Session [10D05] - Novel Computer Applications in Chemical Engineering
http://www.aiche.org/Annualapp/previewmodule/SessionDetail.asp?SessionCode=10D05

Design and Optimization of Microchip Based Electrophoretic Channel Topologies

Anton J. Pfeiffer (1) Yi Wang (2) Qiao Lin (3) Ryan Magargle (4) James Hoburg (5) Tamal Mukerjee (6) Steinar Hauan (7)

(1)(7) Dept. of Chemical Engineering
(2)(3) Dept. of Mechanical Engineering
(4)(5)(6) Dept. of Electrical and Computer Engineering

Carnegie Mellon University
Pittsburgh PA, 15213

Micro-scale electrophoretic separation systems provide a highly effective, versatile and inexpensive method for separating a wide variety of chemical components [1]. Particularly useful applications include separation of biological molecules, chemical sensing, and combinatorial chemistry [2]. Micro-scale electrophoretic separation systems are an integral part of 'lab-on-a-chip' technology.

Efficient and accurate phenomenological models are necessary for the development of 'lab-on-a-chip' technology. Currently designers create micro-scale electrophoretic designs by using laboratory experiments, numerical simulations, or by developing piecewise phenomenological models for specific channel geometries[3-5]. Finite element and experiment based design techniques require a great deal of time and therefore become inefficient for feasibility studies and design optimization. Piecewise phenomenological models, while faster, are limited by assumptions pertaining to initial conditions, boundary conditions, and regions of applicability.

We have implemented a computer-based systematic design methodology that addresses two fundamental problems in the design of electrophoretic microchips: (1) determine a set of feasible designs for a confined chip area (2) determine the minimal area that meets the desired system constraints. This has been accomplished through the creation of a micro-electrophoretic simulation engine [3], channel placement/packing algorithms [4], and numerical optimization. Our methodology is highly flexible and modular. It allows us to investigate multi species systems and complex system layouts. The modular design of the simulation engine allows us to readily exchange, test and verify new models as they become available. Key to our approach is the development of accurate high speed component models that capture phenomena not found in the current literature.

Currently, piecewise algebraic/logic models with phenomenological descriptions taken from the literature [5-7] are implemented within the simulation engine. These descriptions are connected together by the simulation engine to encompass the full design space. While the models from the literature are accurate for single channel sections, the assumptions contained within these models begin to break down when many sections are connected together. Two important phenomena are neglected by the current literature models: (1) dispersion caused by skewed species bands entering channel sections (2) electric field induced dispersion around turns. Both of these effects have been implemented as piecewise algebraic models that can be readily incorporated into the electrophoretic simulation engine.

We will demonstrate the validity of our new models and quantify the impact that these new models have on the design of channel systems. We will show how our methodology can be used to create designs that fit within confined areas and designs that occupy minimal area. Incorporation of dispersion resulting from band skewing and dispersion resulting from electric field effects influence the system design for particular design scenarios and operating conditions. We will show that these effects become of increasing importance for the design of efficient practical designs.

[1] Freemantle, Michael "Downsizing Chemistry" C&EN, December 22, 1999 pg. 27-36

[2] Bruin, G. "Recent Developments in Electrokinetically Driven Analysis on Microfabricated Devices". Electrophoresis, 21, 2000 pg. 3931-3951

[3] Pfeiffer, A.J., Mukherjee, T. and Hauan, S. "A Synthesis Framework for Microscale Electrophoretic Separation Systems". AIChE annual Meeting November 2002

[4] Pfeiffer, A.J., Mukherjee, T. and Hauan, S. "Topology Trade-offs in the Synthesis of Chip-Based Electrophoretic Separation Systems". Proceedings of NanoTech 2003 (MSM '03) pg. 250-253

[5] Paegel, B.M., Hutt, L.D., Simpson, P.C. and Mathies, R.A. "Turn Geometry for Minimizing Band Broadening in Microfabricated Capillary Electrophoresis channels". Anal.Chem. 2000, 72 pg. 3030-3037

[6] Molho, J.I., Herr, A.E., Mosier, B.P., Santiago, J.G., Kenny, T.W., Brennen, R.A., Gordon, G.B. and Mohammadi, B. "Optimization of Turn Geometries for Microchip Electrophoresis". Anal.Chem. 2001 73, pg. 1350-1360.

[7] Griffiths,S. and Nilson, R. "Low Dispersion Turns and Junctions for Microchannel Systems". Anal.Chem. 2001, 73, pg. 272-278

[8] Culbertson, C., Jacobson, S., and Ramsey, M., "Dispersion Sources for Compact Geometries on Microchips" Anal.Chem. 1998, 70, pg.3781-3789