Hierarchical Simulation for Microelectrofluidic System Process Performance Analysis

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ABSTRACT

With the sophisticated development of microelectrofluidic devices and systems, system performance analysis is a key for system optimization and system re-design. Due to the increasing complexity and natural characteristics of microsystems, system performance is intensly related to low-level component design and operation features. This paper presents a hierarchical modeling and simulation method for a micro chemical analysis system. Relationships between overall microsystem capacity and constitutive component performance are analyzed. The objective is to understand quantitatively how variations in device properties influence system throughput and utilization. Such information is useful for system architectural design and manufacturing yield optimization.

Keywords: Microelectrofluidic Systems (MEFS), Hierarchical Modeling and Simulation, Micro Chemical Analysis System, Finite Element Method (FEM), Performance Analysis

1 Introduction

With microelectrofluidic devices and system technology advancing in both design complexity and fabrication integration, system performance analysis is becoming more important for design optimization, enabling new, next generation microelectrofluidic system designs that will seek to push significantly present performance envelopes. For instance, the impact of increasing pump pressure on liquid flow rates and, in turn, on overall reaction and dispensing rates can be investigated. Optimal reservoir utilization and required microvalve settings for time sequencing of fluid transport and channel utilization can also be studied. But due to the special characteristics of microelectrofluidic system, MEFS system performance is still strongly tied to the low-level design component variance. For example, the pressure-controlled check valves with their static and dynamic properties are very important for determining the behaviour and flow rates of a micropump, which determine the performance of a drug delivery system or chemical analysis system. However, increasing the device complexity makes full system with low-level modeling and simulation time consuming, especially if coupled analyses become necessary.

By paying attention to certain more tractable subtasks, encompassing both architectural system simulation with functional macro modeling and circuit component simulation with lumped-parameter nodal modeling, hierarchical modeling and simulation, shown in Figure 1, play a significant role concerning both application complexity and component capacity. Application complexity involves investigating how the performance of the reconfigurable microliquid handling system architecture scales with increasingly complex chemical and biological analyses, and what types of biomedical applications can be practically miniaturized via microfluidic molecular processing. Component capacity involves investigating how the performance of the reconfigurable microliquid handling system scales with advances in constituent microfluidic device technology. This information is useful in projecting how the rapid pace of microfluidic device technology will influence microfluidic molecular systems. Such a hierarchical modeling and simulation methodology reduces model design complexity, shortens model developing time, and allows a designer to explore problems early during the development process. Meanwhile, it provides guidance for future research investment strategies.

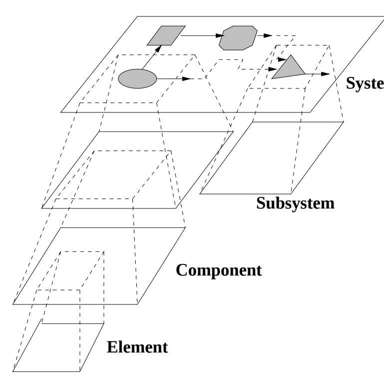

Figure 1: Schematic view of Hierarchical Modeling and Simulation Algorithm

In this paper, our aim is to present a hierarchical modeling and simulation methodology for composite microsystems and to show its application to the system design of a micro chemical system. In section 2, a micro chemical analysis system and its micropump structure are presented. The hierarchical modeling with system-level modeling by an advanced simulation language and micropump dynamic component modeling and simulation results by finite element methods are presented in section 3 and section 4. In section 5, hierarchical simulation results and system performance analysis are discussed. Conclusions and future work are summarized in section 6.

2 A Micro Chemical Analysis System

Refering to the silicon integrated miniature chemical analysis system introduced by Bart H., *et al*, [5], a micro chemical analysis system is presented as Figure 2, which comprises a bidirectional micropump connected with a sensor cell, and a storage buffer with n equal volume cells.

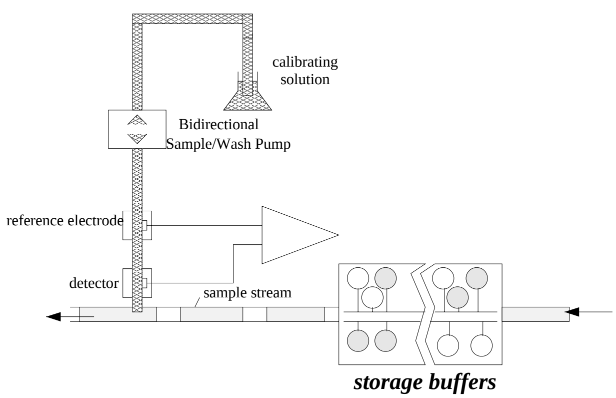

Figure 2: A Micro Chemical Analysis System

With a special valve design and high actuation frequencies, the resonances of the passive check valves become important, which makes a phase shift happen between the movement of the valve and the pressure difference driving the fluid as well as the valve. This effect can be used to cause the micropump to operate in a bi-directional mode. Figure 3 shows the schematic view of an electrostatically driven diaphragm bi-directional pump.

Due to the limited displacement of valves for fluid handling with the micropump, sample solutions have to be carefully filtered or these solutions can not pass the pump valves. When the pump works in the sample direction, it is intermittently used to draw a small sample from the sample stream, just enough to fill the system up to the detector, but not enough to reach to the sensitive micropump valve. After detection, the pump works in the wash direction, and it flushs the detector cell with filtered calibrant solution. Due to the time spent on drawing a sample, and in the detecting and washing pump operations, the chemical samples will be stored in the storage buffer until the detector is free. There are air bubbles to separate different samples.

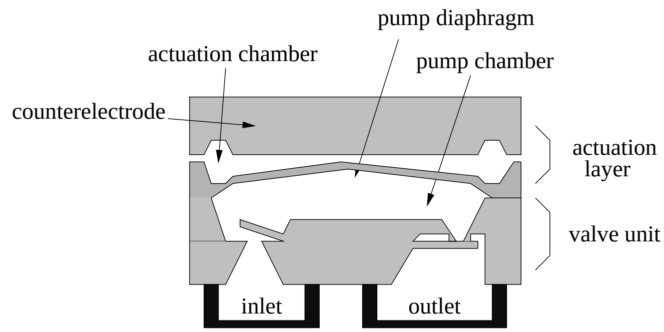

Figure 3: Schematic view of an electrostatically driven diaphragm pump

The working principle of micropumps can be separated into two stages. In the supply stage the voltage is turned off and the pump diaphragm is released. As it tends to return to its first equilibrium position, the ΔV fluid will be rejected out from the pump to the outlet. The output valve will be opened and the input valve will be closed at the same time. During the pumping stage, the active condenser is biased, the pump membrane deflects upward, and an amount of fluid ΔV will flow in from the inlet to the pump. The input valve is opened and the output valve remains closed.

3 System Performance Modeling

Depending on the analysis procedure, the analyzing process can be separated into three stages. In the first stage the fluidic sample is sucked into a detector, which can be equal to a server process. The server time is dependent on the micropump operating parameters. The second stage is the analyzing stage. The fluidic sample is analyzed in the detector, and the process time is determined by the kind of fluidic samples. In the third stage the fluidic sample is ejected out. This is also named the solution clean stage, which is the same as the first stage. The server processing time is dependent on the micropump operating parameters.

Therefore, from the system level modeling view, this micro chemical analysis system can be modeled with an advanced simulation language as a sequential threestep, one server queuing system involving the transfering of a fluidic sample from a storage buffer into the detector chamber for the analyzing operation. Assuming that the chemical analysis system mainly analyzes two kinds of fluidic samples, SS_A and SS_B, the interarrival time of fluidic samples, denoted by $T_1, T_2, \ldots$ are independent, identically distributed (IID) random variables with a certain probabilistic distribution. Some of the fluidic samples are classified as fluidic type A, and some are classified as fluidic type B. The volume for all fluidic samples is the same. It just occupies one storage cell in the storage buffer. A fluidic sample that arrives at the storage buffer and finds the detector chamber (service) idle, enters service immediately. Otherwise, it is queued into a cell of reservoirs located in the storage buffer. When the analyzing process competes for a fluidic sample, another fluidic sample is gated (valved) into the detector using a first-in, first-out (FIFO) discipline. After analysis, the fluidic sample will be sent out of the detector for further processing. Depending on the different kinds of fluidic samples, the analyzing time for the individual fluidic samples may be different for the fluidic sample type A and the fluidic sample type B. The delivery time of fluidic samples in the microchannels is ignored. The detector sample loading time and calibrant solution flushing time are dependent on the sample volume needed and the flow rate of the micropump, which is related to the membrane operating frequency.

4 Micropump Modeling and Simulation

Micropumps usually consist of an actuation unit and two passive check valves. Microchannels are used for connecting the inlet port and outlet port. The pump provides the pressure gradient for moving liquid in channels, reservoirs, and chambers. Piezoelectric, thermopneumatic and electrostatic drives are normally used as driving mechanisms. There are several micropump modeling methods. Static and dynamic flow simulations with the finite element method (FEM) done by J. Ulrich and Zengerle [6] are used in this paper.

Three coupled differential equations, Equation 1, Equation 2 and Equation 3 are used for describing the transient behaviour of the pump chamber pressure driven by an electrostatic mechanism and the passive check valve movement x_{iv}, x_{ov}.

$$\dot{p} = \frac{\Phi_{iv}(p, x_{iv}) - \Phi_{ov}(p, x_{ov})}{\frac{dV_o(p)}{dp} - \frac{dV_{gas}(p)}{dp}} \qquad (1)$$

where iv means the inlet valve and ov means the outlet valve. The inlet flow is Φ_{iv}, and the outlet flow is Φ_{ov}. The volume of the pump chamber is V_0 and the volume of the gas bubble is V_{gas}, which can be derived from the continuity equation. The fluid flow can be calculated depending on the the functions of the total pressure difference and the valve movement. The pressure-dependent volume displacement of the actuation membrane can be simulated by a static FEM simulation.

Equation 2 and Equation 3 describe the dynamics of the valve.

$$m_{iv}\ddot{x}_{iv} + d_{iv}\dot{x}_{iv} + k_{iv}x_{iv} = S_{iv}(p_1 - p) \qquad (2)$$

$$m_{ov}\ddot{x}_{ov} + d_{ov}\dot{x}_{ov} + k_{ov}x_{ov} = S_{ov}(p - p_2) \qquad (3)$$

With the spring constant k taken from the static valve simulation, the damping factor d and the effective mass m could be obtained from a 3D FEM simulation. So with combinations of an analytical solution and the results of FEM simulations, these three coupled differential equations are solved with a numerical solution, and the result with the frequency-dependent micropump rate is depicted in Figure 4 [6].

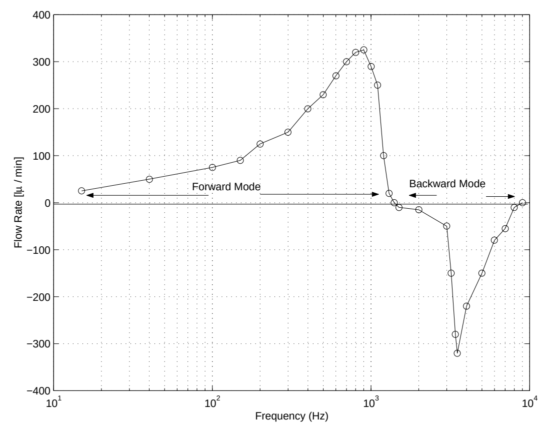

Figure 4: Frequency-dependent pump rate of a bidirectional micropump[6]

5 Simulation Results and Performance Analysis

Depending on the result of the frequency-dependent micropump rate depicted in Figure 4, four frequency selections are made to study the system throughputs and storage buffer capabilities. All simulation ending times are 3500 time units. Related information about the number of jobs waiting in the storage buffer when the kth job is finished, system occupation with time t, and the waiting time of kth job are shown in Figures 5, 6 and 7.

Table 1 shows the comparison of simulation results with all four different frequency selections, and Figure 8

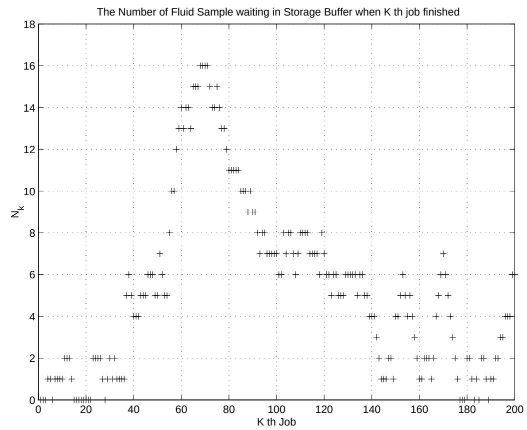

Figure 5: The number of jobs in the system when the Kth job finished

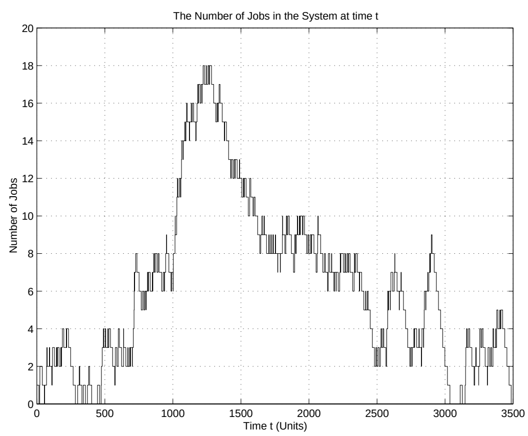

Figure 6: The number of jobs in the system at time t

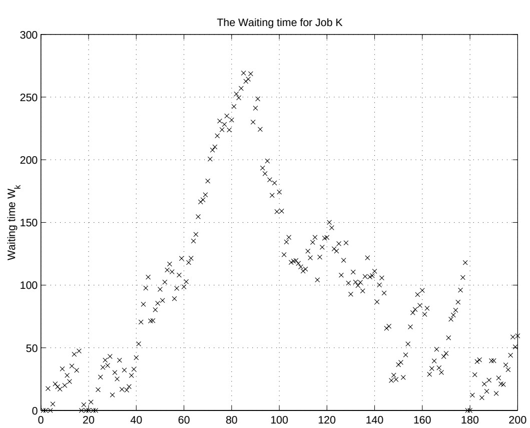

Figure 7: Waiting time of Kth job

and Figure 9 present the system throughput comparison and the storage buffer occupation information with different frequency selection by time t.

These simulation results show that the micropump flow rate is tightly related to the micropump operating frequency, thus the variation of the micropump operating frequency would influence the whole system performance. Therefore, with the appropriate frequency selection, the system can have better performance with higher throughput or on-target performance.

Meanwhile, the hierarchical system performance analysis can also benefit the system architecture design optimization. The simulation results show that system component designs are coupled. Thus, the storage buffer design is related to the design of the micropump, etc. In the meantime, the system component design is also related to the application area when considing the penalty of abandoning the processing fluidic sample due to the capacity of the system, the number of storage buffer cells, micropump, and even the delivery channel length have to be carefully designed to make the system operated at saturation status.

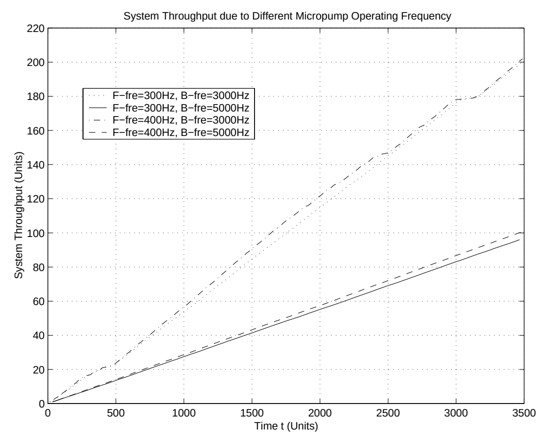

Figure 8: System throughput due to the different micropump operating frequency

6 Conclusion

This paper presents a rapid hierarchical modeling and simulation methodology with an advanced simulation language, analytical solutions and the Finite Element Method. This approach not only decreases the time of design, but also improves understanding of the system performance due to the variance of component parameters, and also provides the optimal design and sensitivity information which are very useful for the further new generation design.

Table 1: System Performance Comparison Due to Different Operating Frequencies

Statistical Parameters	$f_{forw.} = 300Hz$ $f_{back.} = 3000Hz$	$f_{forw.} = 300Hz$ $f_{back.} = 5000Hz$	$f_{forw.} = 400Hz$ $f_{back.} = 3000Hz$	$f_{forw.} = 400Hz$ $f_{back.} = 5000Hz$
Throughput after 3500 time units	200	96	202	101
Average Queue Length	5.45	56.73	2.40	54.63
Standard Deviation	4.36	31.45	3.12	30.25
Detector Average Utilization	0.94	1	0.87	1
Standard Deviation	0.23	0	0.34	0
Average Waiting Time	92.13	959.11	40.50	923.61

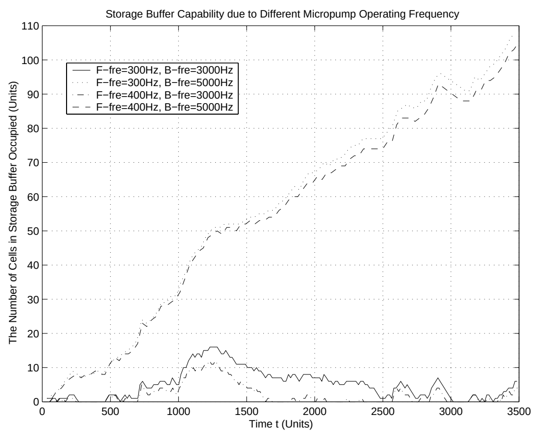

Figure 9: Storage buffer utilization comparison with different micropump operating frequency

The methodology presented in this paper is also helpful for developing Rapid Prototyping and CAD tools for system and design parameter optimization of complicated microsystems, like microelectrofluidic systems (MEFS) and microelectromechanical systems(MEMS).

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