Simulation of (Self-)Priming in Capillary Systems Using Lumped Models

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ABSTRACT

In this paper, a toolbox of lumped models for simulating (self-)priming and emptying of complex capillary networks is presented. Each model is a kind of an all-in-one-model, that considers inertia, friction, gravitation and capillarity and has been implemented on a conventional, commercially available, mixed-signal system-level simulator.

The toolbox contains fundamental microfluidic components which are lines with micromachined geometries, fittings, tees, dispensers and media transition elements.

With these all-in-one-models it is now possible for the first time to layout complex capillary networks by simulating not only the dynamic behavior of filled systems but even the priming and emptying.

Keywords: priming, emptying, capillarity, lumped models, microfluidic simulation.

INTRODUCTION

During the past few years there has been a continuously rising demand on microfluidic systems. In the majority of these systems the fluidic media is guided in complex capillary networks. Capillarity however, does not just mean a complication, which has to be accepted, but rather represents a fundamental working principle.

Due to the complexity and the interconnections of microfluidic components, the dynamic behavior and the priming of capillary networks is quite difficult to understand. Microfluidic systems therefore, must be designed on a simulator. A highly efficient simulation can be achieved by using lumped models, which consider the capillarity.

IMPLEMENTATION

Conventional Lumped Models

The consideration of friction and inertia effects of flow in conventional lumped models by using the LR-concept is state-of-the-art. The pressure drop across a certain line Δp can be calculated by

$$\Delta p = Rq + L\dot{q} + \rho g h \qquad (1)$$

where q is the flow and ρ the density of the fluidic media. With the acceleration due to gravity g and the difference in altitude between both ends of the line h gravitation can be considered. R is a function of the fluid's viscosity and the dimensions of the line. It combines all parameters concerning the pressure drop due to friction and equals an ohmic resistance in electric circuits, whereas L considers all parameters concerning the changes in pressure due to inertia. L therefore is defined by the fluid's density and again by the dimensions of the line. It equals an inductivity in electric circuits. The calculation of R and L is not the scope of this paper and can be found in literature [1-4] in detail.

Capillarity

Gravitation, friction and inertia effects are still applicable in micromachined geometries, but due to the small dimensions capillarity becomes a determinant factor in the behavior of microfluidic systems. In narrow dimensions capillarity leads to another pressure drop each time a meniscus exists. Therefore we have added capillary behavior to conventional models by implementing a pressure drop depending on the geometry as shown in equation 2.

$$\Delta p = x(Rq + L\dot{q} + \rho g h) + \frac{2\sigma}{r} \qquad (2)$$

σ is the surface tension and r the radius of curvature at the contact surface. This pressure drop, however, only occurs if a meniscus is in-between model boundaries, e. g. in the middle of a line. Consequently the new models must be able to deal with partially filled geometries on the one hand and with totally filled geometries on the other hand. In partially filled geometries the effects due to gravitation, friction and inertia must be scaled down with the filling ratio x, whereas in totally filled geometries capillarity must be neglected. x is defined as the ratio of the actual stored volume to the maximum volume of the implemented geometry.

Wetting States

Therefore, a model must determine its wetting state (empty, partially filled or full) by checking whether its connectors are wet or dry. On account of these states each model switches between three different sets of equations. Table 1 shows which pressure drops are considered in the corresponding wetting states.

wetting state		considered pressure drops			
pin 1	pin 2	gravitation	friction	inertia	capilla-rity
dry	dry	no	no	no	no
wet	dry	$f(x)$	$f(x)$	$f(x)$	yes
dry	wet	$f(x)$	$f(x)$	$f(x)$	yes
wet	wet	yes	yes	yes	no

Table 1: Wetting states and considered pressure drops.

Furthermore, connected models must have the same wetting information at joint connectors, because connectors are considered to be ideal and do not have any volume or other physical property.

Propagation of Wetting States

Due to this reason a model has to propagate or receive changes of its internal wetting state to, respectively from linked models in the neighborhood. Propagating this wetting information equals the simulation of digital networks. As shown in figure 1 we combined an analog, fluidic connector with digital, logic connectors. The fluidic media flows through the analog, fluidic net, in which the conservation laws are to be observed. In the meantime, the changes of the state passes through the digital, logic net.

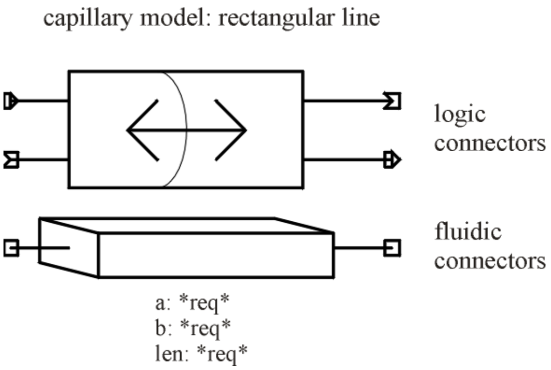

Figure 1: Single model, showing fluidic and logic connectors.

Connected Models

After splitting up the microfluidic system into discrete subsystems it can now be modeled by simply linking up the parameterized instances of the appropriate models as shown in figure 2.

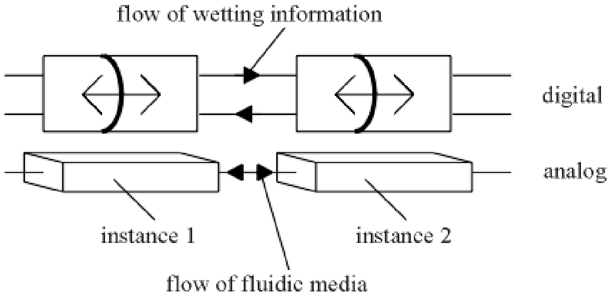

Figure 2: Connected instances showing the flow of wetting information and the flow fluidic media.

The working principle of these coupled networks is as follows: Imagine the meniscus is somewhere in-between the model boundaries of instance 1 and the flow is priming this instance from the left. This means, that the left hand fluidic pin of instance 1 is wet and the right hand pin of instance 1 as well as both pins of instance 2 are dry. Capillarity is considered in instance 1 but not in instance 2. After a certain time instance 1 is totally filled and the wetting state of the right hand pin is switched from dry to wet. With the switching of the wetting states the corresponding set of equations is switched on at instance 1. Now instance 1 throws an event and the new wetting state is propagated to instance 2. Instance 2 compares the external wetting state with its internal one. If an adjustment is necessary it changes the internal wetting state and switches to the appropriate set of equations. At this moment capillary effects are considered in instance 2 whereas they are not considered in instance 1. The meniscus has propagated from instance 1 to instance 2. At every change of the internal wetting state an event is thrown. Therefore instance 2 propagates its new wetting state back to instance 1. Instance 1 compares the new external state with its internal one, finds no discrepancy and decides, that no further actions are necessary. The propagation of the wetting state stops and the flow starts priming instance 2. Now imagine the flow changes its direction and instance 2 falls dry. Again the left hand pin of instance 2 changes its wetting state from wet to dry and capillarity is switched off at instance 2. An event is thrown and the new wetting state is propagated to instance 1. Capillarity is switched on at instance 1 and the wetting state is propagated back to instance 2, where the propagation of states stops.

As shown above the connection of instances seems to be very easy. But instances can only be connected in such an easy way, if neither the capillary pressure drop changes from one instance to another nor menisci have to propagate over branches.

Special Connection Devices

To solve these problems special connection devices are required.

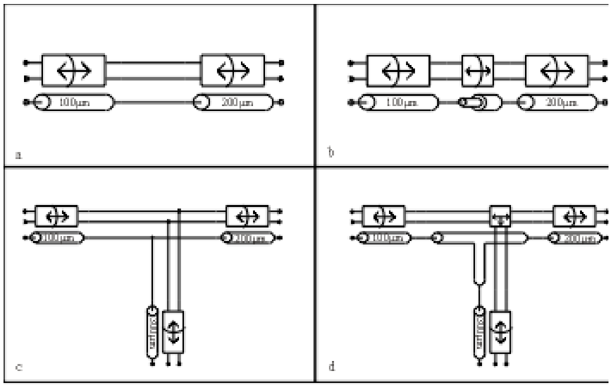

Figure 3: Connection devices used for propagating menisci over changes in diameter and branches.

Instances with different cross-section cannot be connected as depicted in figure 3a, because the meniscus could show an undamped oscillation between the two instances due to the abrupt, discontinuous changes in cross-section and pressure drop. The fitting model between the two lines in figure 3b implements a (very) small but finite volume, so that cross-section and pressure drop can change continuously.

In addition to this, digital shortcuts or incomplete connections (like shown in figure 3c) arise, if three instances are connected to branches. The implemented tee is shown in figure 3d and not only rules the propagation of the states correctly, it also allows the sticking and reconnection of a meniscus at a branch off. There is no need to implement branches with more than three side arms, because the direct coupling of *n* tees allows the connection of *(n+2)* branch offs.

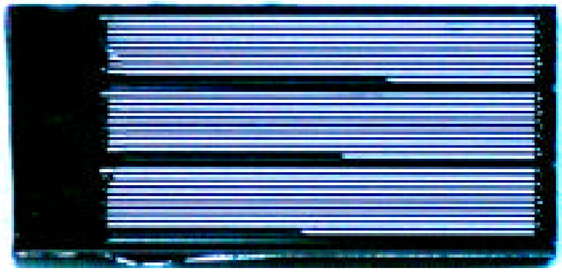

Figure 4: Micromachined meander network used for verifying models. Three menisci travelling through the channels at different positions.

This techniques allow the propagation of menisci across model boundaries so that priming and emptying even over changed cross-sections or branches of microfluidic networks can be simulated.

MEASUREMENTS

To verify the models we measured the speed of priming in micromachined meander channels. Channels with different geometries were etched in Si and sealed with a cover. The cover existed of Pyrex, so that the moving of different fluids could be observed by a camera through a microscope as shown in figure 4. After a drop of the desired liquid had been disposed at the inlet of the channel, the speed of the meniscus was retrieved by simply measuring the time and the traveled distance.

Because there was no simple way to measure the effective surface tension between the different liquids and the combination of Si-walls and Pyrex-cover directly in situ, we simulated a straight rectangular line and used the surface tension as the only fitting parameter to adjust the simulation to the measurements. These adjusted surface tensions were reasonable for all the different liquids and were used for former simulations.

Then we modeled the more difficult structures, which had very different cross-sections and geometries compared to the straight line, that we used for fitting, by simply linking up the corresponding modules from the toolbox as shown in figure 5.

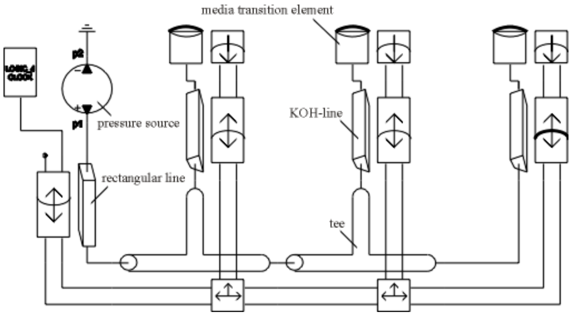

Figure 5: Model of the micromachined meander network forming fluidic and logic nets. Contrary to the drawing, the cross-section of the models used for verifying have had the same shape. The connection of models with different shapes is only shown to present more elements from the toolbox and is not possible without special interconnection devices in reality.

The results of the measured and simulated priming are compared in figure 6. The simulations were in a very good agreement with the measurements and proved the reliability of the models.

DISCUSSION

The consideration of capillarity and the propagation of states by coupling logic and analog fluidic nets are major enhancements in the simulation capabilities of lumped models. Priming and emptying as well as the dynamic behavior of complex capillary systems can be simulated by simply linking up the appropriate all-in-one modules from the presented toolbox. Changes in cross-section, the propagation of menisci over branches and the sticking of menisci in side arms are taken into consideration by special connection devices. The problem of capillarity is solved in a general approach. There is no need from the implementation to fill the fluidic network against air. Microfluidic networks can be simulated for any combination of fluidic media as long as the liquids are not mixable and do build up an interface. All modules have been implemented with a common hardware description language on a conventional, commercially available, mixed-signal system-level simulator.

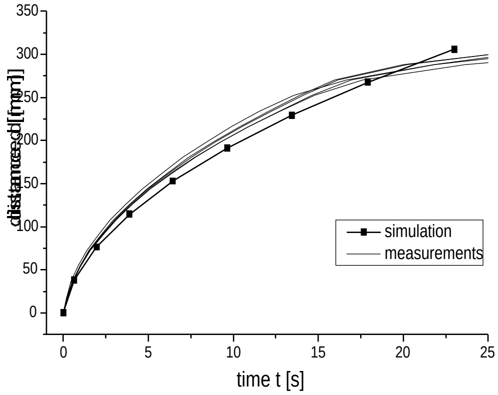

Figure 6: Comparison between measured and simulated (self-) priming.

Limitations

The implemented equations assume, that the fluidic media as well as the lines are incompressible. This is almost always no restriction due to the low pressures used in microfluidic devices. Furthermore, the flow in the channels has to be laminar.

Changes in the effective surface tension due to several priming cycles are not considered. In our implementation the surface tension for priming equals the surface tension for emptying. Hysteresis effects on account of the interaction of the fluid with the walls can not be simulated.

All models, except the tee, are able to handle only one meniscus in-between model boundaries. Nevertheless it is possible to simulate liquid bubbles, if using a lot of instances in such a way, that the size of the liquid bubbles guarantees, that at most one meniscus is for all instances at any time in-between model boundaries. Gaseous bubbles are compressible. Therefore the toolbox cannot simulate gaseous bubbles.

Outlook

In the future hysteresis effects could be considered by tracking the history of the device. The instance has to recall how long a wall has been in contact with the fluidic media (at least at discrete points). The surface tension could no longer be a constant and would have to be calculated as a function of the wetting time and the position of the meniscus in the line. To make the simulation of liquid bubbles more comfortable, a model must be able to handle more than one meniscus at a time in-between model boundaries. At this time, it would be reasonable to modify the equations for at least one compressible fluidic media and gaseous bubbles could be simualted.

ACKNOWLEDGEMENTS

The authors wish to thank the staff of HSG-IMIT for processing the chips used for verifying the models.

The project MikroDos is funded by the German Federal Ministry of Research and Technology BMBF under 16SV736.

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