Computer-assisted modelling, optimizations and data evaluations in electrophoresis

Pavel Dubský[1,*]

[1] *The group of Electrophoretic and Chromatographic separation Methods, Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Hlavova 8, 128 43, Prague 2, Czech Republic*

*dubsky@natur.cuni.cz

Development of scientific software for capillary electrophoresis (CE) has a long tradition in our research group, and the software is publicly available [1]. We summarise a number of software tools and demonstrate their potential for solving various scientific problems in this talk.

Simul, introduced in late 80's, is one of the first simulators of 1D electrophoresis. An adaptive grid algorithm that enables the spatial grid points to concentrate in regions of the biggest computational effort [2] has been incorporated into Simul recently. Simul Complex is the newest update that can account for interactions between analytes or BGE components and one (e.g. chiral) selector in the system, as in the affinity capillary electrophoresis (ACE) setup. Still, the development has not been finished and new upgrades should introduce parallelized computational core, interactions with any number of selectors or multi-platform releases for Linux and Mac OS, to list a few.

PeakMaster calculates BGE properties (pH, buffer capacity, conductivity etc.) and discloses an occurrence of system peaks in capillary zone electrophoresis (CZE). Since its introduction at the beginning of 2000, new theory enabled drawing exact shapes of the system peaks and evaluating simple ACE systems in 2012. The very new CAES model can account for general ACE systems enabling – among others – calculations of pH-shifts in the BGE due to complexation. Predictions of system peaks in general ACE systems is on the way.

CEval is designed for easy data evaluations in CE and ACE. It performs automated HVL fit, a feature essential in CE that is however not provided by CE manufacturers. Automated evaluation of ACE data is already included for obtaining complexation constants, and data transformations for other physical-chemical parameters shall be available in a near future. DualAnalyzer – on the other hand – utilizes complexation constants determined, e.g., by means of CEval and assists in finding optimal dual-selector mixtures for individual separations in ACE, when a single selector does not provide good enough resolution.

Financial support by the Czech Science Foundation grant no. 15-18424Y is acknowledged.

References

[1] http://echmet.natur.cuni.cz

[2] Originally introduced by Dr. Moran Bercovici in SPRESSO, http://microfluidics.technion.ac.il/open-source-simluation-tool-for-electophoretic-processes/