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Review

Software and internet resources for capillary electrophoresis and micellar electrokinetic capillary chromatography

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Abstract

The purpose of the contribution is to show how software and the internet have changed the way in which we carry out research, and what additional possibilities these new resources and tools provide. The internet and e-mail broaden our horizon for cooperation. There are no borders for information exchange: our library is a virtual one, electronic databases are at our fingertips. E-mail discussion groups provide an electronic community of CE users. Such forums have provided a basis for worldwide scientific cooperation amongst scientists; the present contribution is only one of several examples. Estimation software provides us with estimates of component properties in those cases where this information is not available from literature or from experiments (an estimated value is better than no value). Several examples will illustrate the use of estimation software in capillary zone electrophoresis and micellar electrokinetic capillary chromatography. Simulation software presents visualization of experimental results to be expected, both as a training tool and as the first step in method development. Other simulations yield valuable insights into phenomena that are not readily accessible experimentally for reasons of size or time-scale.

Keywords: Reviews; Software resources; Internet resources; Capillary electrophoresis; Micellar electrokinetic chromatography

Contents

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1. Software

1.1. Simulation programs

In an earlier review on computer simulation [1], a distinction was made between steady-state and dynamic simulators. Both are based on mathematical descriptions of all (or most) phenomena taking place in analytical separation methods. Steady-state simulators present a graphical representation of the signal as seen by the detector after the separation. There are several such experiment simulators available for capillary zone electrophoresis (CZE), e.g., HPCESIM [2,3], added chiral options [4,5], CEsight [6] and CESAR [7] and for micellar electrokinetic capillary chromatography (MECC), e.g., MECCSIM [8]. Dynamic simulators [9–15], in contrast to steady-state simulators, are based on solving differential equations for charge and mass transfer by migration, flow and diffusion, and give insight into the dynamics of the separation process during the analysis, often on a very small scale with respect to time and distance. Most of these dynamic simulators were developed for research purposes and consequently lacked a user-friendly interface. Easier to use are the following programs: CZE, based on a DOS user-interface and including a database [16] and Simul [17], a Windows-based program albeit without database access. A screen capture of the latter is shown in Fig. 1, where in the graph concentrations, pH and conductivity are plotted along the capillary length axis.

1.2. Estimation software

Whereas simulation programs presented in the previous paragraph use sample parameters obtained preferably from experimental results, sometimes

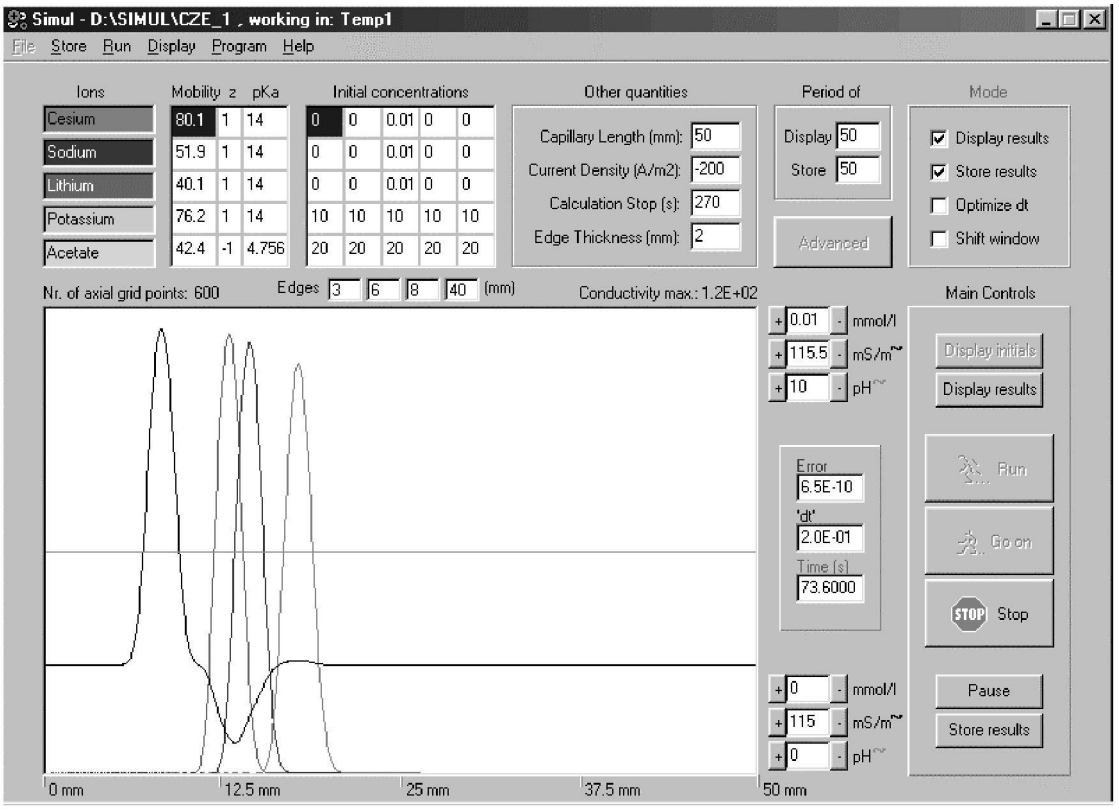

Fig. 1. Screen capture of the Simul program for dynamic simulation of isotachophoresis and CZE [15].

these parameters are not readily available. In these cases, estimation software can sometimes be useful. For example: migration behavior in MECC can be modeled using the octanol–water partition coefficient (log *P*), leading to a fair estimate of MECC migration time order. Several estimators for log *P* are available, admittedly an indication that there is no consensus with regard to the best modeling algorithm. Most algorithms calculate the cumulative effect of all functional groups with certain weighting factors and possibly mutual interference. Table 1 gives an overview of available programs for log *P* estimation.

The accuracy of the estimation software is determined by the quality (and thus the degree of complexity) of the algorithm upon which the calculations are based. Correlations between experimental and calculated values, as claimed by the manufacturers, are in the order of 0.99, depending on the number of components (100–1000). Subselections, such as the homologous series naturally correlate better. More illustrative is the correlation between different algorithms, an example is depicted in Fig. 2. The correlation coefficient is also in the order of 0.99 but there is a systematic difference of 7%.

Syracuse Research Corporation (http://esc.syrres.-com/interkow/kowdemo.htm) is another company whose web site contains an on-line interactive demonstration software of a commercial package on calculating log *P*. Log *P* data may be retrieved from a 13 000-compound database. Queries are submitted in SMILES notation or as CAS numbers. (SMILES stands for Simplified Molecular Input Line Entry System, a chemical notation system used to represent a molecular structure by a linear string of symbols). Also on this site is an environmental fate database of

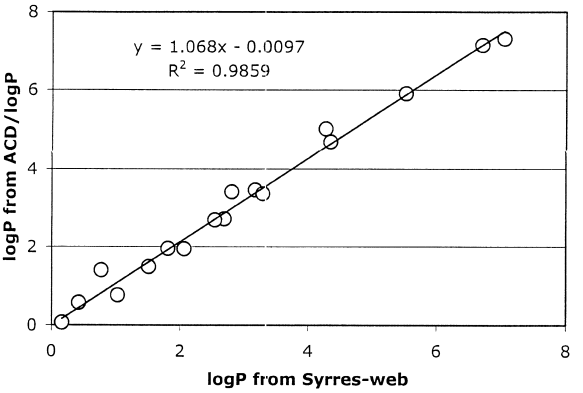

Fig. 2. Correlation between calculated log *P* values from the ACD/logP program and the web-based demo version of K_{OW}WIN.

20 000 chemicals, with full references to 33 000 articles.

1.3. Sources of data

In addition to the traditional literature sources, some selections of databases are integrated into a computer program. A perfect example is Michael Bello's Buffer Workshop program [18] that contains pK_a and mobility values of 475 acids and 66 bases, cited from eight previous collections by other authors [19,20]. Full references are given for each ion. In addition to being a valuable source of relevant parameters for capillary electrophoresis (CE), the pH, conductivity, ionic strength and buffering capacity of any buffer mixture can be calculated. Fig. 3 shows a screen capture of the program.

A simpler interactive program than Buffer Work-

Table 1
List of programs for log *P* estimation

Software	Manufacturer
ACD/logP	Advanced Chemistry Development, Toronto, Canada
CLOGP	Daylight Chemical Inf. Syst., Mission Viejo, CA, USA
K_{OW}WIN	Syracuse Research, New York, NY, USA http://esc.syrres.com/interkow
SciLogP	SciVision, Burlington, MA, USA
AccuLogP	Microsimulations
ProLogP	CompuDrug International, South San Francisco, CA, USA

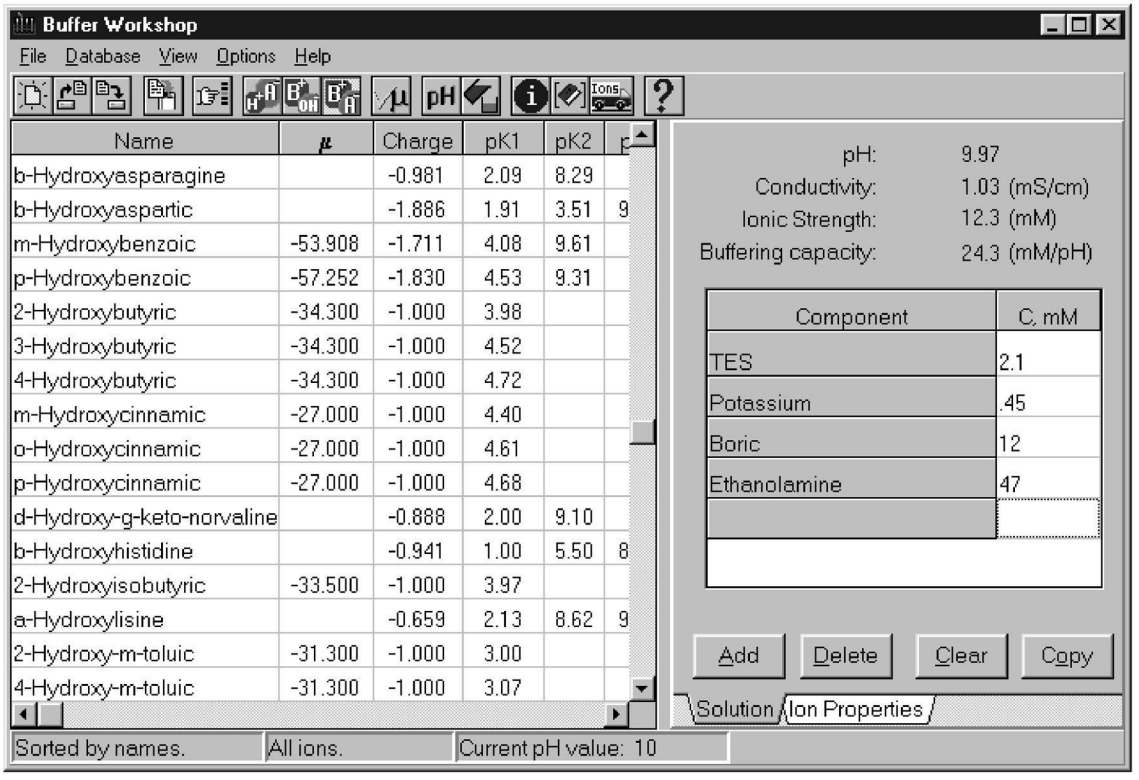

Fig. 3. Screen capture of Buffer Workshop.

shop that allows users to calculate buffer concentrations is available from the University of Manchester Institute of Science and Technology's Department of Biological Sciences web site: http://www.bi.umist.ac.uk/users/mjfrbn/buffers/makebuf.asp.

Apart from providing application notes, etc., the Beckman-Coulter site may also be accessed to download a program that permits calculation of CE parameters such as field strength, injection amount, volume and relative capillary length, corrected for temperature and viscosity. The web address is: http://www.beckmancoulter.com/Beckman/biorsrch/prodinfo/capelec/tst_calclg.asp.

At the site http://www.mobilise.com, one may access a database that allows keyword (analyte, probe, author) searches for background electrolyte, mobility, pK_a, references, probe molar absorptivities. This site also has a discussion forum (see below).

1.4. Sources of literature and theory

Next to traditional sources such as text books and journals, more and more data and resources are now available in electronic form. A searchable selection of 22 000 analytical references (titles, authors) from the period 1989–1997 is available on a CD-ROM from Elsevier Science (Amsterdam, The Netherlands). The database includes subsets for CE, liquid chromatography and gas chromatography. An update for the years 1998 and 1999 will appear shortly. For those without digital access to *Chemical Abstracts*, the above selection is an attractive source.

2. Internet resources

We have compiled a comprehensive, if not

exhaustive, selection of internet sites that offer useful information on CE. In the paragraphs that follow, we provide brief descriptions of these sites.

2.1. Company websites

Table 2 shows a list of web sites of several companies which manufacture CE systems. On some of these, e.g., Agilent Technologies, Beckman-Coulter and Waters, application notes are available for browsing.

2.2. Sites with specific CE information

Another important parameter of buffer and sample components in CE is pK_a. In the case where no experimental or literature value is available, an estimate can be very useful for both initial experiments and method development. Comparable general considerations as in the case of log *P* estimators apply. The results of ACD/pK_a estimation software were correlated for a limited selection of example components. The results, indicated in Fig. 4, show a correlation coefficient of 0.98 and a slight systematic difference with experimental values. Although this may seem reasonable as a first estimate, for some components there is a full pH unit difference.

A software vendor, Advanced Chemistry Development (http://www.acdlabs.com) the developer of the popular ChemSketch chemical structure drawing software also markets products that may be of use to CE practitioners include the Log P calculator, Solubility Calculator and pK_a, Calculator, and Chromatography Laboratory which allows users to deconvolute peaks, set up databases of structures, etc. Users' application notes are available, and there are some useful links to, for example, a Chemistry web-based magazine. The company also markets I-Lab, an Internet-based service for instant access to chemical databases and property prediction programs. Users can obtain nuclear magnetic resonance spectra and systematic names and predict properties such as pK_a or LogP for their chemical structures either through a web browser or from within ChemSketch.

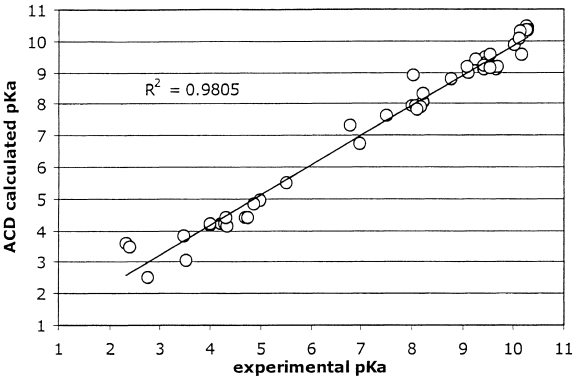

Fig. 4. Correlation between pK_a values calculated by the ACD/pK_a software and experimental values.

http://www.ceandcec.com, is a CE website of general interest. It is a comprehensive and well-designed site devoted to CE and capillary electrochromatography. Almost anything that a novice or experienced practitioner wishes to know about CE and its various guises is available here or through links to other sites. There are many links to journals, conferences, training courses, societies, consultancies, companies selling CE equipment and supplies, troubleshooting techniques and company web sites.

Table 2
List of some CE manufacturers' web sites

Company	Internet address
Agilent Technologies	http://www.chem.agilent.com/cag/products/ce.html
Beckman-Coulter	http://www.beckman-coulter.com/beckman/biorsrch/prodinfo/capelec/caphome.asp
Perkin-Elmer	http://www.pebio.com/ga/3700/features.html
Waters	http://www.waters.com/
Prince Technologies	http://ourworld.compuserve.com/homepages/PrinceTechnologies
CE Resources	http://www.ce-resources.com/index2.htm
BioMolecular Instruments	http://www.biomolecular1.com/

Descriptions of CE theory and applications of the various modes of CE are also available.

2.3. Miscellaneous sites of potential interest

http://www.webmolecules.com/cgi-bin/webmol-page.cgi: Although not specifically for CE, this site is useful because it provides three-dimensional visualization of molecules plus other information. It is fully indexed, and molecules are retrieved in VRML (a general-purpose three-dimensional plug-in) or CHIME (a molecular visualization plug-in) format; both can be downloaded free. The site also offers listings of the ''Top 100 Pollutants'', ''Top 200 Pharmaceuticals'', etc. Compound structures are downloadable. The database is claimed to contain information on 200 000 chemicals.

http://www.scimedia.com/chem-ed/sep/electrop/cap-el.htm: CE website of general interest, a very basic, no-frills site with a short introduction to CE, and a link to the Encyclopaedia of Analytical Instrumentation.

2.4. Discussion lists

The CE discussion group [21] is an e-mail-based isotachophoresis/CZE discussion list, moderated by V. Dolnik. Since 1993 it has provided an electronic community of over 400 expert and novice CE users. The number of contributions varies strongly, ranging from 1 to 10 weekly e-mails. Favorite discussion subjects are separation conditions and troubleshooting. Most contributions result in one or more replies.

Another free discussion forum is hosted by Voyager Info-Systems (http://www.voy.com/1810). It appears to attract a considerable number of respondents.

3. Conclusions

It is clear that the advent of the internet has considerably enhanced the means by which we are able to access information from remote sources, as well as estimate, through use of interactive software, physico-chemical parameters that would otherwise be difficult or even impossible to obtain, to aid us in our scientific work. Additionally, this electronic medium has enabled groups of scientists to discuss topics of common interest effectively without actually having to come together at a physical location. Through the internet, the conduct of science has become truly global.

References

[1] J.C. Reijenga, M.H.P.A. Martens, F.M. Everaerts, Electrophoresis 16 (1995) 2008.
[2] J.C. Reijenga, E. Kenndler, J. Chromatogr. A 659 (1994) 403.
[3] J.C. Reijenga, E. Kenndler, J. Chromatogr. A 659 (1994) 417.
[4] J.C. Reijenga, B.A. Ingelse, F.M. Everaerts, J. Chromatogr. A 772 (1997) 195.
[5] B.A. Ingelse, K. Sarmini, J.C. Reijenga, E. Kenndler, F.M. Everaerts, Electrophoresis 18 (1997) 938.
[6] Information from the author Han Martens at it@oemdata.nl
[7] http://www.chemsw.com/chromat.htm
[8] J.C. Reijenga, M. Hutta, J. Chromatogr. A 709 (1995) 21.
[9] R.A. Mosher, D.A. Saville, W. Thormann, The Dynamics of Electrophoresis, VCH, Weinheim, 1992.
[10] E.V. Dose, G.A. Guiochon, Anal. Chem. 63 (1991) 1063.
[11] S.V. Ermakov, O.S. Mazhorova, M.Y. Zhukov, Electrophoresis 13 (1992) 838.
[12] S.V. Ermakov, O.S. Mazhorova, Yu.P. Popov, Informatica 3 (1992) 173.
[13] S.V. Ermakov, M.S. Bello, P.-G. Righetti, J. Chromatogr. A 661 (1994) 265.
[14] S.V. Ermakov, M.Yu. Zhukov, L. Capelli, P.-G. Righetti, Anal. Chem. 66 (1994) 4034.
[15] B. Gaš, J. Chromatogr. 644 (1993) 161.
[16] J.H.P.A. Martens, J.C. Reijenga, J.H.M. ten Thije Boonkkamp, R.M.M. Mattheij, F.M. Everaerts, J. Chromatogr. A 772 (1997) 49.
[17] C. Schwer, B. Gaš, F. Lottspeich, E. Kenndler, Anal. Chem. 65 (1993) 2108.
[18] Information from the author at mishabello@aol.com
[19] 6th ed., Landolt-Börnstein's Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik, Vol. 2, Springer Verlag, Berlin, 1960, Part 7.
[20] T. Hirokawa, N. Nishimo, N. Aoki, Y. Kiso, Y. Sawamoto, T. Yagi, J.-I. Akiyama, J. Chromatogr. 271 (1983) D1.
[21] To subscribe, submit a request in this format: SUBSCRIBE CZE-ITP<firstname><lastname> to listserv@muni.cz