

## **Towards a Modular Split&Recombine Micro Mixer**

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### **Abstract**

In this paper we discuss a novel approach towards a system-level description for micro reactors. In particular, a compact model for laminar micro mixers for fluids with different viscosities is presented. We show how the well known principle of laminar Split-and-Recombine mixing can be modeled by three elementary geometrical building blocks each of which is treated as separate compact model. This way, the analytical and numerical treatment can basically be reduced to multi-laminar flow in straight channels with square cross sections to a good approximation. The presented model reliably predicts the flow field, the fluidic resistances and the hydrodynamic spreading for multi-laminar flows. The model is validated in comparison with experiments and computational fluid dynamics (CFD) simulations for viscosity ratios as large as 1:20. This way it is possible to map relevant characteristics of a mixer onto a compact model description in order to provide fast network simulations instead of time consuming CFD-simulations.

### **Introduction**

Microfluidic systems have an increasing relevance in life sciences, where the well known benefits such as minimized sample consumption and the potential use in integrated designs have lead to many concepts of “lab-on-a-chip” (LOAC) devices. Micro mixers are essential components for many of these systems [5], e.g., in chemical process engineering. The high surface to volume ratio, short diffusion lengths and an enhanced heat transport improve the quality of chemical reactions in micro dimensions, thus reducing the effort for time consuming successive steps like purification of the chemical products from undesired by-products [9].

Despite all potential and practical advantages, a generalized description of LOAC systems at an adequate level of abstraction is one of the remaining challenges, in particular for micro mixers. In contrast to microelectronics, where large circuits may be represented, designed and tested by lumped element networks, the techniques aiding the design for many fluidic components are mostly based on time consuming, iterative CFD-simulations, often leading to only monolithic applications. Additionally, in arbitrarily specified geometries CFD is often error-prone towards, e.g., numerical diffusion [4] or discretization artifacts. With this work we demonstrate how inefficient use of CFD might be avoided through enhancing the modular character of the whole micro-fluidic environment.

### **Modular Concept**

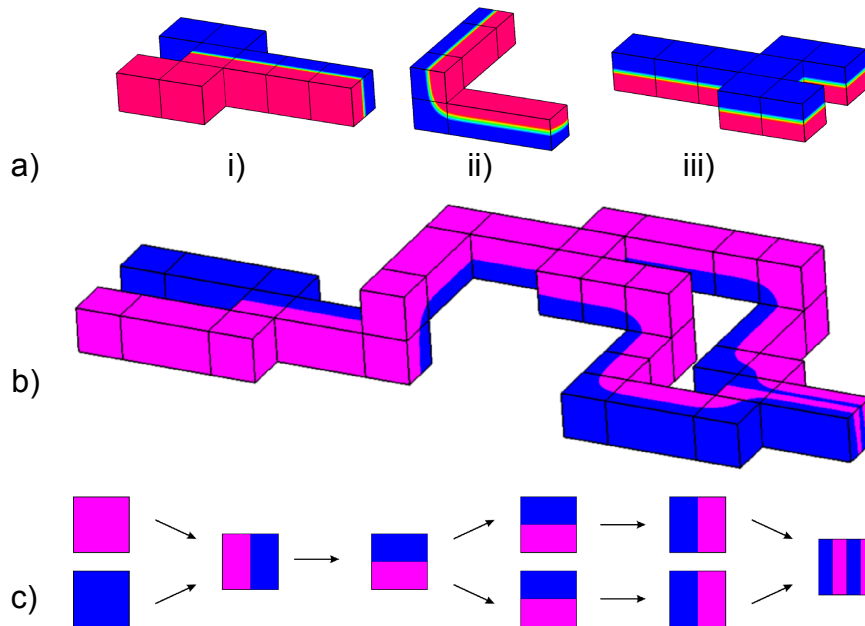
The concept we pursue may be divided into three stages: first, defining a set of fluidic components with possibly restricted, but well-defined operations that are amenable to an analytic description. Second, optimizing and characterizing these operations by a series of “smart” CFD-simulations, establishing strict modularity and connectivity and third, the integration of these informations in a compact model, yielding reliable estimates about efficiency, but also hints for the layout to the designer.

In the following, we will discuss how the so-called Split-and-Recombine (S&R) principle for micro mixers may be reorganized in this way in order to arrive at a lumped element

representation, suitable for integration in a pressure driven fluidic environment. The design may then be reconfigured solely via the compact model.

### Fluidic Setup

Many different Split-and-Recombine mixers, are partly based on complex geometries ([2,4] and references therein). We chose to decompose a whole S&R-step into three different geometric structures, attributed to defined operations on entering fluid streams, see Fig. 1a : i) combining two streams, ii) twisting the flow profile by 90° and iii) symmetric split.



**Fig. 1.** a):Modular components of the S&R mixer: i) combine, ii) twist and iii) split structure.  
b):CFD-simulation of the S&R mixer.  
c):Schematic working principle of the mixer.

Fig. 1b illustrates how the three components are used to create a complete S&R-step, i.e., a doubling of the number of fluid lamellae. Most of the CFD computing time is spent in identifying and optimizing the elementary components, and establishing their modularity. An important point is that in order to allow for an analytic description of the mixing progress, the fluid interfaces should be kept parallel to the channel walls throughout the whole geometry. This is achieved by requiring that each component separately complies with this requirement. Furthermore, the particular assembly of components in Fig. 1b leads to a symmetric distribution of fluidic resistances. Thus, the assembly of fluid lamellae *leaving* the S&R-step may be treated as if the four fluid streams had been introduced into a single channel symmetrically. This is where the strategy outlined above leads to a rather simple analytic description of the mixing process, as described in the next section.

### Analytical Approach and Compact Model

Since a complete analytical solution of the problem of multi-laminar flow in rectangular geometries is not possible [3], we firstly consider a corresponding 2D-approximation of a multi-laminar flow in a slit. This is useful because the flow profile in a square channel is parabolic

near the channel center, where the largest part of the total flux is transmitted. Furthermore, diffusion (and thus a possible blur of the fluid interfaces) is neglected. This is also justified since the averaged lamella thickness is halved after each S&R-step, and the diffusion time decreases quadratically with decreasing lamella thickness; thus one expects significant mixing to set in suddenly, essentially within the time spent in a single output channel after, say, the  $n$ -th S&R-step. The governing equation for the fluid motion is the Navier-Stokes equation, which for the case of two-dimensional, fully developed slit flow of parallel fluid lamellae at low Re numbers, can be reduced to the Poisson equation [6]. For a slit flow with multiple fluid lamellae and possibly different viscosities, the solution for the flow field can be calculated by applying the Poisson equation for the particular domain, i.e.

$$\frac{\partial p}{\partial y} = \eta_i \cdot \frac{\partial^2 u_{y_i}}{\partial x^2} \quad (1)$$

where we assume that the domains are separated by a fluid interface at position  $x_i$ . The different domains are coupled at  $x_i$  via equilibrium of shear forces [3],

$$\eta_i \cdot \frac{\partial u_{y_i}}{\partial x} = \eta_{i+1} \cdot \frac{\partial u_{y_{i+1}}}{\partial x} \quad (2)$$

and the continuity of the flow field,

$$u_{y_i} \Big|_{interface} = u_{y_{i+1}} \Big|_{interface} \quad (3)$$

The solution of the eqn. (1-3) allows to determine all characteristic quantities entering the compact model. In addition to external parameters such as the diffusion coefficients  $D_i$  and the channel length  $l_{ch}$ , these are the fluidic resistance, the diffusion lengths  $l_{Di}$  as estimated from the distribution of lamellae thicknesses, and the mean residence time  $l_{ch}/\langle u_i \rangle$  through the average flow velocity  $\langle u_i \rangle$  for each fluid lamellae. The point where notable progress of mixing sets in may then be estimated by evaluating the Fourier Number  $Fo$ ,

$$Fo = \frac{D_i \cdot l_{ch}}{\langle u_i \rangle \cdot l_{Di}^2} > 1, \quad (4)$$

with a value greater than 1 indicating considerable diffusion in passing a channel segment of length  $l_{ch}$ . Eqn. (1-3) may be solved formally assuming a piecewise polynomial solution for  $u$  with stick boundary conditions, resulting in a system of implicit non-linear algebraic equations for the  $x_i$ , the pressure drop  $\Delta p$  and the flow rate  $\phi$ ,

$$\Delta p \cdot R^{-1}(\eta_1, \eta_2, d, x_{i,interface}) = \phi, \quad (5)$$

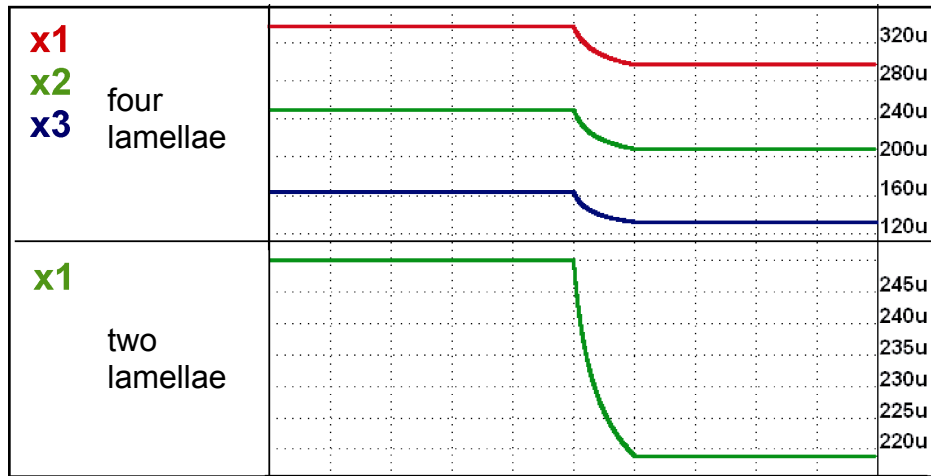
that can be mapped to a network model.

## Numerical Implementation and Validation

Equations (5) constituting the core of the compact model, were implemented in the hardware description language VHDL-AMS with all computations performed with the commercial software SMASH 5.2.0 from Dolphin Integration. The analytical model was validated by CFD-simulation with the commercial software CFDRC-ACE+ for square channels applying the Volume of Fluid (VOF) method. In order to extend the analytical model to a full 3D-model the fluidic resistance and the diffusion lengths for square channels were investigated and compared with the analytical model.

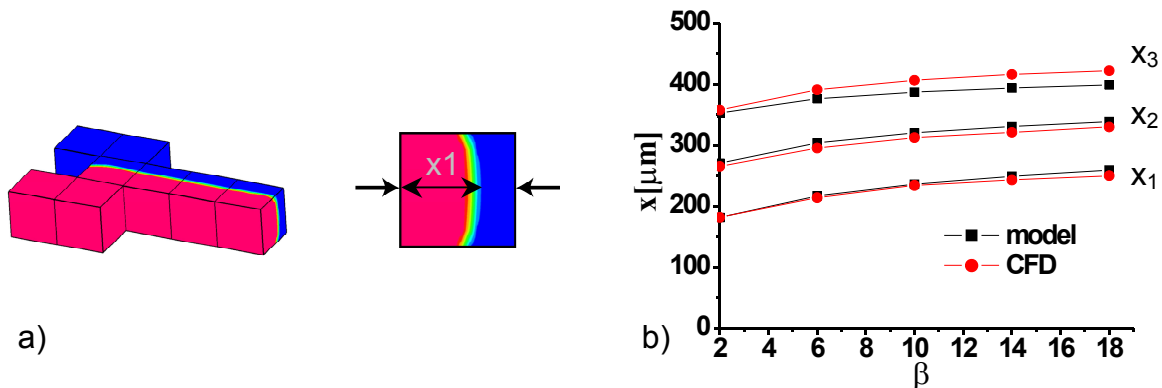
The system (5) has many solutions; in order to stick to the physical one, parameters such as the  $\eta_i$  are varied continuously with time, starting from a known solution for the  $x_i$  at a defined operation point of the network model. Changes in  $\eta_i$ , for instance, due to temperature changes, may be emulated by ramping the corresponding parameter to the new value. This

process is illustrated in Fig. 2, where a change in viscosity ratio  $\beta$  from 1 to 4 is accomplished, with the  $x_i$  changing from a symmetric configuration to an asymmetric one due to hydrodynamic spreading. The time scale at which the transitions occur may be chosen either according to a specific model or in order not to conflict with other time scales in the system. This leaves some space for the level of abstraction the model is operated at.



**Fig. 2.** Network simulation of the position of fluid interfaces  $x_i$  for a complete S&R-step with  $\beta$  changing from 1 to 4 ( $1u$  corresponds to  $1\mu m$ , with the right channel wall located at  $0u$  and the left one at  $500u$ ).

The convergence of the network model was verified for a variety of parameters, and up to viscosity ratio as large as 1:20. The analytical model for the slit flow was compared to a full three-dimensional CFD-simulation for two as well as four fluid lamellae.



**Fig. 3. a):** CFD-simulation for a viscosity ratio  $\beta = 10$ . The position of the fluid interface was evaluated at the middle of the channel cross section.  
**b):** Positions  $x_i$  of fluid interfaces of the network model vs. CFD-simulation.

Fig. 3a shows that in contrast to a slit, the fluid interface between two adjacent lamellae are characteristically bended [5]. This effect influences the hydrodynamic spreading in confined geometries and consequently the accuracy of the model. The accuracy of the model for the fluidic resistance and the diffusion lengths was validated up to a viscosity ratio 1:20. Fig. 3b sketches the positions of the fluid interfaces for an increasing ratio of viscosity. The model

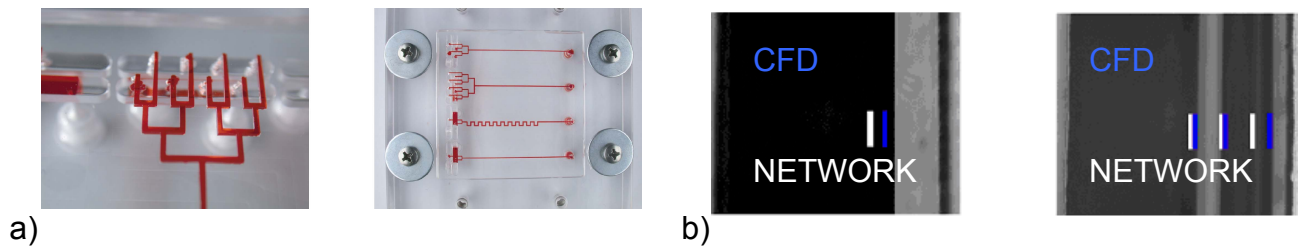
reliably predicts the asymmetry of the lamination pattern for four fluid lamellae as  $\beta$  increases. In order to account for the three-dimensional geometry, the fluidic resistance of the compact model was adjusted by a geometric factor which for uni-laminar flow is [11]

$$\gamma = \frac{\Delta p_{square}}{\Delta p_{slit}} \approx 2.4 . \quad (6)$$

The pressure drop  $\Delta p$  in the model scaled by  $\gamma$  was compared to a full 3-D simulation, and only a weak dependency of the geometric factor  $\gamma$  on the viscosity ratio  $\beta$  was found.

## Experiments

In order to validate the model, experiments were performed with water and glycerol mixtures with different mass fractions of water and glycerol. A rapid prototyping technique based on SU-8/PDMS [7] was used to manufacture the microfluidic structures with a lateral size of 200 $\mu\text{m}$  and 500 $\mu\text{m}$ , respectively. The channel structures were fixed with a PMMA bracket in order to access the fluidic channels by external connection. In order to investigate the multi-lamination for different conditions, a tree-shaped channel structure in one plane was realized, see Fig. 4a, with flows being controlled by a syringe pump. For optical measurements a microscope (Zeiss Axio Phot) was used. For visualization of the fluid lamellae, the glycerol-water mixture with higher mass fraction of glycerol, i.e. the fluid of higher viscosity was dyed with ink.



**Fig. 4. a):** Tree-structures of microfluidic channels for generating regular flow profiles including up to eight fluid lamellae.

**b):** Lamination pattern of multi-laminar flow for a viscosity ratio  $\beta=10$ . The flow direction is in plane.

The agreement between numerical results and experiments is best between CFD-simulation and experiments, see Fig. 4b. As predicted by the model and CFD-simulation, the lamination pattern shows an increasing asymmetry for an ascending viscosity ratio  $\beta$ . Deviations between model and experiments are mainly caused by the curvature of fluid interfaces not taken into account by the compact model.

## Summary and Conclusion

In summary, our results suggest that it is possible to implement compact models and reliably predict the performance even of complex microfluidic systems such as mixers, by keeping their design modular and reconfigurable. The procedure was demonstrated for a specific design of a laminar S&R micro-mixer. Through the modular approach, the analysis of the flow patterns could be reduced to regular, multi-laminar flow in straight channel segments, which in turn was approximated by two-dimensional slit flow. This way, a model of nonlinear algebraic equations was developed that estimates the thickness of fluid lamellae, the fluidic resistance and the flow field even for strongly varying viscosities at least up to a ratio of 1:20. Good agreement

between compact model, CFD-simulation and experiments was achieved. Using this information, effective diffusion times can be estimated, allowing to trace the progress of mixing. Reconfiguration of the mixer layout in order to optimize the design is possible within the framework of the compact model parameters.

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