Use of Numerical Methods for Modeling and Simulating Capillary Driven Flows in Microchannels

A. Quinte, S. Halstenberg and H. Eggert

Forschungszentrum Karlsruhe, Institut für Angewandte Informatik, Germany, quinte@iai.fzk.de

ABSTRACT

Today, medical test strips are used for rapid diagnostics and the quick and easy determination of biomedically relevant parameters, such as the content of glucose of the blood. For the transport of the test fluid into the test strip the capillary effect will be made use of. The technical progress achieved in microsystems engineering in the past years allows to fabricate precisely microchannels with defined structures using microstructuring techniques. Consequently, a selective control of the flow on the basis of an adequate geometrical design is possible. The use of computer-based simulators during the development of the medical test strips can reduce the costs and the time-to-market significantly. In this article the validation of the simulation tools FLOW-3D by FlowScience and CFX4 by AEA Technology will be discussed with regard to capillary driven flows. For this purpose, simple basic models have been applied. For the modelling and simulation of a medical test strip, a concept has been developed. It shall also be described in the present article.

Keywords: capillary driven flows, simulation of free surfaces, model coupling, microchannel

1 INTRODUCTION

The development of medical test strips still is often based on the knowledge and experience of the developers and expensive trial-and-error methods. With the use of simulation tools for the calculation of the propagation of flow in microstructures many different designs can be tested and the system can be improved. Spreading of the test fluid in the structure cannot be described sufficiently in an analytical way due to the complexity of the structure. So, it is necessary to use simulation methods which discretise the flow space to calculate the shape of the fluid/fluid interface, for example finite volume methods (FVM) or finite difference methods (FDM). As information on the validity of the capillary models within the above simulation tools is still lacking, some basic structures have now been evaluated. For these structures the flow behaviour could be described analytically. For one of the structures we also used measurement results for the comparison with the simulation results.

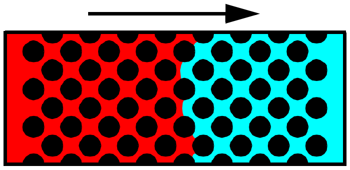

Figure 1: Microchannel with integrated columns

2 PHENOMENOLOGICAL CHARACTERISATION

Figure 1 shows the schematic representation of a microchannel with integrated columns. From the left, the test liquid will penetrate into the structure because of the capillarity and this liquid displaces another liquid or a gas (initialisation fluid) out of the channel. Thus, the flow is a flow of two phases, this means that two immiscible fluids are involved. The typical velocities which occur are relatively small. So the flow can be considered laminar and incompressible. But because of the spreading of the interface, the problem is a transient problem which is associated with variations of the interface form.

3 VALIDATION OF THE SIMULATION TOOLS

The present problem requires the simulation tool to contain physical models for investigating a flow of two fluids under the influence of capillarity. A research of various simulation tools showed that, for instance, the simulation tools FLOW-3D by FlowScience and CFX4 by AEA Technology meet this requirement. For this reason, these simulation tools have been validated. For the validation we used test problems which could be described analytically. From the comparison of the simulation results with the theoretical data, we learned more about our problem and physical influences and we detected some problem areas that might occur when simulating the real system. With the help of these basic models, experience was gained with regard to accuracy of the simulation results and the influence of the numerical parameters.

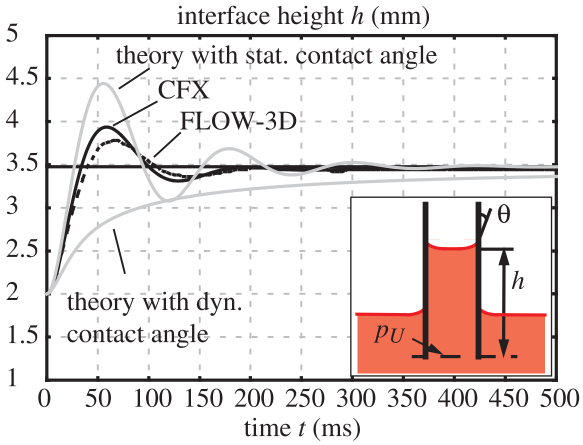

Figure 2: Opened plates: simulation results in comparison with theory

3.1 Opened plates

As a test model, the opened plates were applied to check whether the simulation results reflect the advancement of the fluid front with time and whether the maximum height h_{max} will be reached (Figure 2). The capillary rise as a function of time can be described by the following nonlinear differential equation of second order:

$$\ddot{h} + \frac{12\eta}{d^2\rho}\dot{h} + g - \frac{p_U}{\rho h} - \frac{2\sigma\cos(\theta)}{d\rho h} = 0 \qquad (1)$$

with $\dot{h}(t=0) = 0$ and $h(t=0) = h_0$ as initial conditions. The behaviour is influenced by the material parameters of the viscosity η and density ρ. The contact angle θ depends on the velocity of the interface (dynamic contact angle). Several authors investigated the dynamic contact angle for various conditions and materials. Bracke [1], for example, derived an empirical relation from the experimental data for a partial wetting of a fluid at a dry wall:

$$\cos(\theta_d) = \cos(\theta_0) - 2(1+\cos(\theta_0)) \cdot \sqrt{\frac{\eta\dot{h}}{\sigma}} \qquad (2)$$

Both curves calculated with the simulators show an overshoot and are located between the two theoretical curves. They reach the maximum height (final value) of 3.48 mm with a deviation of < 1 % (Figure 2).

3.2 Test structure

The company microParts GmbH produced some test structures which consist of a single rectangular microchannel without obstacles (Peters [1]) with the following geometrical data: length $s_K = 20$ mm, width $w = 3$ mm, height $d = 40$ μm (Figure 3). They measured the behaviour of the flow of black ink inside this channel. Therefore, they stopped the time which was needed by the ink to pass a test section (s_1 or s_2) of 7 mm. As the result of an investigation of ten channels, an average velocity of 17.3 mm/s was obtained. Because of the horizontal position of the channel, the hydrostatic pressure can be neglected. From the equilibrium of pressures, the following differential equation is obtained for the spreading of the interface in the microchannel:

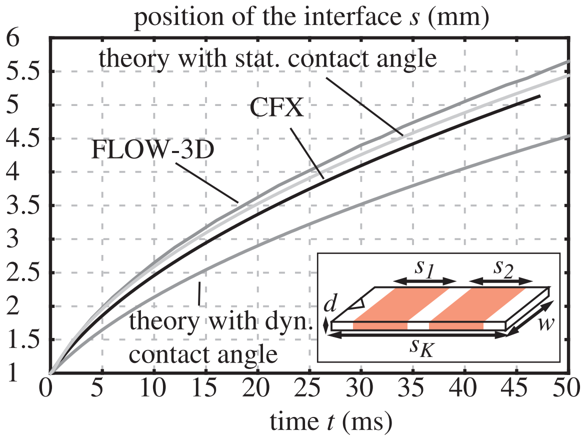

Figure 3: Behaviour of the ink interface in the microchannel with time.

$$\ddot{s} + \frac{12\eta\left[1+\left(\frac{d}{w}\right)^2\right]}{d^2\rho}\dot{s} - \frac{p_U}{\rho s} - \frac{2\sigma(w+d)\cos(\theta)}{wd\rho s} = 0 \qquad (3)$$

Due to the great width in comparison to the small height of the channel ($w \gg d$), the behaviour can be described by a two-dimensional model of the microchannel. This leads to a simplified differential equation:

$$\ddot{s} + \frac{12\eta}{d^2\rho}\dot{s} - \frac{p_U}{\rho s} - \frac{2\sigma\cos(\theta)}{d\rho s} = 0 \qquad (4)$$

A comparison of the simulation results with the theoretical values shows that the simulation results are close to the theoretical curve which is calculated with the stationary contact angle (Figure 3). The values for the interface velocities determined from measurements, theory and from the simulation results are listed in the

Table 1: Velocities of the ink interface

Method	v_{ink} (mm/s)
measurement	17.3
theory: θ_{dyn}, two-dim., s_1, σ_{water}	38.9
theory: θ_{stat}, two-dim., s_1, σ_{water}	51.8
theory: θ_{dyn}, three-dim., s_1, σ_{water}	39.3
theory: θ_{stat}, three-dim., s_1, σ_{water}	51.85
FLOW-3D s_1, σ_{water}	56.45
FLOW-3D s_1, 1/3 σ_{water}	38.9
FLOW-3D s_2, 1/3 σ_{water}	14.9

Table 1. The velocities listed in the table show that the use of a two-dimensional model is justified. The values only slightly differ from the values calculated with a three-dimensional model. However, the measurements clearly show lower values than the theory or the simulations. One reason could be that the value of the surface tension is not known. Hence, we used the surface tension of water, $s_{water} = 0.072$ N/m, which might differ from that of black ink. The density $\rho = 1.0322$ g/cm^3, viscosity $\eta = 0.00137$ Pa·s and the stationary contact angle $\theta_0 = 36°$ are measured data. With the simulator FLOW-3D the simulations with a reduced surface tension (about one third of that of water) lead to lower velocities. And the calculated velocities for the first or the second range in the channel also show clearly different values. This means that the simulation results strongly depend on the boundary conditions.

4 MODELLING OF THE ENTIRE SYSTEM

Both simulation tools, FLOW-3D and CFX4, have in common that due to the numerical methods used, the necessary computation time is too expensive especially for complex systems. For the elementary structures alone, the computation times range from about some minutes to hours. For simulating the entire system of the medical test strips with columns in the flow channel the models needed will be much larger and, consequently, a higher simulation expenditure is necessary. This cannot be justified during system optimisation. The steps taken to reduce the computation time, such as the implementation of a dynamic control of the time steps, were not sufficient to obtain an entire system model that can be applied for the optimisation of the medical test strips. Therefore, a general model concept was developed for optimising the system (Figure 4). To meet the requirements of low simulation times and high accuracy, the entire model consists of three components. These three components are models for the following ranges:

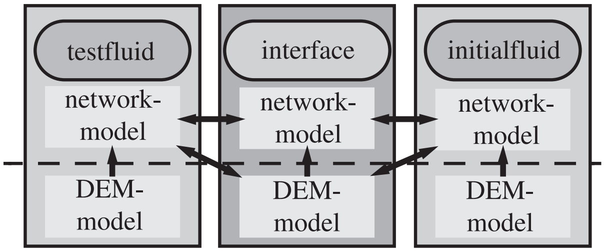

Figure 4: Concept for the modelling of the entire system

- Single-phase flow behind the interface (test fluid which will penetrate into the channel because of the capillarity),
- Two-phase flow in the range of the interface,
- Single-phase flow in front of the interface (initial fluid which is displaced from the channel).

This segmentation is chosen because the single-phase flow can be described by a higher model (for example, a network model or a black-box model) which will be generated or improved with the help of simulation results using physical models, e.g. FVM models or FDM models. Higher models (model on a higher model level) require less computation time than models on the physical level. The range with the interface of the test fluid and the initialisation fluid requires a high discretisation, even if the range possesses many structures. Such complex structures, for example various types of columns, cause strong variations of the shape of the interface. In case a higher model can be generated for this range, the behaviour of the entire system can be modelled on a high level. But if the structure is too complex, it is necessary to couple models on different model levels. Sometimes, a coupling of different simulation tools is necessary. Such a simulator coupling leads to special simulator requirements in terms of the control of convergence, the control of the simulation run, the exchange of the values between the models, the dynamic control of the boundary conditions and the post-processing of the simulation results. In contrast to CFX4, the simulator FLOW-3D does not meet these requirements in the desired manner. For this reason, we will use the simulator CFX4 for the coupling. Using the microchannel as an example, a first model coupling has been realised. Here, the total model of the channel consists of two components. The range with the interface is represented by a CFX model (Figure 5, right). For the range behind the interface with only the test fluid inside, an analytical model was used (Figure 5, left). In this analytical model the pressure drop caused by the inertia of the test fluid p_T and the pressure drop caused by friction p_R are considered. The range in front of the interface, which

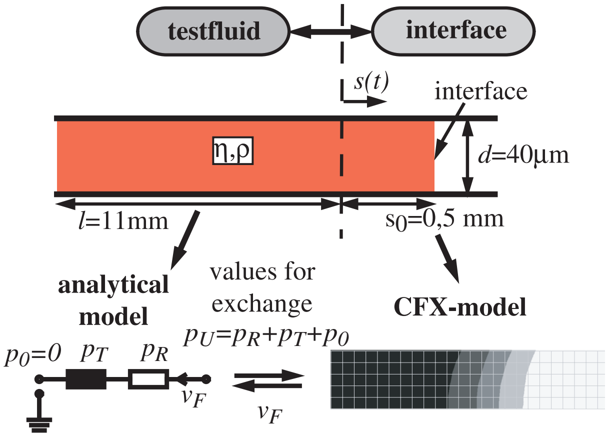

Figure 5: Model coupling with CFX

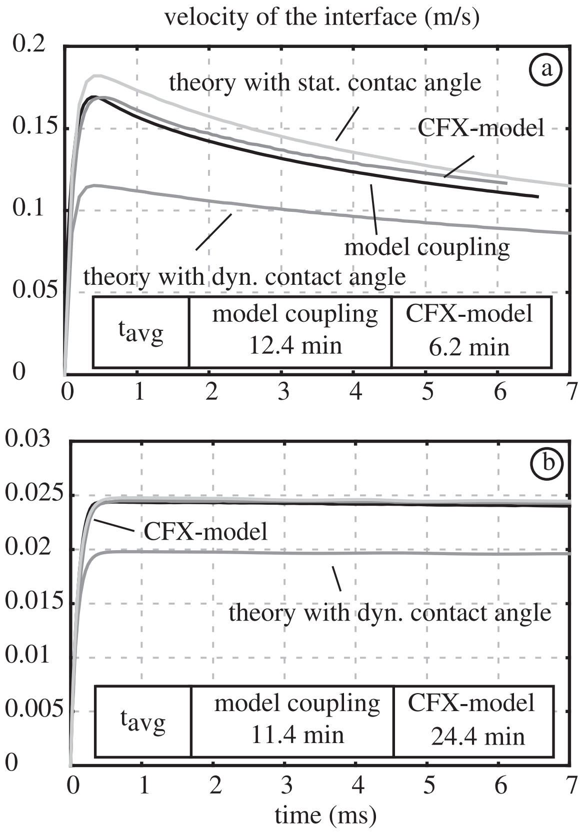

Figure 6: Model coupling with CFX: a) short channel (l = 1.5 mm), b) long channel (l = 11.5 mm)

is only filled with gas, does not have any significant influence on the behaviour of the test fluid and, hence, this range was neglected. Both component models are coupled via the exchange values of pressure p_U and interface velocity v_F. The analytical model as well as the control of the simulation run for model coupling are implemented with Fortran user routines in CFX. The coupled problem is solved by an iterative method. Various methods have been checked for convergence. For a channel with a total length of 3.5 mm and an initial occupation of 1.5 mm by the test fluid some results are shown in Figure 6a. The figure shows the comparison of the velocity of the interface calculated from theory (for the stationary and dynamic contact angle) and the simulation results. On the one hand, a simulation with a CFX model for the total channel (2150 elements) is performed and, on the other hand, the simulation results for model coupling are represented. Both curves are in good agreement and they are located near the curve for the stationary contact angle. An averaged computation time t_{avg} was calculated and converted to 1 ms simulation time for comparison of the values. For this short channel the analytical model only represents a length of 1 mm. The length of the coupled CFX model is 2.5 mm (1550 elements). The simulation with model coupling takes longer than the simulation with the total CFX model because model coupling needs more iterations per time step than the total CFX model. For a longer channel with a different ratio of the analytical model to the coupled CFX model, the results are plotted in Figure 6b. The total length of this channel is 13.5 mm (8150 elements) with an initial occupation of 11.5 mm. Now, the analytical model represents a channel length of 11 mm and the coupled CFX model is 2.5 mm long (1550 elements). The computation time for model coupling is about half of the computation time needed by the total CFX model. These first results, however, have been obtained with a model coupling that is not yet optimised. Such an optimisation of the coupling can be achieved by using a shorter CFX model for the coupling or by the reduction of the necessary iterations.

5 SUMMARY AND OUTLOOK

The validation of the simulators FLOW-3D by Flow-Science and CFX4 by AEATechnology showed that the results for the opened plates are in good agreement with the theoretical results. For the dynamic contact angle some further investigations have to be performed to obtain a mathematical equation which can be implemented and by means of which the capillary model can be improved. The discrepancy between the simulation and the measured data for the rectangular microchannel has to be checked in more detail. Due to the complexity of the medical test strips, the model will consist of several components. A concept for the modelling of the total system was described and a first vertical model coupling was implemented. Based on the example of a rectangular microchannel, it could be shown that with model coupling the necessary computation time can be reduced. In the future, the coupling will be improved, higher models will be built for some structures with single-phase flow and the concept will be applied and, if necessary, extended for the case of the medical test strips.

REFERENCES

[1] Bracke, M., de Voeght, F., Joos, P., "The Kinetics of Wetting, The Dynamic Contact Angle" Progr. Colloid Polym. Sci., Vol. 79, pp. 142-149, 1989.

[2] Peters, R.-P., Schön, C., Halstenberg, S., Quinte, A., Eggert, H., "Entwicklung medizinischer Teststreifen" Tagungsband 7. GMM-Workshop, Methoden und Werkzeuge zum Entwurf von Mikrosystemen, Herausgeber W. John, W. Groß, R. Laur, Paderborn, S. 119-126, 1999. (in German)

[3] Berg, J.C. (Editor),Wettability. Surfactant science series, Vol. 49, Marcel Dekker, 1993.