Simulation and Design Optimization of Microsystems Based on Standard Simulators and Adaptive Search Techniques

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Abstract

The concept of a partial automated design optimization and the improvement of a micropump as a first application is described. Starting with a parametrizable simulation model the parameter values are modified with evolutionary algorithms until the simulation results which describe the behaviour of the system satisfy the defined goals. As the quality of the optimization depends strongly on the quality of the simulation model we give an outlook on a concept for improving the simulation model or components of this model by using FEM-simulation results.

1. Introduction

The industrial application of microsystems requires short development times as well as reliable designs comparable to the state of the art in microelectronics. To achieve this goal CAD based design techniques and simulation are necessary but not sufficient as outlined below. During the design process the engineer is faced with an extremely large search space of possible design solutions and parameterizations. Although a great percentage of the design directions can be dismissed based on the available knowledge and the experience gained from previous designs in most cases the remaining search space will be far too large to be systematically investigated. Usually the search process is a trial-and-error process and the result depends on the skill of the engineer but also on luck. This is an unsatisfactory situation and a systematic exploration of the search space will be aspired. Our concept shows a search method for an improved investigation of the design alternatives.

One property of an intelligent microsystem is the existence of various physical domains such as microelectronics, micromechanics, microfluidics, microcalorics and microoptics. Several simulators exist to investigate the behaviour of the microsystem but in most cases it is possible to consider only one physical domain of the system. For most microsystems it is not sufficient to investigate and to simulate each domain separatly because the different phenomenas depend strongly on each other. Thus for the investigation of the behaviour of a total microsystem it is necessary either to couple different simulators or to build a model containing the description of all phenomenas in a common description language so that the overall system can be simulated with one simulator. We focus on the latter alternative.

An often applied method is the description of the physical effects in analogy to the electronics. This type of model is a network model and can be simulated with a circuit simulator. Analytical studies are necessary to build the model and often it is unavoidable to make simplifications as for example to neglect the friction or to make the assumption that the fluid do not possess a temperature gradient. Depending on the complexity of the system component and its mathematical description the devices of the network can be formulated preferably as usual electronic devices like resistors, capacitors or sources or as HDL-A[1]-models.

1. HDL-A is a trademark of ANACAD EES Ltd.

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With the hardware description language HDL-A both simple devices and more complex components can be described. For the description of components with known nonlinear behaviour the HDL-A-language is very comfortable. This language permits to build a model with differential equations or implicit equations in a simple way. The advantage of such models is that they are relatively fast but the disadvantage is that the accuracy of the simulation results often leaves to be desired. Another simulation method is based on the Finite Element Method (FEM). The FEM-model is more exactly because of the discretization of the space, but the simulations are very time consuming and in many cases the system possess such a complexity that it is not practicable to build a FEM-model of the entire system. To overcome these limitations only system components are investigated with this method. Another property of FEM-models is that they are non parametrizable. Thus it is necessary to build a new model if a model parameter like a geometrical or a material parameter should be modified.

2. A simulation and optimization tool environment

We developed a concept for the partial automated design optimization of microsystems by using the advantages of several simulation methods: Our **SIM**ulation and **O**ptimization **T**ool Environment **SIMOT** consists at present of four tools: GAMA (Genetic Algorithm for Model Adaptation), GADO (Genetic Algorithm for Design Optimization), ANSYS[2] (FEM simulator) and ELDO[3] (circuit simulator). The simulation tools ANSYS and ELDO are standard tools, the optimization tools GAMA and GADO are based on adaptive search techniques and both are developed at our institute.

For the investigation of the behaviour of a microsystem a macromodel of the total system has to be built. This model has to enclose the most important properties of the system and it is necessary that the model is valid over the total search space of possible designs. During an optimization process many simulations with various design parameters have to be done. Therefore the time required for one simulation run should be short enough. On the other hand the optimization results depend strongly on the accuracy of the model. These two requirements contradict each other: A model which needs short simulation times can not be too complex and so it is likely to be not accurate enough. To get a model which meets these requirements macromodels of the system components will be built. In case of a structural model the model will be improved by making an adaptation with respect to the results of FEM simulations. In case of a macromodel consisting of mathematical equations only the FEM simulation results will be used to estimate the coefficients of the used functions. This method is an alternative if the structure or an approximate mathematical description of the system component is unknown. These macromodels of the different components are combined to get an overall simulation model of the entire microsystem on which the design optimization is based. The resulting model is of sufficient accuracy, it is parameterizable and the duration of one simulation run is short enough for the optimization process. For example in our environment the duration is about one minute.

The engineer is faced with an extremely large search space of possible designs and thus the engineer is not able to investigate the search space systematically because during the conventional design process the engineer performs some simulations with different design parameters and after that he evaluates the simulated design. The knowledge of the engineer, previous experiments with similar (micro)systems and luck are the foundations for his search (Fig. 1a).

2. ANSYS is a registered trademark of SAS IP
3. ELDO is a trademark of ANACAD EES Ltd.

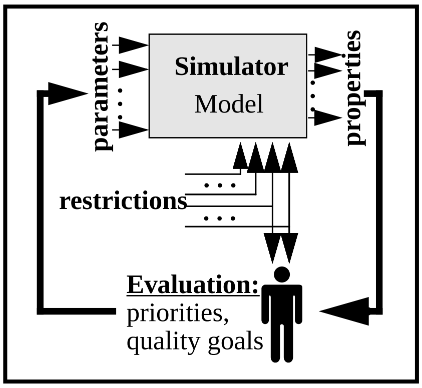


Figure 1a. Conventional Design Process

For a more systematic investigation of the total search space it is necessary to make numerous simulations. The engineer cannot start all required simulations by hand. For such an extensive search he depends on technical support. The idea of our concept is to substitute the human by an automated explorer (Fig. 1b). The task of the explorer is

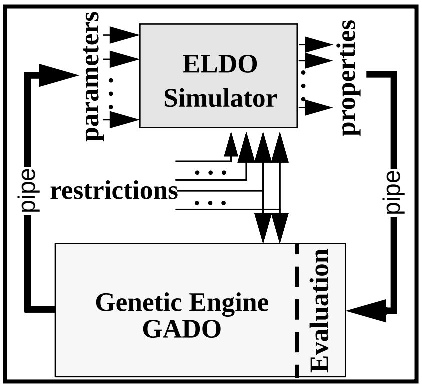


Figure 1b. Design Optimization with GADO

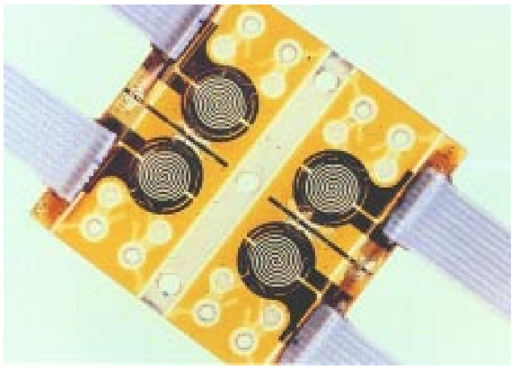
to implement an ‘intelligent‘ search focusing on promising areas of the search space, avoiding suboptima and adapting itself to the search landscape. The explorer is based on the evolutionary algorithm GLEAM (Genetic Learning Algorithms and Methods) [1], which integrates traditional adaptive search techniques like Genetic Algorithms [2] and Evolution Strategies [3]. The task of the engineer is now on a higher level than before. He develops the basic designs and models and fixes the goals of the optimization by defining the functions for the evaluation of the designs. For every property of the simulated system he defines a class and its weight, so he graduates the different properties. Based on the results of prior optimizations the evaluation functions may be subject of readjustments. Therefore the design process is an iterative process and the engineer controls the direction of the optimization.

3. Design optimization of the micropump

3.1. The micropump

Before an optimization run can be done the engineer has to build a macromodel of the system, to define the goals for the optimization and to specify the limits of the design parameters. These limits and the accuracy of the parameters determine the magnitude of the search space. The description of our first application will illustrate this:

At the IMT (Institute for Microstructure Technology), another institute of our research centre, a thermo-pneumatic-driven micropump was developed [4]. Figure 2 shows a unit of four pumps and



Typical properties of a micropump:

flow rate (air)	200	µl/min
frequency	20	Hz
max. outlet pressure	100	hPa
geometry	9×10×1	mm^3

Figure 2. Modul of four micropumps

their electrical contacts. These micropumps have two working states. One is the heating phase: The heating coil which is located on the membrane warms up the gas in the closed actor chamber. The expansion of this gas is the reason of the elastic deformation of the pump membrane. The gas in the channel will then be pressed through the outlet valve. The inlet and the outlet valves are passive valves and they direct the fluid flow. They consist of a valve seat and a membrane with an orifice. The valves open when the pressure at their inlet increases the pressure at the outlet. Otherwise the valve membrane will be pressed on the seat. During the second phase, the cooling phase, the inlet valve opens because of the decrease of the pressure in the actor chamber and gas streams into the micropump. A schematic view of the micropump is shown in Figure 3.

3.2. The model of the micropump

The first macromodel, we used for our opimization run, was written for the circuit simulator PSPICE: It includes the description of the thermal and of the pneumatic behaviour in analogy to the electronics. Therefore the thermal resistance and the fluidic resistance will be compared with an electric resistance and the temperature flow and the volume flow are comparable with the current. The main devices of this first macromodel are resistors, capacitors and sources. The voltage at the network nodes represents the temperature in the thermal domain and the pressure in the fluidic domain and the current through the network devices represents the heat flow rate respectively the volume flow rate. The behaviour of the passive valves, the gas in the actor chamber (air) and the gas in the pump chamber (at present air) and the behaviour of the membranes are nonlinear and as mentioned above their description in PSPICE is long winded. This model contains controlled sources with tables to describe the nonlinear behaviour. Because of the existance of this model we used it for our first optimization runs. Such network models are rough models but on the other hand they satisfy the requirements for an optimization: the models are parametrizable and the simulation is considerable fast.

3.3. First design optimization runs

To define the goals for the optimization of the micropump design we have to answer the following question: How important are the different properties? For us the most important properties are a high flow rate by holding a low temperature of the pump. As optimization parameters which are modified during the optimization process we select the five parameters of the power supply: the magnitude of the heating impulse, the rise time, the fall time, the width of the pulse and the period (Fig.4).

After fixing the limits of the optimization parameters we started our first optimization runs. The genetic engine GADO and the simulator ELDO are linked via pipes to achieve a fast communication between them. The genetic engine delivers a parameter set to the simulator and after the completion of one simulation run the values of the fluid flow rate, the pressure over the valves, the maximum of the temperature, the electrical power consumed and the efficiency are calculated out of the results and returned to GADO. Afterwards the genetic engine computes a quality value dependent on the userdefined goals being used to generate a new parameter set with an evolutionary

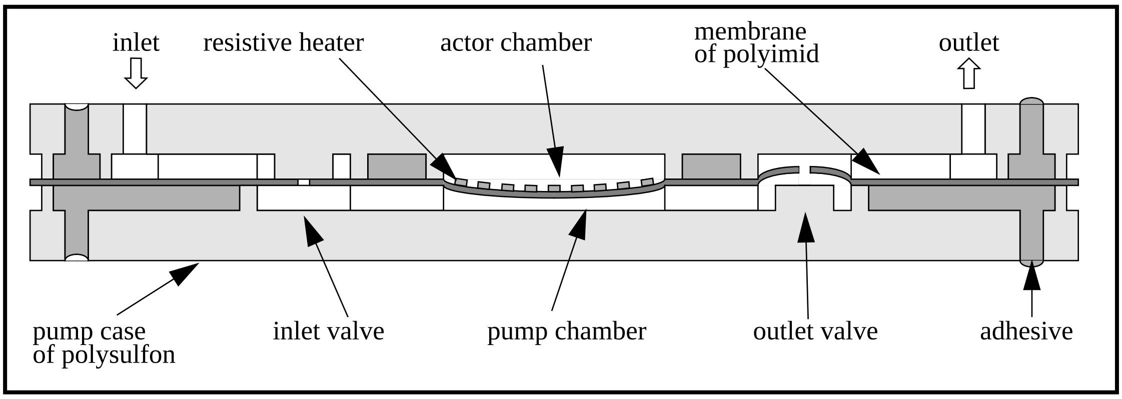


Figure 3. Schematic view of the micropump

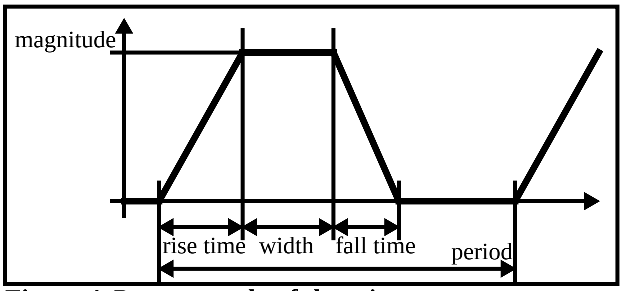


Figure 4. Power supply of the micropump

algorithm. The process continues until a termination criterion is reached.. Starting with an initial population of pump designs these become better from generation to generation and the result of the optimization is a set of pump designs with an improved quality. These first optimization runs have delivered the results shown in Fig. 5.

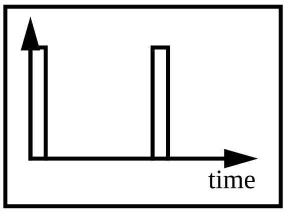


Figure 5a. Original power supply

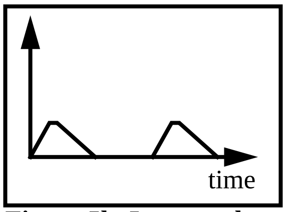


Figure 5b. Improved power supply

The optimization of the design of the micropump is a very complex problem, so it is not sufficient to find the solution with trial-and-error. Although our first optimization example considers only five control parameters of the power supply the search space has already a magnitude of about 10^{22}. As first experiments show it is multimodal and due to its restrictions discontinuous. Furthermore other parameters are of interest for the optimization too, especially the geometrical parameters. If these parameters are taken into account the complexity grows very rapidly. This recommends the utilisation of GLEAM rather than simpler techniques like local hill climbing [5].

For our first optimization runs we selected the parameters of the power supply as optimization parameters. The reasons were the existing macromodel was parametrizable in these five parameters as well as the existing pumps can be used to check the optimization results by measurements. Therefore it is not necessary to produce new pumps. The optimization results showed that they strongly depend on the quality of the used model. In our case the micropump model was not accurate enough because it consists of some components for which we had to do many assumptions to build a model. So it is necessary to build improved models of these components. The next chapter describes a method we used to get a model with higher quality. Therefore we adapt a network model to FEM-simulation results which mean we improve the existing network model. Another method is to build a mathematical macromodel out of the FEM-simulation results, but such a 'black box'-model possess no structural information.

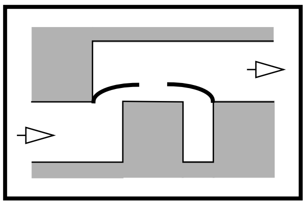
4. Building of a high qualified macromodel

4.1. The concept of the model adaptation

The idea of the concept of the model adaptation is to improve a network model with the help of the results of FEM simulations. Thus we need both, a network model as well as FEM-simulation results or measurement results. Firstly it is necessary to build a network model with an approximate structure to the real system or system component. Secondly we need FEM-simulation results. As mentioned above FEM-models are complex, time-consuming and very accurate models. The complexity of these models derives out of the discretization of the space and in many cases this make it more practicable to investigate only some system components. The creation of the behaviour reference values with FEM requires a lot of computing power. But this has to be done only once and the resulting improved simulation model of a microsystem component can be reused for investigations of further systems containing this component.

4.2. The passive microvalve

One component of the micropump with a nonlinear behaviour is the passive valve. Physical effects of different domains like fluidics, mechanics and calorics influence each other and the geometry of the valve is too complex to be described



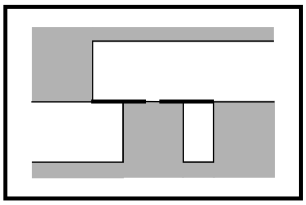


Figure 6a. Opened valve **Figure 6b. Closed valve**

with exact mathematical equations (Fig. 6).

The passive valves are of a rotational symmetry with the exception of the inlet and the outlet channel. A circular valve seat and a circular membrane with an orifice are the main valve components. If the pressure at the valve outlet is smaller than that at the inlet the valve opens and the fluid can flow through an opened annular gap. This gap depends on the form of the elastic deformation of the membrane. When the inlet pressure decreases under the outlet pressure the membrane will be pressed on the valve seat and the valve is in closed position. The flow through the valve also depends on the temperature of the fluid and the components. Another effect which should be considered is the dynamic behaviour. If pressure difference over the valve changes immediately the valve does not open at the same time. The membrane first has to overcome the adhesive forces of the seat.

4.3. The network model of the microvalve

As already stated some simplifications had to be done for creating our first analytical network model which was built for a SPICE simulator. The space of the valve was divided into several areas and for each area the volume flow is described. One disadvantage of this model is that the flow rate through the membrane would be described by a controlled current source in form of a table. Advanced models possess HDL-A-models instead of the tables of the controlled sources. The mentioned models are founded on the same equations, so both models possess the same assumptions and simplifications but the network model with the HDL-A-model causes better simulator behaviour.

The following equation describes the mechanical behaviour of a membrane without an orifice if a pressure difference ($p=p_1-p_0$) over the valve exists. It is assumed that the behaviour of a membrane with an orifice is approximately the same. Another equation describes the flow through the resulting gap. Therefore we assume that the flow is laminar, incompressible, stationary and one-dimensional.

The behaviour of a circular membrane was investigated by J. W. Beams [6]. He stated an equation for the bulged film dependent on the adjacent difference of the pressure

$$p = \frac{8}{3} \cdot \frac{h \cdot D^3}{a^4} \cdot \frac{E}{1-\nu} + 4 \cdot \frac{h \cdot D}{a^2} \cdot \sigma_i$$

where h is the thickness of the film, a the radius, D the height of the center of the bulged film, E the Young‘s Modulus, ν the Young‘s ratio and σ_i the tension. His theory assumes that the bulged film is a hemispherical cap.

With the calculated height D the flow rate through the annular gap can be determined. Because of the hemispherical form of the membrane an average of the distance between the membrane and the seat will be estimated.With the calculated resistance of the gap [7] the flow through the valve can be estimated from the quotient of the pressure difference p and the resistance R. The fluidic resistors of the valve chambers and the capacitors can also be calculated out of the geometrical and material parameters. The advanced model is a network model which includes a HDL-A-model. This model integrates all geometrical and material parameters explicitly and so it is parametrizable. It contains both HDL-A and SPICE syntax. With the HDL-A language the model may include differential and non-differential, as well as explicit and implicit mathematical relationships. Areas of application of the HDL-A package include electrical, mechanical, structural, thermal, fluid and other systems [8].

A great advantage of the new model is that it is easy to understand and to handle because one can identify the mathematical equations which describe the behaviour of the system component.

4.4. Model adaptation of the microvalve model

We have done several investigations of the valve with the FEM-simulators ANSYS and FLOTRAN. The results were only considered qualitatively because for the quantitative consideration some material parameters have to be determined more exactly. These first results show that the usage of a constant Young‘s Modulus is justified and that the flow is laminar and incompressible. For the stationary case some FEM-simulations were done with various geometrical parameters for different pressures. The simulation results are among others the maximum tension of the membrane, the maximum deflection and the volume flow rate through the valve. These results are used for the improvement of the existing network model. To improve the network model we use an adaptation method which is similar to an off-line parameter estimation [9] which is usually used for the calculation of unknown model parameter values. The standard off-line parameter estimation method is based on the variation of unknown parameter values of an analog simulation model until the desired coincidence of the model behaviour with a behaviour reference, e.g. a set of measured values of a real system, is obtained.

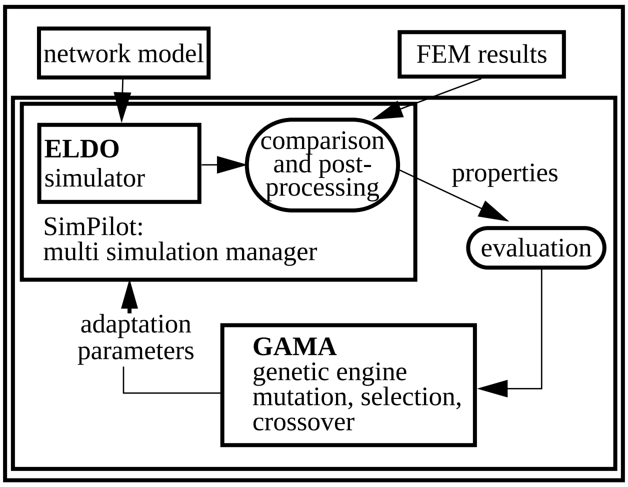


Figure 7. Scheme of the model adaptation process

Using this procedure the FEM simulation results will be used to determine the values of the devices for example the value of the fluid resistance. The advantage of our concept is that we use a parameterizable model. Functional dependencies of design parameters are included in the model explicitly and the unknown disturbances are taken into consideration as correcting factors.To every device a correction factor is attached. These factors are the adaptation parameters which will be modified during the adaptation process GAMA (Fig. 7).

The genetic engine GAMA delivers such a set of adaptation parameters to the simulator. With the help of SimPilot several simulations for every FEM-investigated geometry were done. The simulation results will be compared with its reference values and the relative error is calculated. For all errors the variance is also a good and helpfull parameter to qualify the model. For further design optimizations it is necessary to have a model which is valid over the total search space. This is given if the average relative error is small and the variance is insignificant. For the further design optimization we need a parametrizable model which allows the variation of the geometrical parameters of the system.

4.5. First adaptation results

First adaptation runs presents the following results: We got improved models with a reduced deviation of their simulation results from the corresponding reference values. That means that we got macromodels of the microvalves with a lower error over the total parameter space.

The improvement of the network models depend on the structure of these models and on the used mathematical equations. The adaptation results show if a modification of the structure or of the mathematical equations is necessary or if the parameter space is too large to use only one model structure. Then the total parameter space should be partitioned and it is better to use a special structure for every section of the parameter space. One cause for such a measure can be that the used structure is not a sufficient approximate description of the real behaviour. Another cause is that for different sections of the parameter space various physical effects with various intensity can exist. The usage of the mentioned adaptation method requires to know approximately the structure and the physical behaviour of the system component.

5. Summary

For the design optimization of the micropump it is necessary to have a parametrizable model with a low average error over the total search space. Therefore our first analytically built model was not accurate enough so we improved our network model with the mentioned method.

During our first design optimization the optimization parameters are restricted to the five parameters of the heating impulses. These optimization runs showed that the results are improved designs of the existing micropumps. Further investigations will integrate the modification of some geometrical parameters especially of the parameters of the microvalves. Therefore we use a model which is parametrizable in the geometrical and materisl parameters of the microvalves. Investigations of the microvalves with FEM-simulations showed that the used macromodel of the valve was not accurate enough because of the assumptions which had to be done for building the network model. The complexity and the coupling of physical effects of different domains are the causes for the difficult model building. We improved the network model with the adaptation method. For further design optimization runs improved microvalve models help to get optimization results with higher quality.

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