Computational Study of Microfluidic Two-Fluid Mixing

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ABSTRACT

In the past few years, microfluidics have become a very powerful tool for physical analysis of fluids. Indeed, microdevices yield accurate control on the laminar flows, and it allows one to build genuine *labs-on-chip*. Original microfluidic experiments combined with mathematical models offer possibilities to measure different physical properties, from rheological behavior to surface tension [1].
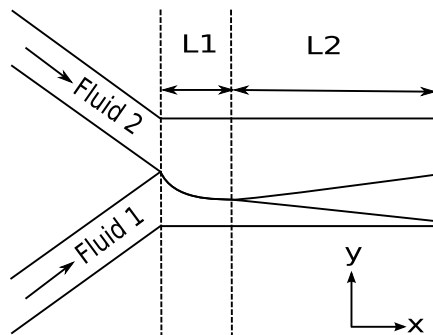
Figure 1: Schematic view of a typical co-flow interdiffusion experiment. $L1$ represents the characteristic length for the viscous displacement phenomenon, $L2$ represents the characteristic length for the diffusion phenomenon. Usually we have : $L1 \ll L2$.

The aim of this study is to compute the interdiffusion coefficient of two fluids by using microfluidics experiments and numerical simulations on simple mathematical models.

The following experimental setup is considered : two miscible fluids are injected at a constant flow rate in a Y-shaped microchannel (see Fig.1). At these very small Reynolds numbers, the two fluids mix slowly by molecular diffusion. The evolution of the mixing width along the stream direction should contain all the mixing features, including the interdiffusion coefficient.

At this point, models are needed to estimate the interdiffusion coefficient from the comparison between experimental results and numerical computations. However, as full 3D simulations on the Stokes model of mixing may be rather long, it is useful to simplify the model using several assumptions.

The evolution of the local composition (volume fraction in our case) is described using the classical convection-diffusion equation for two fluid mixing [2]. The convective term of this equation involves a velocity which is given by a 3D stationary incompressible Stokes model. We take into account the specific geometries of microfluidic channels : the height of the channels is small compared to the other length scales. We therefore use the Hele-Shaw assumption that allows us to reduce

the complexity of the 3D model to a simple 2D Reynolds model. The viscosity of the fluid depends non-linearly on the local composition of the mixing. The dependance of the viscosity on the local volume fraction is provided by literature [3].

Numerical computations on such a model show good agreements with the experiments [4] for the viscous displacement that occurs quickly in the channel (as in Fig.1, $x < L1$). We also highlight the fact that for such short lengths, the effects of the diffusion are neglectable. Simple physical arguments relying on the flow rate conservation can predict the widths of the two streams that are not significantly mixed ($x < L1$).

For simulations involving larger lengths (as in Fig.1, $x \sim L2$), numerical diffusion affects significantly the concentration profiles. This is related to the fact that both viscous displacement and diffusion phenomena occur on different time scales. We solved this problem by introducing a new set of inlet boundary conditions. Thanks to this new inlet conditions, we ensure that the flow rates are equal in each phase at the entry of the channel. The absence of flow rate gradient at the entry of the channel reduce drastically the displacement of the fluid in the transverse direction and therefore the numerical diffusion.

When using experiments performed on the mixing of glycerol and water, one can measure the displacement and the spread of the interface on a long space scale (for $x > L1$, see Fig.1). After fitting the result with an error function, one obtains an effective diffusion coefficient. This coefficient cannot be linked analyticaly to the one used in our model. However, it is possible to recover it through numerical simulations. We hence built up a tool that can deduce the interdiffusion coefficient from the experimental data.

Thanks to the very simple behavior of the hydrodynamics in this type of experiments, it is possible to write an asymptotic model from the 2D Reynolds model. Such a model contains an equation depending only on the local composition of the mixing :

$$\partial_t \varphi + F(\varphi)\partial_x \varphi + G(\varphi)\partial_y \varphi = D\partial_{yy}^2 \varphi,$$

where $F(\varphi)$ and $G(\varphi)$ are provided by the asymptotic analysis. This 2D non-linear parabolic equation that can be solved numerically in a very simple way. With regards to the evolution of the mixing width, comparison between the numerical solutions of the complete Reynolds model and this equation shows a very small difference. A similar analysis involving models of chemical reactions could also be designed for estimating chemical kinetics of miscible reactive fluids.

REFERENCES

[1] P. Guillot, P. Panizza, J.-B. Salmon, M. Joanicot, A. Colin, C.-H. Bruneau and T. Colin. "Viscosimeter on a Microfluidic Chip". *Langmuir*, 22, 6438-6445, 2006.

[2] Daniel D. Joseph, A. Huang and H. Hu. "Non-solenoidal velocity effects and Korteweg stresses in simple mixtures of incomressible liquids". *Physica D*, 1996.

[3] D.R.Lide, G.Baysinger, L.I.Berger, R.N.Goldberg, H.V.Kehiaian, K.Kuchitsu, G.M.Rosenblatt, D.L.Roth, D.Zwillinger, "Handbook of chemistry and physics 85th edition 2004-2005", *CRC Press*, 2004.

[4] J-.B. Salmon, A. Ajdari, P. Tabeling, L. Servant, D. Talaga and M. Joanicot. "In situ Raman imaging of interdiffusion in a microchannel". *Appl. Phys. Lett.* 86, 094106, 2005.