G	H	I
1	Number of components in solution			1			Result pH		4,48
2	Ionic strength			0,01					
3	Component No.					1	2	3	4
4	NUMBER OF POSSIBLE ACIDIC PROTONS					1			
5	ACID/BASE [A/B]					A			
6	CHARGE OF MAX. PROTONATED FORM					0			
7	CONCENTRATION (MOL/L)					1,00E-04			
8									
9	Dissociation constants								
10					pK1	4,76			
11					pK2				
12					pK3				
13					pK4				
14					pK5				

Figure 1 The sheet “Input-Output”

	A	B	C	D	E	F	G	H
1	Component No.					1	2	3
2	Dissociation constants (Stoichiometric)				pK1	4,67		
3					pK2			
4					pK3			
5					pK4			
6					pK5			
7					pK6			
8								
9	Distribution							
10			maxH		0	60,79%		
11					1	39,21%		
12					2			
13					3			
14					4			
15					5			
16			minH		6			
17								

Figure 2 The sheet "Distribution"

The text on the screen explain the contents of the cells. Briefly, on the sheet "Input-Output" the cells D1 and D2 contain input values of the number of components in solution and ionic strength, respectively. The properties of each component represent the input values in the columns F - N, each property in the lines 4 - 15.

The result of the calculation is the output value in the cell I1. As the sheet is recalculated after each input, sometimes, when the set of the input values is not complete, the error message can appear as the output value. The result will be calculated correctly after the input set of data is completed.

The sheet can also be used to calculate another "input" number, e.g. concentration of one component at fixed pH value by using the "Goal seek" tool implemented in EXCEL. It will be simple for a person moderately familiar with EXCEL.

Each recalculation of the pH values leads automatically to the recalculation of the distribution. The sheet "Distribution" shows the percentage of different protonated forms of a given base and the values of pK's at the applied ionic strength.

The above mentioned VBA program module contains the calculation kernel - it is not necessary to know how it works in detail. It takes the input values from the sheet "Input-Output", calculates the pH values. After each change on the sheet "Input-Output", the macro recalculates and rewrites also the values on the sheet "Distribution".

The ionic strength is not a calculated value - it is given as input value influenced and controlled by the salt concentration. The "ideal" values can also be used as input - lower than caused by dissolved species, for example zero value. The activity coefficients are calculated according to the Davies equation.

Implementation as the means for visualization of titration curves (file name pH-titr.xls)

The appearance of the sheet "Input-Output" (Fig. 3) is similar as above, the properties of the used components are in the same cells. Important is the setup in the columns. The first component(s) is(are) components of solution in the burette. The number of these components can be chosen by the value in the

cell D1. The number of sample components is then in the cell D2, ionic strength in the cell D3. The values of pH as a function of the composition of titration mixture are in the table (sheet "table" (Fig. 4)) and they are displayed as the graph on the sheet "Input-Output".

On the sheet "Input-Output", the cell H1 is the pK value of indicator, the function range is then delineated on the graph as the value $pK \pm 1$, the values "sensitivity X" (cell H2), and "from" (J1) and "to" (J2) serve to manipulate the X range displayed (to show more long or short titration "experiment" and more detailed part of titration curve). The displayed titration curve or its part is constructed from 200 points, this value was chosen as reasonable value for the used PC and can be easily changed if appropriate. Two buttons associated with corresponding macros help to change the scale of the axis X and axis Y when it is necessary (mostly when the values "from" and "to" were changed).

The second sheet contains titration curve in the table form, which is used as the basic for the graph construction. The values in the table can also be used to estimate the titration error and for this reason it is necessary to display them and found the points where the used indicator changes its color. The macro associated with button "End points" can be used for this to highlight the cells of interest. In the case shown on Fig. 3, the value in column "Detail", where indicator start the change of color, is 46, true value derived from stoichiometry and concentrations of components is 50, so the end points was indicated -8 % before the true value and this method of indication is probably not acceptable. In the case of more steep curve, for more accurate identification of the end points, the values "from" and "to" have to be adjusted in the near neighborhood of expected end point.

For particular educational reasons, the workbook can be further extended, e.g. with derivative curve, distribution diagram of indicator, etc. The file with derivative curve is named "pH-titr.xls" and differ only by presence of derivative curve and "End points" macro in this case search also maximum on this derivative curve

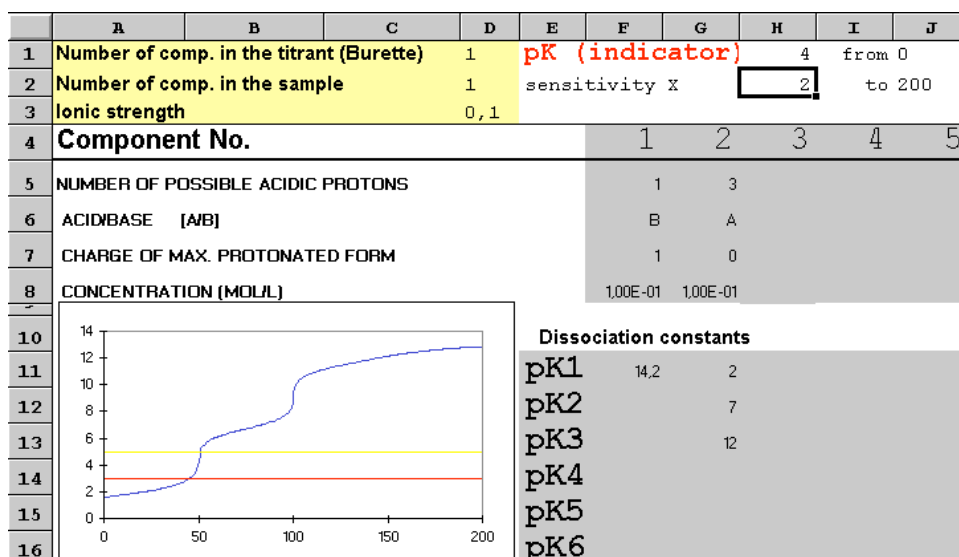


Figure 3 The sheet with the titration curve graph

	A	B	C	D	E	F	G	H
1	No.	DETAIL				pH	LIM. 1	LIM. 2
2	1	1				1,6	5	3
3	2	2				1,62	5	3
4	3	3				1,63	5	3
40	39	39				2,54	5	3
41	40	40				2,59	5	3
42	41	41				2,65	5	3
43	42	42				2,7	5	3
44	43	43				2,77	5	3
45	44	44				2,84	5	3
46	45	45				2,93	5	3
47	46	46				3,03	5	3
48	47	47				3,16	5	3
49	48	48				3,34	5	3
50	49	49				3,64	5	3
51	50	50				4,33	5	3
52	51	51				5,02	5	3
53	52	52				5,32	5	3
54	53	53				5,5	5	3
55	54	54				5,63	5	3
56	55	55				5,74	5	3

Figure 4 The sheet with the titration curve table

Application in the classroom

The typical goals of equilibrium calculations in teaching in analytical chemistry are:

1. practising in description of chemical equilibria which are important in analytical procedures
2. understanding of chemical equilibria description in general
3. better understanding of the principles of analytical procedures
4. exercising of the solution of similar problems, especially with respect to future possible

generalizations

5. understanding of relations between properties of the components of the system and the final composition of the system.

The goals 1 and 2 require the use mainly “pen and paper” method, but the point 3 or higher requires lot of calculations, sometimes not simply realized by calculator, and so the exercises are limited to the first two goals, and application into analytical chemistry is insufficient.

The use of PC and such tools as above can bring significant improvements to this area, algebra and numeric calculation can be removed from the exercises and the arrangement can be directed to the explanation of the relations in the system, or more advanced description of equilibria and more complex calculations.

Calculation of pH of a strong and weak acid or base

Unlike the common calculation of pH of strong or weak acid with obvious simplifications (the only one source of H^+ ions...) made by method “pen and paper”, the procedure presented here enables to study the:

- influence of the value of dissociation constant,
- influence of dilution,
- influence of ionic strength,
- relation in the mixture strong and weak acids, etc.

Example 1: The influence of dilution on strong or weak acid solutions

The teacher asks the students to complete the following table for hydrochloric acid and for acetic acid, first as estimate without calculation and then verify their guess by calculation for concentration from 0,01 mol/L to 10^{-8} mol/L

Concentration of acid	Estimated pH	Estimated ionic strength (I)	pH at I = 0	pH at I = estimated	Distribution %HA/%A
0,01 mol/L					
....					

Solution and comments

The students first will look for equilibrium thermodynamic constants of these acids

Hydrochloric acid : $\log K_H = -7$ ($=pK_a$)

Acetic acid : $\log K_H = 4,76$

Then the properties of both acids have to be considered. In solutions, these compounds exist as monoprotic base species, i.e. chloride or acetate – these species bind 1 acidic proton and in that acidic form, the charge is zero after protonation. These values are used as input parameters for solution by spreadsheet application described above.

First, the estimates are input to the table. Hydrochloric acid is strong, fully dissociated 1 to 1 protolyte that means that the ionic strength is equal to its concentration. Then pH and distribution are calculated for each point, the table is completed with calculated values and the results can be evaluated.

Table 3 Solution of the problem Example 1 for hydrochloric acid

Concentration of acid	Estimated pH	Estimated ionic strength (I)	pH at I = 0	pH at I = estimated	Distribution %HA/%A
10^{-2} mol/L	2	10^{-2}	2,00	2,05	0/100
10^{-4} mol/L	4	10^{-4}	4,00	4,01	0/100
10^{-5} mol/L	5	10^{-5}	5,00	5,00	0/100
10^{-6} mol/L	6	10^{-6}	6,00	6,00	0/100
10^{-7} mol/L	?	10^{-7}	6,79	6,79	0/100
10^{-8} mol/L	?	10^{-8}	6,98	6,98	0/100

Similarly, acetic acid can then be calculated.

Table 4 Solution of the problem Example 1 for acetic acid

Concentration of acid	Estimated pH	Estimated ionic strength	pH at I = 0	pH at I = estimated	Distribution %HA/%A
10^{-2} mol/L	>2	$<10^{-2}$	3,39	3,39	95,0/5,0

10^{-4} mol/L	>4	$<10^{-4}$	4,47	4,47	66,1/33,9
10^{-5} mol/L	>5	$<10^{-5}$	5,15	5,15	28,8/71,2
10^{-6} mol/L	>6	$<10^{-6}$	6,02	6,02	5,2/94,8
10^{-7} mol/L	?	$<10^{-7}$	6,79	6,79	0,9/99,1
10^{-8} mol/L	?	$<10^{-8}$	6,98	6,98	0,6/99,4

The “true” ionic strength values can be calculated by an iterative procedure – from estimated value of the ionic strength and subsequent distribution values a better estimate of ionic strength can be obtained, however, the values imply that it is not necessary.

The first estimates will be probably not good, but the students can easily calculate the right values and correct their own opinion. In this process, the students can understand the relation between the true pH value and the strength of acids at the same concentration, they can see that an another source of H^+ ions, water, plays role at low acid concentrations and the term “low” in this sense depends on the strength of the acid. They can see the relation between the distribution of species and pH, ionic strength, acidity strength, charge of species... To check such knowledge, teacher can formulate questions and sub-questions and ask students conclusions about system of interest. It is evident, that skilled teacher will be able to design a variety of similar problems.

The above problem can be extended with the same compounds as a mixed system of a strong and a weak acids. The “Input-Output” sheet will be changed only in the cells D2 (number of components) and G4-G10 (properties of the second acid).

It can thus be shown, that at the same concentration of both acids, e.g. 10^{-2} mol/L, the strong acid depresses the dissociation of the weak acid, only 0,2 % of acetic acid is dissociated while HCl is fully dissociated and the pH is virtually the same as in pure HCl solution, the contribution of acetic acid to the pH value is negligible.

The sheet can also be used for inverse direction of such calculation, i.e. to calculate concentration of one component from a known pH value. For this reason can be simply used the standard EXCEL tool “Goal seek”. This is useful, for example, in calculations pH changes due to dilution of strong or weak acids.

Example 2 The influence of ionic strength on the pH of H_2SO_4

The sulfuric acid is often considered as strong diprotic acid - that means fully dissociated at usual concentrations. At a concentration of $c = 0,005$ mol/L and provided that it is fully dissociated, the estimated pH is 2. The calculated values based on the protonation constants $\log K_{H1} = -3$, $\log K_{H2} = +2$ are listed in Table 5.

Table 5 The influence of ionic strength on H_2SO_4 solutions

Ionic strength	pH	Distribution %H ₂ A/%HA/%A
0	2,11	0/44/56
0,01	2,13	0/33/67
0,1	2,16	0/20,5/79,5
0,3	2,18	0/16/84

If the obtained distribution is used to calculate ionic strength due to sulfuric acid, the corrected value of ionic strength in the second row is 0,012 (moderately skilled worker with EXCEL easily make the sheet that calculate ionic strength from distribution and concentration), the value in the first row is the ideal case, the second row is almost real and next two can be realized using an indifferent salt background. From the values, students learn about paradox – with the increase of ionic strength in this case, value of pH increases although the extent of dissociation increases too. The differences in pH above are commonly measurable and so in such type of calculations it is worthwhile to consider non-ideality.

Salts

A salt can be considered as stoichiometric mixture of an acid and a base, e.g. NaCl is the mixture NaOH and HCl (Fig. 5).

	A	B	C	D	E	F	G	H	I
1	Number of components in solution			2			Result pH		7,000
2	ionic strength			0,1					
3	Component No.					1	2	3	4
4	NUMBER OF POSSIBLE ACIDIC PROTONS					1	1		
5	ACID/BASE [A/B]					B	A		
6	CHARGE OF MAX. PROTONATED FORM					1	0		
7	CONCENTRATION (MOL/L)					1,00E-02	1,00E-02		
8									
9	Dissociation constants								
10				pK1		14,2	-7		
11				pK2					
12				pK3					

Figure 5 The sheet “Input-Output” for NaCl

If we take a weak base instead of a strong one, e.g. NH_4OH , the result is NH_4Cl . The only change is in the pK value (Fig. 6).

	A	B	C	D	E	F	G	H	I
1	Number of components in solution			2			Result pH		5,730
2	ionic strength			0,1					
3	Component No.					1	2	3	4
4	NUMBER OF POSSIBLE ACIDIC PROTONS					1	1		
5	ACID/BASE [A/B]					B	A		
6	CHARGE OF MAX. PROTONATED FORM					1	0		
7	CONCENTRATION (MOL/L)					1,00E-02	1,00E-02		
8									
9	Dissociation constants								
10				pK1		9,24	-7		
11				pK2					
12				pK3					

Figure 6 The sheet “Input-Output” for NH_4Cl

The mixture of acid and hydroxide in ratio different from stoichiometric - buffer

If there is an excess of the weak components, for example hydrochloric acid and ammonium hydroxide in the ratio of 1:2, the result is a buffer. The only change in the previous sheet is the concentration of the base component.

A14									
	A	B	C	D	E	F	G	H	I
1	Number of components in solution			2			Result pH		9,340
2	Ionic strength			0,1					
3	Component No.					1	2	3	4
4	NUMBER OF POSSIBLE ACIDIC PROTONS					1	1		
5	ACID/BASE [A/B]					B	A		
6	CHARGE OF MAX. PROTONATED FORM					1	0		
7	CONCENTRATION (MOL/L)					2,00E-02	1,00E-02		
8									
9	Dissociation constants								
10				pK1		9,24	-7		
11				pK2					
12				pK3					

Figure 7 The mixture of acid and hydroxide in ratio different from 1:1, i.e. buffer

The values on the sheet "Distribution" further offer nice possibilities to assemble questions and possible answers about such systems and to explain behavior of such mixtures.

Titration curves - calculation of individual points

The each point of titration curve in the case acid-base titration represents the mixture of titrant, i.e. acid or base, and sample, i.e. base or acid. Because the sheet can calculate such cases immediately, it is necessary only manipulate the concentration of components according the mixing procedure. The sheet can be used for rapid calculation of several points by following procedure which shows titration of acetic acid (sample) with ammonium hydroxide (titrant) (Fig. 8).

A												
	A	B	C	D	E	F	G	H	I	J	K	L
1	Number of components in solution			5			Result pH		8,760			
2	Ionic strength			0								
3	Component No.					1	2	3	4	5	6	7
4	NUMBER OF POSSIBLE ACIDIC PROTONS					1	1	1	1	1	1	1
5	ACID/BASE [A/B]					A	B	B	B	B	B	B
6	CHARGE OF MAX. PROTONATED FORM					0	1	1	1	1	1	1
7	CONCENTRATION (MOL/L)					1,00E-01	3,33E-02	3,33E-02	3,33E-02	3,33E-02	3,33E-02	3,33E-02
8												
9	Dissociation constants											
10				pK1		4,76	9,24	9,24	9,24	9,24	9,24	9,24
11				pK2								
12				pK3								
13				pK4								
14				pK5								
15				pK6								
16												

Figure 8 The sheet "Input-Output" for calculation individual points of titration curve in the system of acetic acid (sample) with ammonium hydroxide (titrant)

The properties of sample compound are in the cells F4-F10, the properties of titrant are in the cells G4-G10, where the concentration of titrant is only a part of the concentration of sample, adjacent cells H4-H10... can be loaded very quickly by copying group of cells by usual method. The calculation of another point is then realized by changing the value in cell D1 - number of components: if it is 1, result is pH of the sample before titration, in the case 2, result is pH after first addition of titrant, in the case 3, result is pH after second addition of titrant (total concentration of titrant represents sum G7+H7), etc. The results summarized in the Table 6 can be obtained very quickly.

Table 6 Individual points of titration curve in the case of acetic acid (sample) titration with ammonium hydroxide (titrant)

1	2	3	4	5	6	7	8	9
2,88	4,46	5,06	7,00	8,76	9,06	9,24	9,36	9,46

Titration curves graphically

More convenient is, however, a special book that applies the same function as the base to design complete titration curve - as a table and subsequently as a graph (Fig. 3). This book is described above and it is very similar as the book for simple calculation of pH and so it will be not difficult to use it, if students are familiar with the previous one.

The presentation of the curves for different conditions - ionic strength, concentration level... - allows to discuss influence of such parameters on the analytical process. Such calculations are impossible by using a calculator and even maximally simplified they require a lot of time. Application of already pre-prepared solutions in the "paper" form causes passivity of students, like at listening to the lecture or reading the textbook. An interactive approach with PC is surely a better alternative.

The workbook can easily be supplemented with a derivative curve, and the discussion can relate to instrumental indication vs. visual indicators.

The workbook also enables to display titration of amulti-component sample with a multi-component titrant. This enables to discuss, for example:

- the possibility of separate or conjoint titration of the mixtures due to difference in equilibrium constants,
- the titrability of the mixtures,
- the influence of the presence of carbon dioxide in the sample or in the titrant,
- the particular arrangement of analytical procedures, such as standardization of NaOH by the Bruhns method,
- the influence of polyphosphates in hydrogenphosphate samples,
- the influence of dilution and possibilities of indication,
- presentation of less common titration systems - maybe academic, such as titration of sodium dihydrogenphosphate with sodium phosphate.

It is evident, that skilled teacher can prepare many similar suitable examples.

Conclusion

The calculation of equilibrium composition of acid-base systems can be relatively easily implemented as general algorithm into spreadsheet, that makes it user friendly for students in the classroom. By the use of such tools, it is possible:

- to solve not only simple systems but also very complex ones,
- to solve the problems which explain chemical basis of analytical procedures, without inadequate simplification (or even rough estimation), or it is possible to show the influence of such simplifications on the determination of the composition of such systems without time consumption calculations,
- to understand the relation between table values of equilibrium constants and properties of appropriate solutions,
- to explain the mutual influence of species in the system.

Such an enhancement of the efficiency facilitates a more effective teaching of principles of analytical chemistry without teaching algebraic and numeric procedures.

Literature Cited

1. Ault A., *J. Chem. Educ.*, **1999**, 76, 936.
2. Barnum D., *J. Chem. Educ.*, **1999**, 76, 938.
3. Hawkes S.J., *J.Chem.Educ.*, **2000**, 77, 1183.
4. Billo E.J., *EXCEL for chemist*, Wiley-VCH: New York, 1997.
5. de Lavie R., *J. Chem. Educ.*, **1999**, 76, 987.
6. Beinrohr E., *Chem. Lett.*, **1991**, 85, 1176.
7. Jones R.B., *J. Chem. Educ.*, **2000**, 77, 1085.
8. Sillen L.G., Martell A.E., *Stability Constants of Metal-Ion Complexes*, Spec. Publ. No. 17, The Chemical Society, London, 1964, and
Smith R.M., Martell A.E., *Critical Stability constants*, Plenum Press, 1977.