Spreadsheet universal algorithm for acid base equilibrium calculation in analytical chemistry

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Overview

The calculation of equilibrium composition of acid-base systems implemented as a general algorithm into spreadsheet (as a user defined function) is the base of attached Microsoft Excel workbooks:

1. the pH calculation for any mixture of protolytes (workbook name ”pH-mix), and
2. the calculation and presentation of titration curves (names pH-titr and pH-titrd, without and with derivative curve, respectively).

The both workbooks use a very similar system of input data about acid-base properties of the components in solution(s). They require only basic knowledge about EXCEL and almost no calculation abilities, but on the other hand they require description of chemical properties of the system components, that means they represent the tools to learn more about chemistry without laborious algebra and arithmetic.

The first type of calculation is intended for pH calculation and for calculation distribution of all protonated/deprotonated species in the solution. The second one calculate integral and derivative titration curves. The workbook enables also to display titration of multi-component sample with multi-component titrant.

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 the chemical basis of analytical procedures, without inadequate simplification, or it is possible to show the influence of such simplifications on the determination of the composition of such systems without adverse time consumption,
- to build perception of the relation between the equilibrium constants and the properties of appropriate solutions,

and to explain:

- the mutual influences of species in the system,
- the influence of the presence of carbon dioxide in the sample or in the titrant,
- the problems related to the end point of titration using visual indicators, or to discuss instrumental indication vs. visual indicators,
- the possibility of separate or conjoint titration of the mixtures due to difference in equilibrium constants,
- the particular arrangement of analytical procedures, such as standardization of NaOH by the Bruhns method….

Skilled teacher can use these tools to more effective teaching of the principles of (analytical) chemistry without teaching algebraic and numeric procedures.