Extract: A new Simulation Software for Liquid-Liquid Extraction Process

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ABTRACT: *The aim of this work is to develop software to predict the value of yield and distribution coefficient in the process of reactive liquid-liquid extraction of chemicals components, using mathematical models expressing these entities, based on equations equilibrium between organic and aqueous phases, and predict the conditions under which the extraction operation is favorable, unfavorable or impossible to realize, by studying the variation of the entities cited, based on the parameters influencing the extraction, which are: initial concentrations, rate of solvent and pH, in the case of a simple extraction (extraction of neutral products) or when it is reactive (extraction of complex acids or bases) for one or more components. The programming language used is "Delphi" which is a very powerful oriented object programming under Windows.*

Keywords: Liquid Extraction, Partition Coefficient, Yield, Solvent, Solute, Delphi

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1. Introduction

To estimate the yield of the liquid-liquid extraction of a chemical compound, and predict the value of its distribution coefficient between organic and aqueous phases are the most critical parameters of the operation of extraction [1], these entities vary depending on several parameters including the volumes of the two phases, the nature of the medium and of the constituents, concentrations of the various compounds present in solution as well as the partition coefficients of the substances to be extracted [2, 3].

Modeling and optimize the extraction process, the computer design of such processes requires a model for chemical liquid-liquid equilibria of constituents. This topic was widely discussed by many researchers and various solvents and substances have been studied [4-6].

The objective of our work is to develop software to predict the yield and the distribution coefficient of liquid-liquid extraction using models expressing these entities [7] and to study the influence of various parameters governing the extraction process, to provide conditions in which this operation is favorable, unfavorable or impossible in the case of a simple extraction (extraction of neutral products) or when it is reactive (complex extraction, acid or bases), for one or more components [8-10].

The software was compiled using the Delphi programming environment which is a very powerful language programming on Windows [11].

2. Presntation of Extract Software

2.1 Presentation of EXTRACT software

EXTRACT software was designed to facilitate calculation of certain parameters for a liquid-liquid extraction, especially to estimate the yield and distribution coefficients of components to be extracted by calculations based on computer simulation, and provide in what conditions the extraction operation of these components is favorable, unfavorable or impossible, by studying the variation of these entities based on the most parameters influencing the extraction, ie, initial concentrations, rate of solvent and ligand concentration of complex (pH for acid-base components). The software even allows viewing changes in these entities by diagrams using a graphical representation [12].

The software is valid for an extraction of one or more components, in the case of a simple extraction (extraction of neutral products) or when it is reactive (extraction of complex, acids, bases or ampholytes).

EXTRACT software also compiles a database containing more than 2000 values of partition coefficients of chemicals commonly used in laboratories, in a wide range of solvents 36 in number, the user can easily view and access the database to modify or add new substances, other values of partition coefficients, new solvents or other information about these substances, such as: chemical formula, molecular weight, density, boiling point ... etc..

2.2 Software installation

EXTRACT software can be easily installed in Windows by double clicking the Setup icon from its installation folder and following the instructions that appear on the screen. The icon of the application form of a funnel is automatically placed in the start menu of the computer.

2.3 Software description

2.3.1 Access to the software

The application is launched from the icon EXTRACT program, a home screen of the application appears (splash) for a few seconds and then plug the main menu appears, it looks like the following (Figure 1).

Figure 1. Main menu of the software EXTRACT

Access to the program is possible through the first button at top Access to the program, a form entitled Calculation of yield and distribution rate is enabled, it consists of three separate worksheets: The first case for a simple extraction, the second for a reactive extraction of single compound and the third for the reactive extraction of a mixture. In such case, it is important to clarify first the nature of the extracted compound (acid, base or complex). The inputs entities are: volumes of aqueous and organic

phases expressed in liters, initial concentration of the extracted substance in mol / l. The value of pH of the substance in solution is determined automatically, a message attracts the attention of user that he can change this value and repeat the calculations while indicating the optimum value for efficient extraction.

Finally access to a graphical mapping of the parameters influencing the extraction is done by pressing the Graph values of the distribution coefficients and the yield of extraction at different values of pH are displayed in tabular form as soon as the worksheet is activated, the variation curves of these entities will be plotted on the plan in pressing graph R or LogKD button.

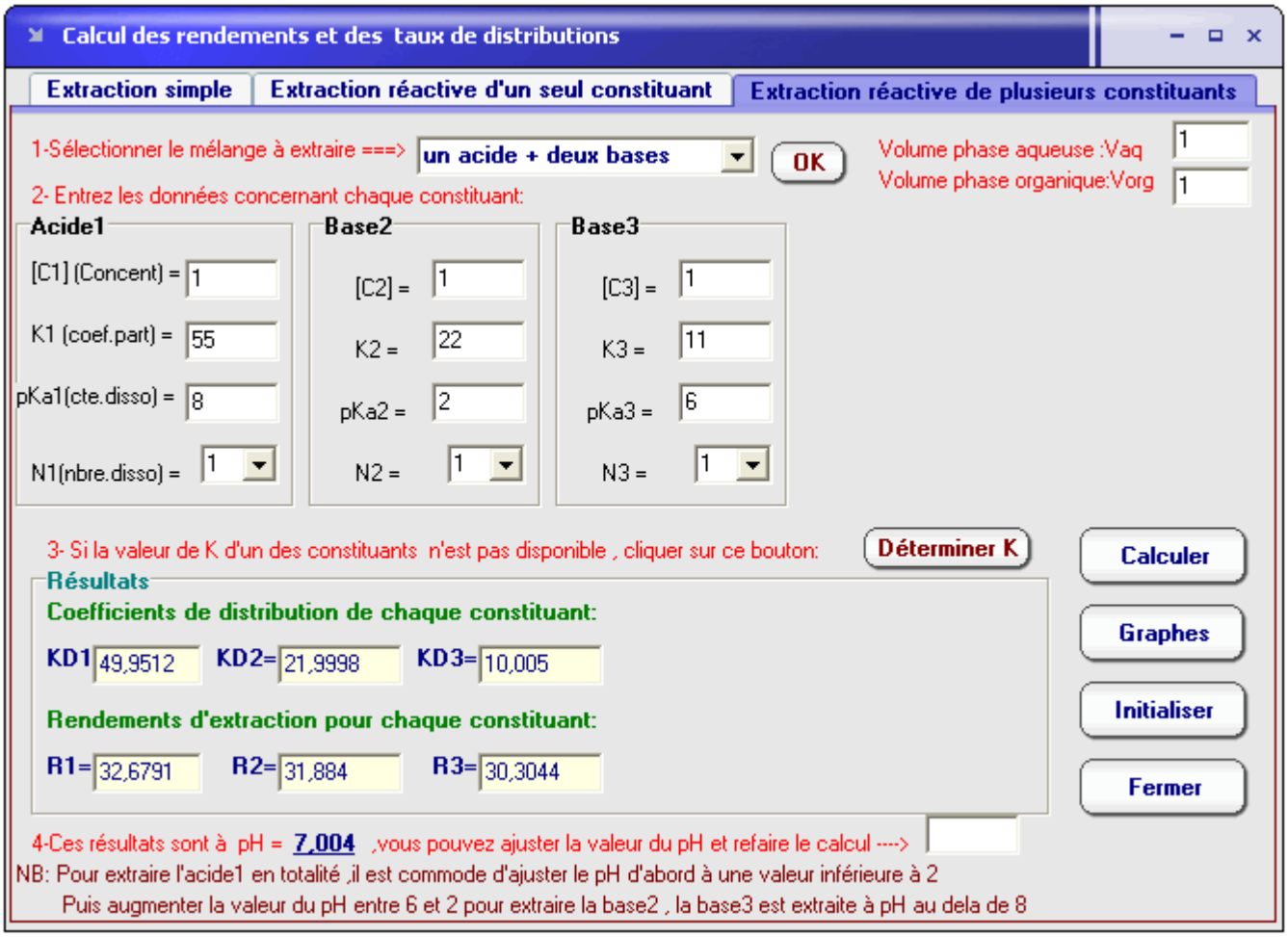

Figure 2. Worksheet of calculation of yield and distribution coefficients for the case of extraction of a mixture of constituents

2.4 LogK database

EXTRACT software has a database containing values of more than 2000 partition coefficients (logK) to about 1000 substances, in 36 most common solvents extraction. This database offers the user the advantage of being amended or supplemented by other values of logK or new solvents, it can contain up to 100.000 values .

2.4.1 Research of K in the database

You must click on the button Determine K, a worksheet entitled "*Finding K in the database*" is enabled (see figure below), it remains to select the solvent and substance in the context menu and click the OK button, once the value of K is displayed, the user can take it to the place he wants to use it after selecting it and pressing the OK button.

2.5 Experimental validation of the software

An experimental validation of results compiled by the software has been applied to the influence of pH on the extraction of a carboxylic acid (0.1 N formic acid HCOOH) from its aqueous solution with an organic solvent (butan-1-ol). 10 ml of aqueous

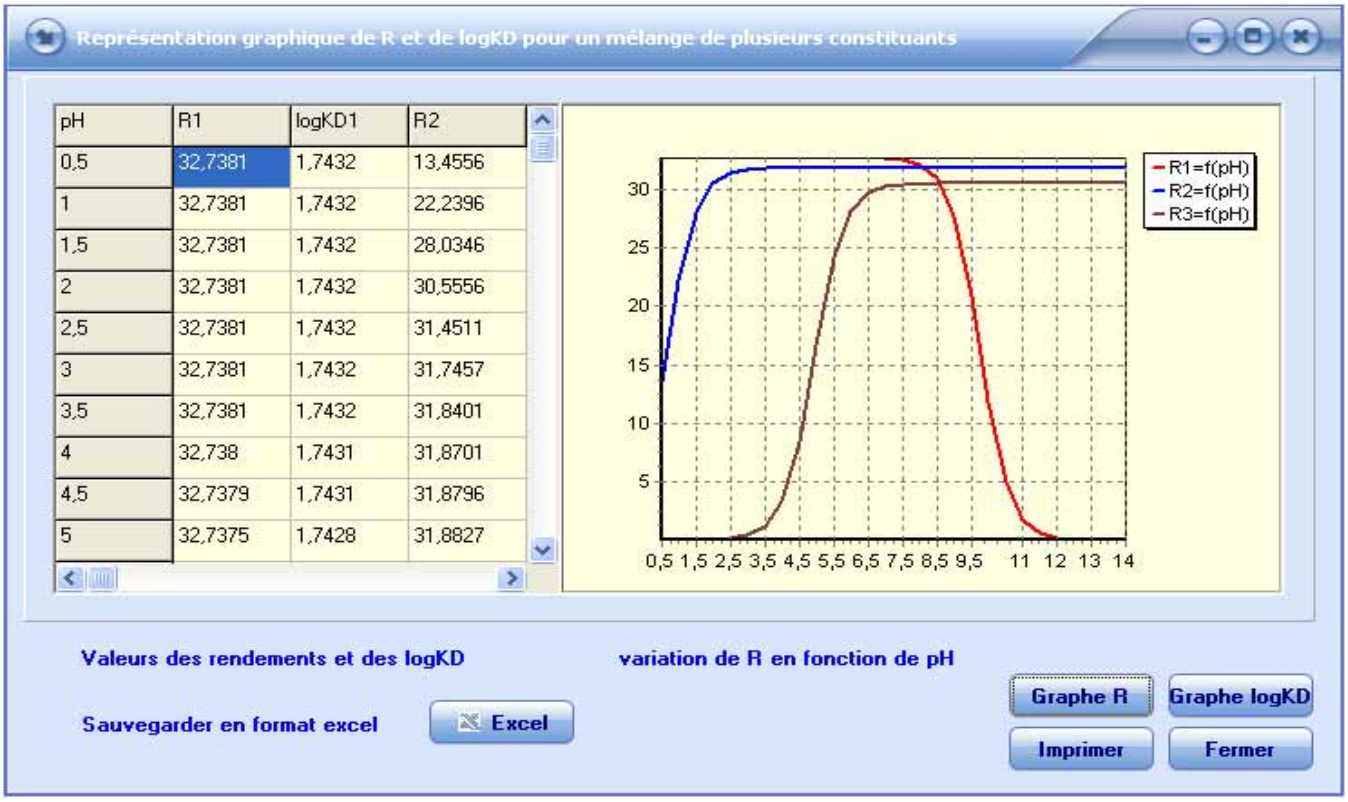

Figure 3. Variation of yield versus pH for a reactive extraction of several components

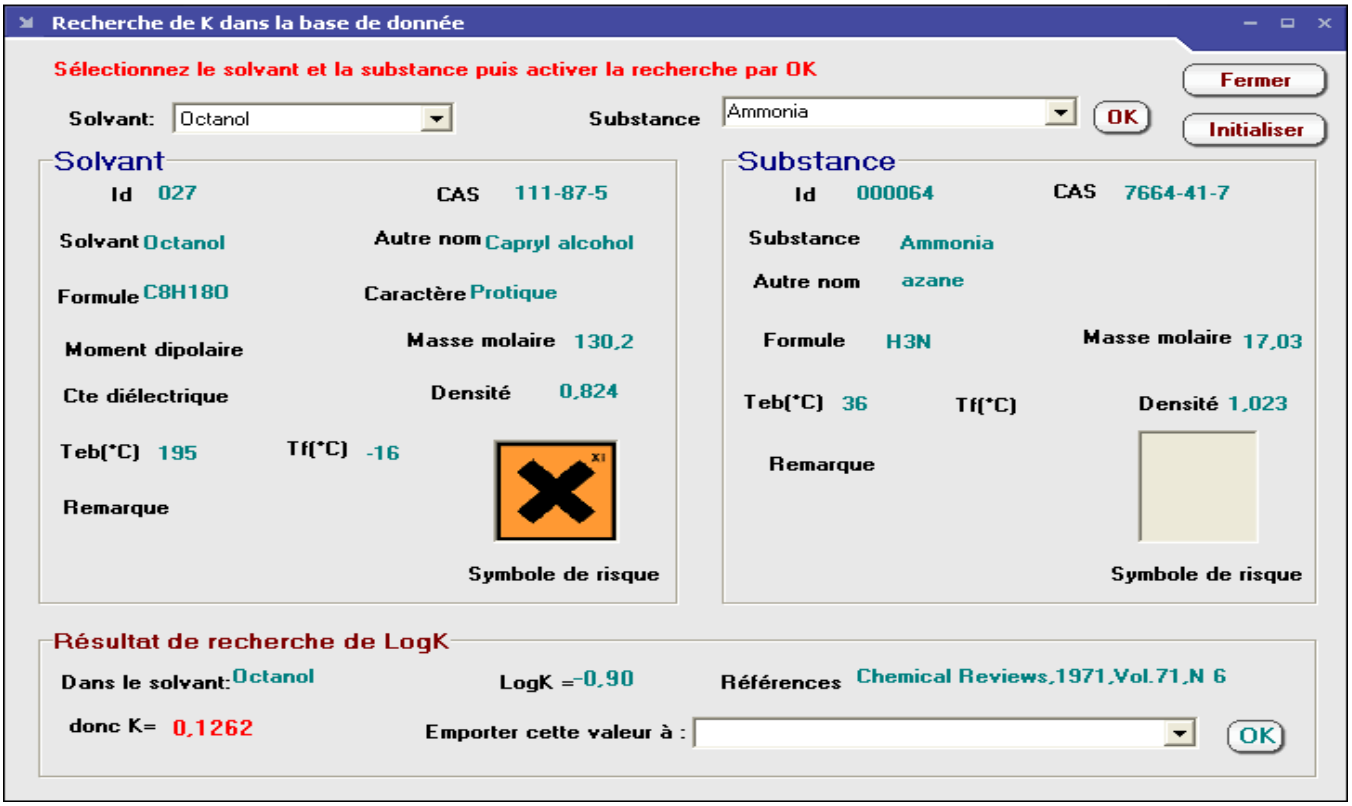

Figure 4. Search of K in the database

solution were stirred by an equal quantity of solvent, after separation, the concentration of acid in the aqueous phase was determined by UV spectrophotometry, and in the organic phase by mass balance, the values of the distribution coefficient and the yield of extraction were deduced and compared with those compiled by the software.

Table 1, below, contains the values of distribution coefficient and the yield of the acid extraction for deferent values of pH. It is of course remarkable that values of experimental D_{exp} and modulated D_{mod} distribution coefficient, in one hand, and experimental R_{exp} and modulated yield R_{mod} in the other hand are in good agreement. The highest yield of the extraction of formic acid is 46.15 % at pH less than pKa value (i.e., 3.75), beyond this value; the acid can not be extracted. Figures 5 and 6 represent the variations of the yield of the extraction and the logarithm of the distribution coefficient as function of pH values. Results show a good correlation between experimental and modulated coefficient distribution and yield of extraction for formic acid, table 1 shows the errors between cited entities.

	Distribution coefficient			**Yield of extraction %**		
pH	D_{mod}	D_{exp}	***Error***	R_{mod}	R_{exp}	***Error***
1.48	0.90	0.85	0.0497	47.29	45.87	1.4176
1.84	0.89	0.84	0.0483	47.12	45.73	1.3854
2.29	0.87	0.86	0.0146	46.57	46.15	0.4192
2.85	0.80	0.73	0.0715	44.47	42.18	2.2977
3.5	0.58	0.40	0.173	36.60	28.79	7.8116
3.85	0.40	0.37	0.0249	28.54	27.25	1.2926
4.2	0.24	0.09	0.1521	19.12	7.77	11.3473
5	0.05	0.04	0.0084	4.60	3.83	0.7661
5.6	0.01	0.00	0.0126	1.25	1.47	0.2215
6.4	0.00	0.00	0.002	0.20	0.89	0.6895
7.1	0.00	0.00	0.0004	0.04	0.06	0.0193
8	0.00	0.00	0.0000	0.01	0.00	0.0051

Table 1. Experimental and Model Values of R and D for Formic Acid Extraction as a Function of pH (Solvent:Butan-1-OL; Vaq/Vorg = 1:1; T = 20 °C)

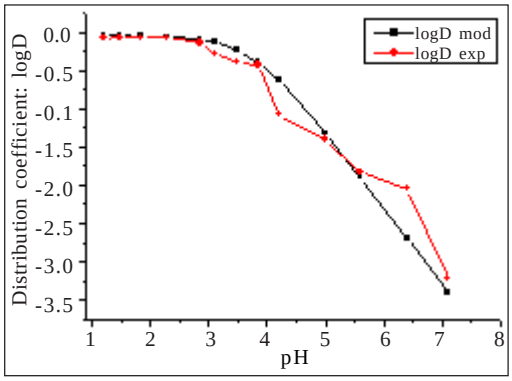

Figure 5. log (D) as a function of pH for extraction of formic acid (initial concentration Ci = 0.1 mol/L)

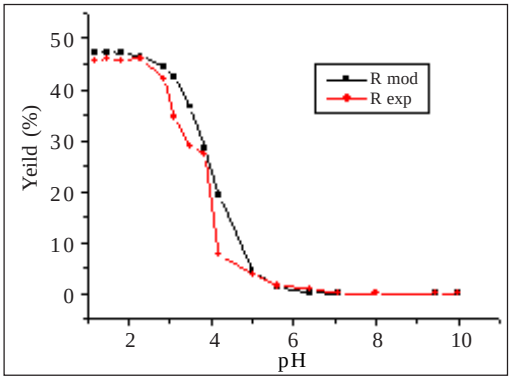

Figure 6. R as a function of pH for extraction of formic acid (initial concentration Ci = 0.1 mol/L)

2.6 Conclusion

Modeling and computer design equations of liquid-liquid equilibrium of a multi-component system allows us through the EXTRACT software developed using oriented object environment DELPHI, in order to optimize the process of extraction, the

distribution coefficient and yield of the operation were simulated and calculated with a good approach by comparing the experimental values .

The results of the software for the case of extraction of formic acid from its aqueous solution for varied values of pH are very consistent with those determined experimentally, the results show that the highest yield of the extraction of formic acid is 46.15 % at pH less than pKa value (i.e., 3.75), beyond this value; the acid can not be extracted, witch is in good agreement with estimated results and confirm the authenticity and the validity of the developed software.

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