570e A Modular Simulation Framework for Microfluidic Chips

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Microchip structures represent an attractive platform for microscale chemical sensing and analysis. These chips, often called Labs-on-a-Chip (LoC), are typically made using glass, plastic or silicon substrates, and can be fabricated inexpensively using mature technology adapted from the semiconductor industry. They have been used throughout the life science and biomedical industries for applications in genomics, proteomics, drug discovery, and forensics [1]. LoC's have the potential to be fast, accurate, and readily automated. Here we present a system-level simulation framework for channel-based microfluidic devices in which unit processes including mixing [2], reaction, separation [3], and injection [4] are connected together to simulate complete LoC's.

Currently, the bulk of work in microfluidic simulation focuses on a single part of a larger system and is carried out using computational fluid dynamics (CFD) or finite element modeling (FEM) packages [1,5]. While CFD/FEM simulations provide highly accurate detailed results, they are computationally expensive for system simulation and can be prohibitive for complex system optimization. Simulation tools that use high-speed reduced order models [6,7] have been created. However, these simulation frameworks often require CFD/FEM pre-solves to extract model parameters. While this restriction is only moderately inconvenient for system simulation, it greatly impedes design optimization and synthesis. Finally, colleagues [2,3,4] have created models that make system simulation possible without CFD/FEM pre-solves. However, these models were implemented in a pre-existing circuit simulation tool [10] that is difficult to incorporate into an optimization framework. Here, we develop a simulation framework that solves these problems.

Our simulation framework is both simple and flexible. It is tailored to microfluidic design and can be readily implemented using standard programming languages. We specifically focus on electrokinetically driven systems, although our approach can also be extended to pressure driven systems. Our simulator is capable of addressing the complex physiochemistry, transient behavior, and channel layout effects that occur in a microfluidic chip. We accomplish this by combining key concepts from process flowsheet simulation, such as sequential modular unit operations and stream tearing, with key concepts from electrical circuit simulation, such as Kirchoffian network analysis and topological sorting.

We illustrate the flexibility of our framework by showing how a microscale reactor model is interfaced with the simulator. This reactor model uses a system of nonlinear ODE's to describe 2D reacting flow within a microchannel over a wide range of flow and reaction regimes. We show that by requiring the reactor model to satisfy a compact set of general information-passing parameters, the model can be interfaced with any other model in the system. We demonstrate our simulation capabilities by systematically analyzing experimental designs taken from the literature [11] and designs generated using FEM. We show that our simulator can estimate key system design variables quickly and accurately. Finally, we discuss how our simulator can be incorporated into a design optimization framework.

[1] Geschke, O., Klank, H., and Tellemann, P., "Microsystem Engineering of Lab-on-a-Chip Devices", Wiley-VCH, 2004.

[2] Wang, Y., Lin, Q., and Mukherjee, T., "Analytical Models for Complex Electrokinetic Passive Mixers", MicroTAS 2004, pp. 596 - 598.

[3] Wang, Y., Lin, Q., and Mukherjee, T., "System-oriented Dispersion Models of General-shaped Electrophoresis Microchannels", Lab-on-a-Chip (LOC), 2004 pp. 453 - 463.

[4] Magargle, R., Hoburg, J.F., Mukherjee, T., "Microfluidic Injector Models Based on Neural Networks", NanoTech 2005, Vol. 1, pp. 616 - 619.

[5] CFD-ACE+ Multiphysics modeling package, CFD Research Corporation, http://www.cfdrc.com, May 2005.

[6] Karam, J.M., Courtois, B., Poppe, A., Hofmann, K., Rencz, M., and Glesner, V., "Applied Design and Analysis of Microsystems", European Design and Test Conference, (ED&TC 1996), 1996, pp. 528 - 532.

[7] Korsmeyer, T., Zeng, J., and Geiner, K., "Design Tools for BioMEMS", Design Automation Conference (DAC 2004), 2004, pp. 622 - 627.

[8] Virtuoso Spectre Circuit Simulator, Cadence., http://www.cadence.com, May 2005.

[9] Tang, T., Badal, M.Y., Ocvirk, G., Lee, W.E., Bader, D.E., Bekkaui, F., and Harrison, D.J., "Integrated Microfluidic Electrophoresis System for Analysis of Genetic Materials Using Signal Amplification Methods", Analytical Chemistry, 2002, pp. 725 - 733.

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