Mixed-Dimensionality, Multi-Physics Simulation Tools for Design Analysis of Microfluidic Devices and Integrated Systems

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ABSTRACT

Computational design of microfluidic devices and integrated microsystems involves several strongly coupled physical disciplines, including fluid mechanics, heat transfer, stress/deformation dynamics, electrokinetics, biochemistry and others. CFDRC is developing a mixed-dimensionality, multi-physics CAD system, CFD-ACE+, using high-fidelity field solvers on unstructured, solution-adaptive grids and reduced dimensionality modeling tools for both detailed design of devices and rapid prototyping of complete fluidic microsystems. The paper presents overall description of the software architecture and the design flow in CFD-ACE+. It describes current status, ongoing efforts and future plans for the software. The paper also discusses new concepts of mixed-level and mixed-dimensionality capability in which 1D microfluidic networks are simulated concurrently with 3D high-fidelity models of discrete components (e.g., pumps, mixers, valves, reactors, etc). The concept is illustrated on selected examples of microfluidic devices and microsystems.

Keywords: microfluidics, MEMS, bio chips, multiphysics, modeling and simulation, CAD.

1 INTRODUCTION

It is generally recognized the microsystems technology will be the focus of intense international competition, and exciting new MEMS-based products will drive the commercial markets [1]. From the microsystems standpoint, conventional microelectronic chips are extremely simple: a large number of silicon based transistors interconnected by a complex system of metallization lines. The new generation of microfluidic chips will host mechanical devices, fluidic channels, chemical mixers and reactors, bioanalytical devices, photonic devices and circuits, and a myriad of others, all integrated with the electronics. We contend that the success of the microsystems industry to a large extent will be determined by the availability of Computer Aided Design (CAD) tools. High prototyping costs, long product development cycles, and time-to-market pressure create acute demands for sophisticated, commercial quality design tools. In electronic (IC) CAD, where a small set of standard devices (e.g. transistors, capacitors) are used in large numbers, then design tasks include placement, routing, and electrical analysis. In microsystem CAD, the problem is much more complex. There are no standard devices, there are a large number of disciplines involved (fluidic, thermal, mechanical, electric, electrokinetic, bio-electro-chemical, optical, controls, ...), there are no simple compact models for system level simulation, there are no standard fabrication processes, and there are several different kinds of materials used (from Si to glass, to plastic). It will take a significant effort to establish commercial quality Microsystem CAD tool.

This paper presents a comprehensive microsystem CAD environment, CFD-ACE+, for bio and microfluidic devices and complete microsystems. The tool provides high fidelity 3D multiphysics modeling capability, 1D fluidic circuits modeling for system level simulations, and mixed-dimensionality design. It combines tools for layouts and process fabrication, geometric modeling, and automated grid generation, and interfaces to EDA tools (e.g. Cadence).

2 FROM LAYOUTS TO MODELS

Simulation process of microsystems involves two challenging steps: geometric modeling and mesh generation. Since geometrical configurations of microsystems are often very complex, typically the grid generation task is performed manually with mechanical CAD tools, which is a tedious and time-consuming effort. A fully automated mesh generation procedure from 2D layouts and fabrication process specifications has been developed and implemented in CFD-Micromesh [2]. Figure 1 illustrates a sample 2D layout of a micromixer and the resultant 3D mesh.

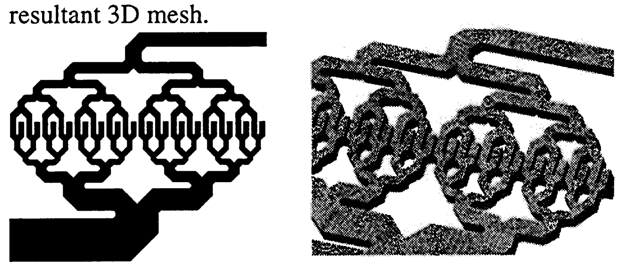


Figure 1: Layouts a Micromixer and 3D Mesh Generated in CFD-Micromesh [2].

The layouts are imported in standard formats (CIF, GDSII, and DXF). However, image formats (GIF, JPG) can also be used. The code generates a 3D model using operations specified by the fabrication process data (deposit, etch, bond) or directly by the user. A 3D finite element mesh with tagged material properties, boundary and volume conditions is then automatically generated. The complete model description is saved in a standard DTF format [11]. The automatic generation of the 3D model and mesh typically takes a couple of minutes on a current PC machine.

3 HIERARCHY OF MODELS

Simulation and design of microfluidic systems requires at least two levels of modeling:

- high-fidelity models (usually three-dimensional finite element or finite volume) for multiphysics design and optimization of particular elements and devices (e.g. their geometrical structure); and
- system-level models for simulation of complete microsystems integrated from a large number of devices, for which reduced or compact models are necessary to make such system simulations computationally feasible.

Generation of compact models for microfluidic devices is one of the most challenging and time consuming tasks in the design process. The difficulties arise from the nonlinearity of physical processes, and from the coupling between physical disciplines e.g. structures, fluid, electrostatic, thermal. There are several approaches to generating compact models ranging from simplified analytic description with algebraic expressions, to functional curve fits to experimental performance characteristics, to equivalent electrical (RLC) circuit models. Compact models can be generated from experimental data for existing devices or from detailed parametric simulations using high fidelity models. Figure 2 illustrates high-fidelity and compact model representations for a fluidic Tesla valve.

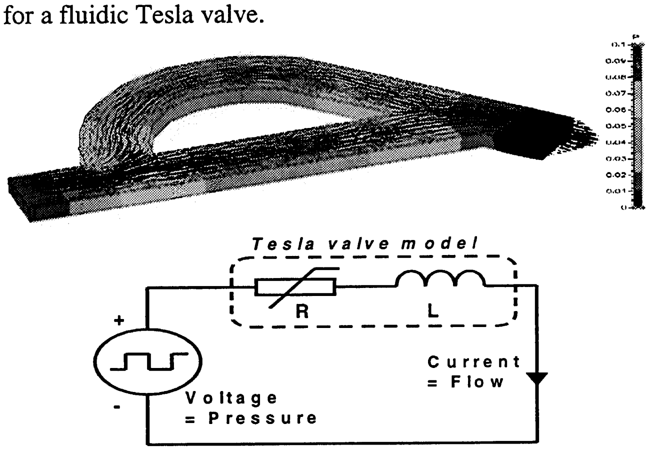


Figure 2: CFD-ACE+ high-fidelity model and a nonlinear compact (circuit) model of a fluidic Tesla valve

A comprehensive library of reusable compact models for electronic, fluidic, and mechanical devices will have to be established for system-level simulations such as SPICE or SABER. Circuit models for fluidic channels, valves, pumps, mechanical membranes, comb drives, microheaters, and others have been demonstrated. For example, circuit models of air damping for inertial sensors and for synthetic jets have been recently demonstrated by the authors [2-5]. 3D models can be used for modeling larger components of fluidic microsystems but computational time (hours per case) will limit the number of design parameters. Circuit models, once validated, allow for rapid parametric simulations of a large number of designs. Figure 3 demonstrates component level modeling for a membrane pump with multiple inlet/outlet valves using 3D models as well as equivalent circuit models.

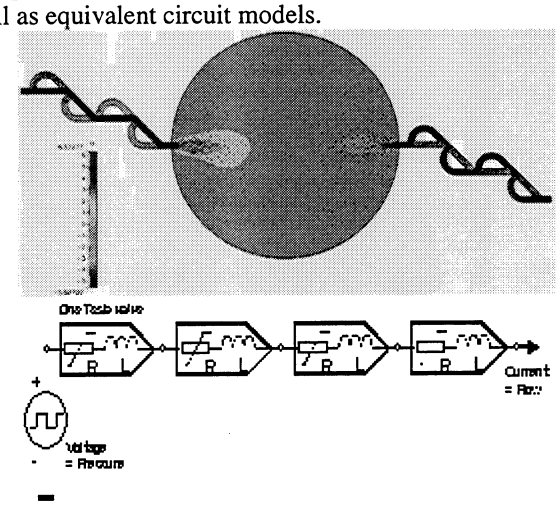


Figure 3: A 3D Model of the Micropump with Eight Tesla Valves and an Equivalent Circuit Model of a Micropump Branch with the Four Tesla Valves.

For some processes e.g. mixing, diffusion there is no clear way to generate the compact model. In those cases a mixed-dimensionality modeling technique can be used. CFD-ACE+ environment allows to link 3D device models, point models described with algebraic/differential equations, and circuit (SPICE, SABER) models to perform system level simulations. Coupling between the simulation levels is facilitated by integrating boundary conditions of the 3D model and using them as contact I/O signals for the system level simulator.

4 MULTIPHYSICS MODELS IN ACE+

Fluidic microsystems in biodiagnostic applications include broad range of devices such as valves, pumps, mixing chambers, electrokinetic channels, detection devices, and several types of microreactors (e.g. PCR, hybridization). Computational design of such systems requires multiphysics modeling capability. CFD-ACE+ environment offers a comprehensive suite of models including:

- Fluid mechanics equations with convection, diffusion, electromigration of mixtures, electrolytes, and biomolecules,
- Energy with conjugate heat transfer in solids, liquids and multiphase flows,

- General Multi-step Chemical Kinetics handling stiff reaction mechanisms,
- Free surface flows in 3D using VOF method with surface tension and Marangoni effects for hydrophobic, hydrophilic liquid filling, microdispensing, liquid wicking in membranes and microcapillaries;
- Multiphase flows solved with Eulerian-Eulerian or Eulerian-Lagrangian method to simulate particle, bubble, droplet, macromolecule transport in microchannels,
- Finite Element Method Stress/Deformation and dynamics model,
- Electrostatics, Electrodynamics, Electromagnetics, and Solid State Electronics,
- Electrokinetics of polyelectrolytes for electrophoresis, dielectrophoresis, and bioelectrochemistry; and
- Surface chemistry to simulate multi-protein binding, antigen-antibody, receptor-ligand, and enzyme-substrate interactions.

A detailed description of mathematical models, numerical methods, validation results, etc., has been presented in previous publications, e.g., [2-7]. In the next section we present examples of computational models of key microfluidic devices of microreaction systems

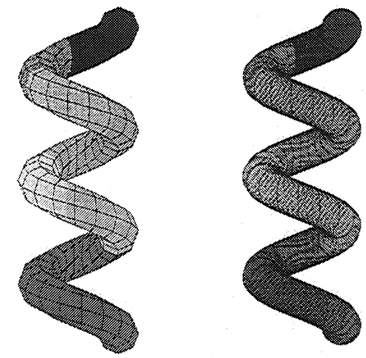
5 MODELING OF MICROFLUIDIC DEVICES AND SYSTEMS

5.1 Modeling Embedded Filaments

In microfluidic-thermal applications large aspect ratio (long) channels need to be modeled along with the surrounding substrate. A common computational mesh for channels and for the substrate would be prohibitive. CFD-ACE+ offers an embedded filament model with polyhedral mesh and coupled numerical-analytical integration of transport equations to solve the multiphysics fluidics channels problems. In a generalized polyhedral element used for filaments flow equations are integrated numerically in the stream-wise direction and analytically in the cross-stream direction. Very good solution accuracy has been achieved for flows in rectangular channels, bends, and even general tubes. Figure 4 demonstrates the flow in a spiral microchannel with two geometrical resolutions of the channel shape, 8-and 64-face polyhedra. Predicted pressure drop in this channel is within 7%, and 1%, of the analytical solution for the two-cell types. This technique can be used for fast simulation of complete fluidic microsystems.

5.2 Modeling Embedded Microheaters

Operation of a microfluidic T-shape reactor [8] is shown in Figure 5. Cold reactants entering through the upper portion require thermal energy to initiate a chemical reaction. Energy is provided using fine heating elements embedded in the wall of the upper portion of the mixing channel, as shown. Typical geometrical scales associated with the problem are 500 μm for the channel cross-section and 0.1 μm for the heater elements. Due to the large disparity in geometrical scales, domain gridding using conventional meshing techniques would be prohibitively difficult, resulting in an unnecessarily large number of grids. In the filament approach [9], each heater element was modeled by combining six straight sub-filament segments. Thermal energy was transferred to the surrounding wall through conduction. For simplicity, constriction effects were ignored. Figure 5 also shows the resultant temperature distribution in the reactants, and the upper wall containing the heaters.



8-face polyhedral 64-face polyhedral

Figure 4: Polyhedral Filament Model of a Spiral Tube

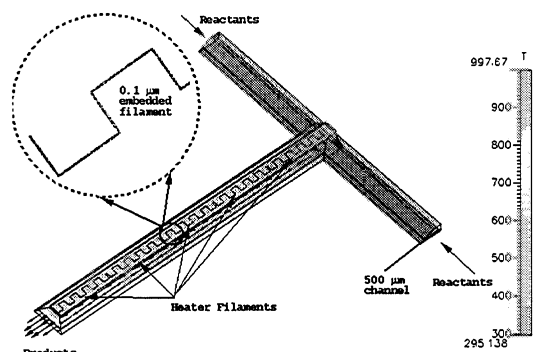


Figure 5: Filament Heating in Micro-Fluidic Reactor

5.3 Electrokinetics DC, AC, and TD

Coupling between electric field and multicomponent flow of ionic solution is encountered in electroosmosis, electrophoresis, electrochemistry, electrolysis, etc. Computational coupling between electric field equations, charged species transport, and chemistry is very strong. In CFD-ACE+, a direct nonlinear coupling procedure has been implemented for electrokinetics. The electric field can be solved for steady DC, time domain, and frequency domain AC problems.

AC electric fields can be creatively used in microfluidics to control flow patterns, enhance mixing, control residence times, promote surface chemistry, and transport and manipulate macromolecules, cells, beads, etc. Figure 6 demonstrates the flow in a channel with wall embedded interdigitated electrodes with localized electric actuation for top and bottom walls. Predicted time dependent electric fields and flow patterns show capabilities of flow control. Vastly different flow pattern are observed in these two test cases.

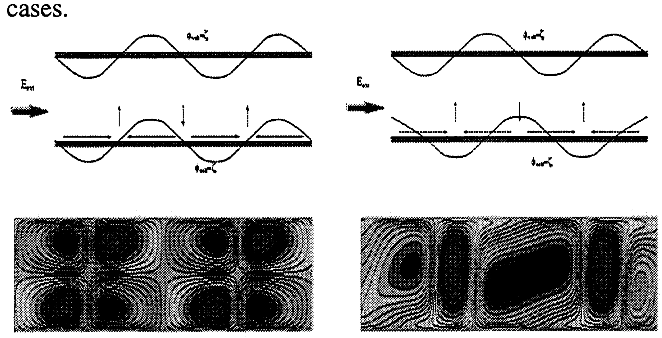


Figure 6: Electrokinetic Flow Control with Wall Electrodes and Localized Electric Actuation.

It is anticipated that a myriad of novel microfluidic, electrokinetic, and biochemical phenomena in very high frequency fields will be discovered in the near future. Computational modeling of these processes may play a major role in scientific discovery and commercial success. The major difficulty in modeling high frequency electrokinetics is the time scale disparity between electric (very short) and fluidic (very long) fields. In CFD-ACE+, a new concept of multi-time stepping and Time Domain – Frequency Domain (TD-FD) techniques have been implemented to solve this problem. Figure 7 shows the electric field and particle dynamics in a "dielectrophoretic vortex" with four wall electrodes at the microchannel wall actuated with AC field and phase shifts of 0, 90, 180, and 270 deg, respectively. The E-field is solved in FD and flow and macromolecule transport are solved in the TD mode field.

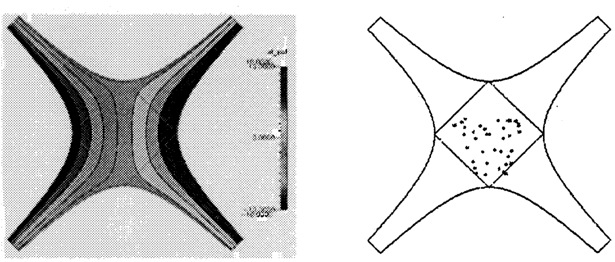


Figure 7: Particle Dynamics in an Electrokinetic Vortex

6 CONCLUSIONS

Comprehensive computational design tools will play a prominent role in the fluidic microsystems design process by providing optimal designs at reduced cost with shorter time to market.

The design tools will have to offer modeling capabilities for detailed 3D multiphysics analysis of individual devices (pumps, mixers, reactors) and fast system-level simulation of integrated microsystems. Unlike in the conventional engineering design, where each discipline is separately analyzed (flow, structures, thermal, electrical, controls), in microsystems all disciplines have to be analyzed in a coupled form. Such tools do not yet exist. This paper presents potential candidate software, CFD-ACE+, for multiphysics simulation of microfluidic and bio devices.

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7 REFERENCES

1. McWhorter P.J. "Intelligent Microsystems: Key to the Next Silicon Revolutionn", MST News, 4/1999.
2 Z.Q. Tan, M. Furmanczyk, M. Turowski, and A. Przekwas, "CFD-Micromesh: A Fast Geometrical Modeling and Mesh Generation Tool for 3D Microsystem Simulations", *Int. Conf. MSM 2000*, San Diego, California, March 27-29, 2000.
3. M. Turowski, Z. Chen, and A. Przekwas, "Automated Generation of Compact Models for Fluidic Microsystems", *CAD, Design and Test Conference*, Paris, France, 9-11 May 2000.
4. A. Przekwas, M. Turowski, and Z.J. Chen, "High-Fidelity and Reduced Models of Synthetic Microjets", *Int. Conf. MSM 2000*, San Diego, March 27-29, 2000.
5. Athavale, M.M., Yang, H.Q., and Przekwas, A.J., "Coupled Fluid-Thermal-Structural Simulations in Microvalves and Microchannels," Proc. MSM'99, San Juan, Puerto Rico, 1999, pp.570-573.
6. Athavale, M.M., Yang, H.Q., and Przekwas, A.J., "Coupled Fluid-Thermo-Structural Simulation Methodology for MEMS Applications," Transducers '97, Chicago, IL, 1997.
7 Yang, H.Q., and Przekwas, A.J., "Computational Modeling of Microfluidic Devices with Free Surface Liquid Handling," Proc. Int. Conf. MSM '98 April 1998.
8 Jensen K. F., Microchemical Systems: Status, Challenges, and Opportunities", AIChE J., V.45, 10, 1999
9. Pindera M.Z. and Przekwas, "Computational Framework For Modeling One-Dimensional, Sub-Grid Components and Phenomena In Multi-Dimensional Microsystems", Proc. MSM2000
10 Przekwas, A.J., "An Integrated Multi-Disciplinary CAD/CAE Environment for Micro-Electro-Mechanical Systems (MEMS)," Int. Symp. On Design, Test and Microfabrication of MEMS, France, 1999.
11 CFD-ACE+, CFD Research Corporation, 1999, Huntsville, Alabama, USA, (for detailed software description, see http://www.cfdrc.com).