AN OPEN-SOURCE RAPID SIMULATOR FOR CONCENTRATIONS IN CHANNEL-BASED MICROFLUIDIC NETWORKS

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We present an open-source[*] rapid simulator for species concentrations in channel-based microfluidic networks to accelerate the simulation step in the design cycle for microfluidic devices. The concentration of species is important in many microfluidic devices, and simulating it is an important step in their design cycle. Simulating concentrations is usually done using *Computational Fluid Dynamics* (CFD) methods, which are costly and time-consuming, especially for large microfluidic networks. Here, we present an open-source abstract simulator for concentrations in microfluidic devices that rapidly provides reliable results [1]. With this simulator, the (automatic) design and validation of larger microfluidic devices becomes feasible.

Simulations can operate at multiple levels of abstraction, i.e., with different correlations between the computational model and the physical world. Methods on a low level of abstraction, such as those in *Computational Fluid Dynamics* (CFD), usually model a device better but are costly and take time, especially for larger networks. Based on the Advection-Diffusion Equation, an abstract model for concentration in a microfluidic channel has already been used to calculate the time required to obtain a full mixture in channels [2]. However, this is only sufficient for applications that consider *fully mixed* mixtures. A simulator that exploits this abstract model for general applications must take the network topology into account, as well as the propagation of the concentration distribution to channels downstream.

To use the simulator, a geometry must be abstracted to a set of channels, as shown in Figs. 1a and 1b. Based on the abstract network topology (Fig. 1b) and the flow direction, the concentration distribution is merged, propagated, or split. The merge operation occurs when multiple inflow channels come together, as in Fig. 1c, and the multiple concentration distributions are concatenated. The newly formed concentration distribution is the initial condition for the propagation in the subsequent channel, see Fig. 1d. Here, the diffusion is modeled using the Advection-Diffusion Equation. If a channel splits into multiple channels, the concentration distribution is split, as shown in Fig. 1e.

To validate the simulator, we compared it to CFD results of an arbitrary microfluidic network, shown in Fig. 2, along cross-sections A-F. The concentration distribution along those cross-sections is given in Fig. 3 for the abstract simulations and the CFD simulations. The distributions mostly align, but it should be noted that CFD does not necessarily always provide the ground-truth. Therefore, we also compared the simulator to experimental results from Jeon et. Al. [3]. The network of this case is illustrated in Fig. 4, and the experiments were performed with a flow speed of 1, 10 and 100 mm/s at the inlets. The concentration distribution is shown and compared to results from the simulator for all three cases in Fig. 5. The results are well in line with experimental data. Overall, the abstract simulator has proven to be reliable, and it can be deployed to simulate concentration in general applications, in a matter of seconds. Beyond that, given its fast execution, it is appropriate for simulating concentrations in large networks of microfluidic channels.

REFERENCES

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2. Wu, Zhigang, Nam-Trung Nguyen, and Xiaoyang Huang. "Nonlinear diffusive mixing in microchannels: theory and experiments." *Journal of Micromechanics and Microengineering* 14.4 (2004): 604.
3. Jeon, Noo Li, et al. "Generation of solution and surface gradients using microfluidic systems." *Langmuir* 16.22 (2000): 8311-8316.

[*]Available at: https://github.com/cda-tum/mmft-simulator

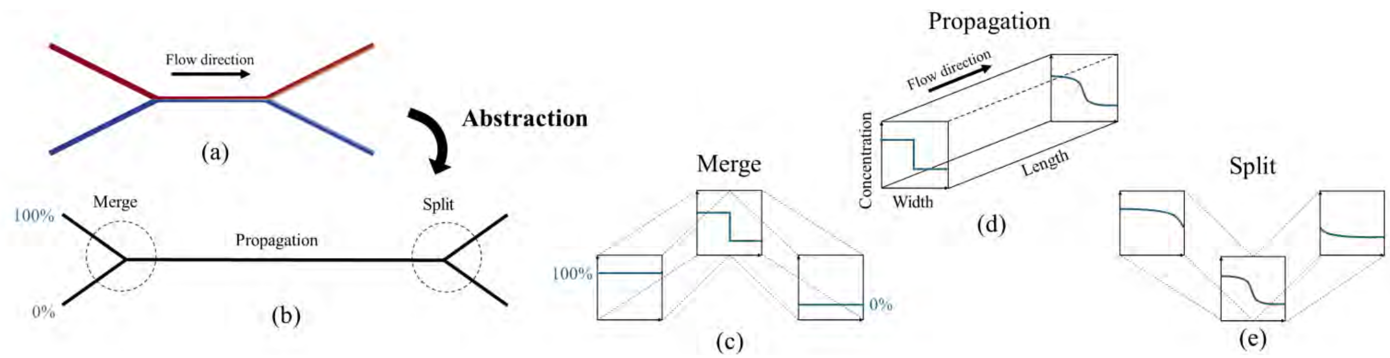

Figure 1: A schematic representation of the abstract method. Instead of doing (a) a CFD simulation, the geometry is abstracted into (b) a network of channels. The concentration distribution in the network is derived using a combination of (c) merge, (d) propagation, and (e) split operations on the inflow concentrations.

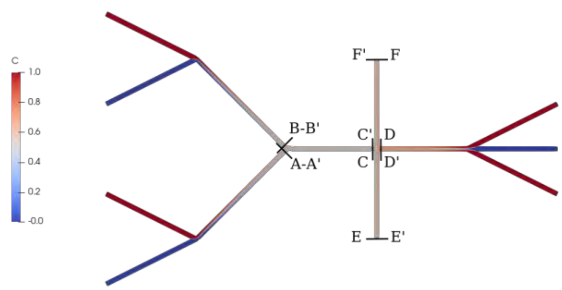

Figure 2: The CFD result for an arbitrary geometry. The simulators are compared at cross-sections A-F.

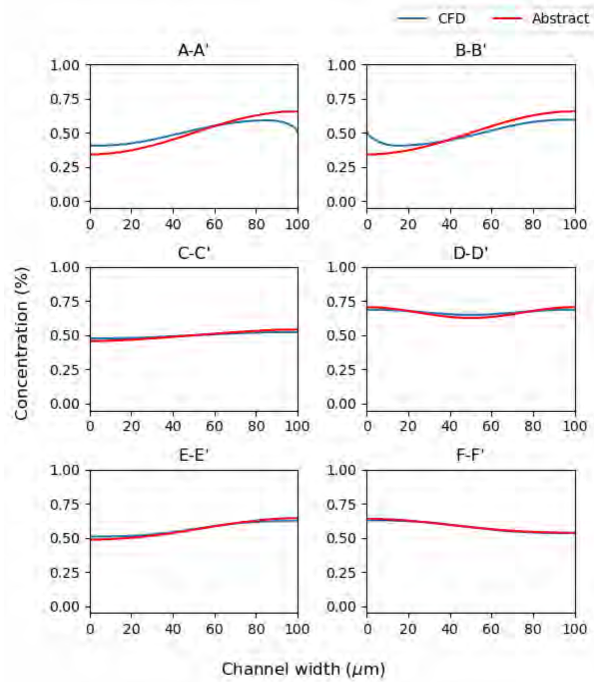

Figure 3: The concentration profiles at various cross-sections given by a CFD simulation (in blue) and the abstract simulator (in red).

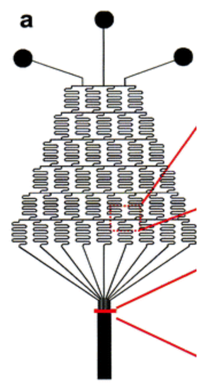

Figure 4: The network of the experimental case from Jeon et. al [3]. The three inlets on top have respectively a concentration of 0%, 100%, and 0%. The concentration distribution is taken at the red cross-section. Image adapted with permission from [3].

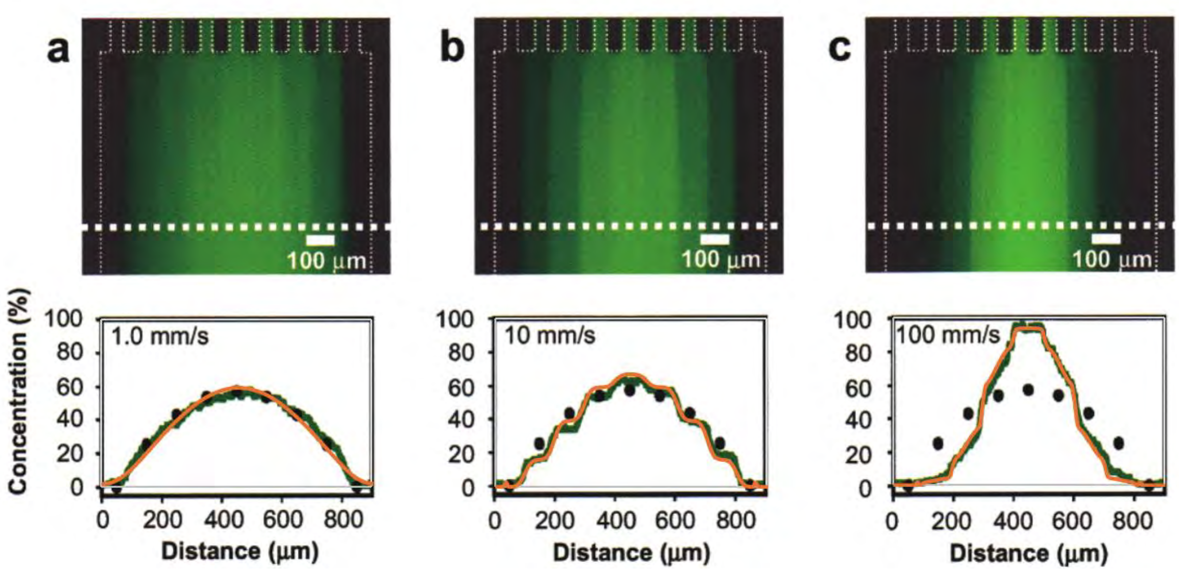

Figure 5: The resulting concentration distributions of the abstract method (in orange) compared to the concentration distribution from Jeon et. al [3] (in green), for inflow velocities of 1mm/s (a), 10 mm/s (b) and 100 mm/s (c). Image adapted with permission from [3].