About stability condition for bifluid flows with surface tension

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Outline

Microfluidics : What ?

- study of multifluid flows
- channels the width of a single human hair
- sections : 10 - 100 μm

Microfluidics : Why ?

Allows :

- handling of nanoliters (good if expensive)
- good control of the flow
  ➜ reproducibility, monodisperse emulsions
- very fast chemical kinetics : 10^{-4} s

Applications :

- genome sequencing
- droplets = chemical-reactors

Motivations :

- simulate bifluid flows in microchannels
- explore/improve mixing processes

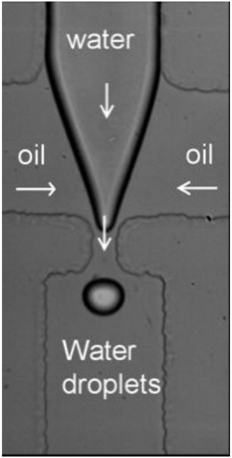
Specificities of the problem

Experimental Framework :

- geometry : cross of channels
- device to create droplets
- typical speed : 0.01 - 1 m/s

Physical specificities :

- low Reynolds number Re = 0.1 - 1
  ➜ inertia forces negligible
- surface tension predominates
  ➜ curvature-driven flows, "simple" shape
- dynamics with vortices

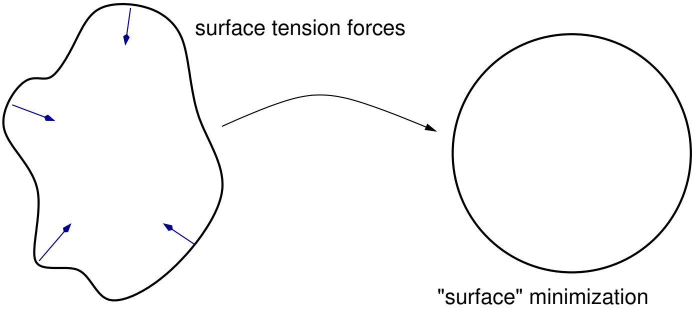


Courtesy G. Cristobal (LOF)

Surface tension

- What ? A force at the interface between 2 fluids
- Linked to the curvature of the interface
- Thus, predominant in Microfluidics

Effect of surface tension : Minimize the interface energy



Mathematical modelling (1)

Hypotheses

- immiscible bifluid flows
- Reynolds < 1
- fluids : incompressible, viscous, homogeneous, newtonian
- sharp-interface : zero interfacial thickness
- constant surface tension

➜ **Flow equation : Stokes**

- moving interface & topological changes (droplets)

➜ **Interface capturing by Level Set method**

Mathematical modelling (2)

Based on Sussman *et al.* (1994)

$$(\mathcal{S}) \left\{ \begin{array}{rl} div(2\eta Du) - \nabla p & = \sigma\ \kappa\ \delta(\phi)\ n \\ div(u) & = 0 \\ + \quad \text{B.C.} & \end{array} \right.$$

$$\eta = \eta_1 + (\eta_2 - \eta_1) H(\phi) \quad n = \left.\frac{\nabla\phi}{|\nabla\phi|}\right|_{\phi=0} \quad \kappa = \nabla . \left.\left(\frac{\nabla\phi}{|\nabla\phi|}\right)\right|_{\phi=0}$$

$$(\mathcal{T}) \left\{ \begin{array}{rl} \phi_t + u \, . \nabla\phi & = 0 \\ + \quad \text{B.C.} & + \quad \text{I.C.} \end{array} \right.$$

Geometry and Boundary Conditions

Geometry : 2D simulations on a cross

Boundary Conditions

- wall :

$$\begin{cases} u.\tau = \alpha u_s(\eta) + \beta L_s(\eta) \frac{\partial (u.\tau)}{\partial n_w} \\ u.n_w = 0 \end{cases}$$

  interface touches the wall or not
- classical B.C. at inlet & outlets

Level Set Tools (1)

(a) Curvature

Easy handling thanks to Level Set function : $\kappa^n = div \frac{\nabla \phi^n}{|\nabla \phi^n|}$

(b) Reinitialization

Better results when keeping ϕ a distance function : $|\nabla \phi| = 1$

- $d_\tau + sign(\phi)(|\nabla d| - 1) = 0$ with I.C. $d|_{\tau=0} = \phi$
- Fast Marching : direct solving of eikonal equation

(c) Mass correction

- translation of ϕ to enforce mass conservation

Level Set Tools (2)

Why does Level Set method well lend itself to Microfluidics ?

Because interfaces' shape

- are close to circular shape
- are not thin compared to the computational domain

Thus, we can use legitimately

- reinitialization
- mass correction by translation of ϕ

to achieve.

- **good mass conservation**
- **accurate curvature computation**

Discretization - Solvers

Time

$$\kappa^n = div \frac{\nabla \phi^n}{|\nabla \phi^n|},$$

$$-div(2\eta(\phi^n)(Du)^{n+1}) + \nabla p^{n+1} = -\sigma \kappa^n \nabla (H(\phi^n)), \quad (1)$$

$$div\left(u^{n+1}\right) = 0, \quad (2)$$

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} + u^{n+1} \cdot \nabla \phi^n = 0. \quad (3)$$

Space

Finite-Volume method on staggered grid (cartesian)

Solvers

- Stokes : Augmented Lagrangian for $div(u) = 0$
- Transport : RK 1,2 or 3 (time), WENO 5 scheme (space)

Time step is restricted by convective, viscous and source terms

Previous model and its discretization are consistant and follow Brackbill et al. approach of 1992 :

surface tension handling by CSF method

Today, most of formulations based on CSF method use the following surface tension-induced stability condition :

$$\Delta t_\sigma \sim \sqrt{C\left(\frac{\rho}{\sigma}\right)\ \Delta x^3} \text{ (Brackbill \textit{et al.}, 1992)}$$

Problem for our model : there is no density.

We therefore present a new stability condition for low flow velocities.

Proposition

Assume that (Navier-Stokes) (2) (3) is discretized in time by an explicit discretization of the surface tension term. Then, a numerical scheme, associated to such a time discretization and all space discretizations, is stable under the condition

$$\Delta t \leq min\left(\Delta t_c, \Delta t_\sigma\right), \text{ with } \Delta t_c = c_1 \|u\|^{-1}_{L^\infty(\Omega)} \Delta x \text{ and } \Delta t_\sigma = c_2 \frac{\eta}{\sigma} \Delta x \tag{4}$$

where Δt is the time step, Δx is space step of the discretization, and c_1, c_2 do not depend on the data of the problem.

Sketch of the proof 1/4

First constraint : $\Delta t \leq c_1 \|u\|^{-1}_{L^\infty(\Omega)} \Delta x$ is the standard CFL condition induced by transport term.

Second condition

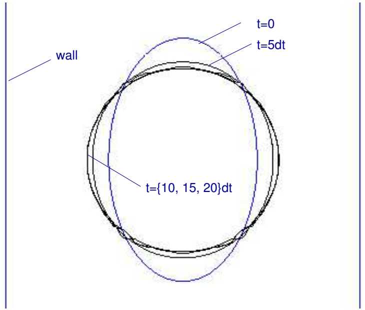
- is induced by the surface tension term
- avoids oscillatory behaviour of the interface around an asymptotic shape of interface, due to the explicit discretization of the surface tension term

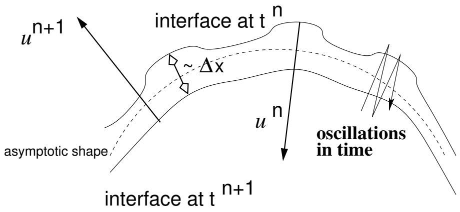
We perform the analysis on the continuous problem instead of the discrete problem, assuming that the numerical scheme approximates consistently the continuous problem.

Keypoint of the analysis : Estimation of the perturbed velocity

Sketch of the proof 2/4

Stability problem if standard CFL is used

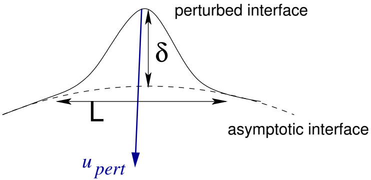




Droplet is globally immobile in the channel

Sketch of the proof 3/4

An explicit time discretization of the source term obliges to consider sufficiently small time step so that the displacement (during the time step) of the interface is smaller than the size δ of the perturbation of the interface. Oscillations are removed if :



$$\Delta t_\sigma = \frac{\delta}{\|w\|_{L^\infty(\Omega)}}, \text{ i.e.}$$

Energy estimate + Hypothesis : $\|\nabla w\|_{L^2(\Omega)} \sim \frac{1}{L}\|w\|_{L^2(\Omega)}$ ➜ velocity

$$\Delta t_\sigma \leq c' \frac{\eta}{\sigma} \frac{L}{1 + \|\partial_\tau \kappa_0\|_{L^\infty(\Gamma_0)} \frac{L^3}{\varepsilon}}, \tag{5}$$

where c' does not depend on the physical parameters.

Sketch of the proof 4/4

As the wavelength L is upper bounded and ε is chosen of size Δx, this condition is restrictive for the smaller wavelength admissible in the numerical process. We are then concerned with $L \sim \Delta x$, and it reads :

$$\Delta t_\sigma \sim \frac{\eta}{\sigma} \Delta x. \tag{6}$$

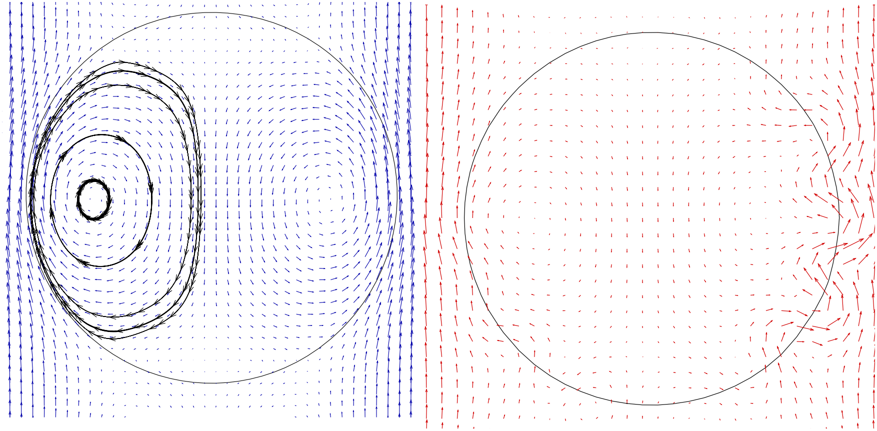
Remark 1 :
If the flow velocity is very low then the previous condition on the time step is very restrictive since $\Delta t_c \gg \Delta t_\sigma$ (*e.g.* in microfluidics : $\Delta t_c = 100 \Delta t_\sigma$).

Remark 2 :
Other way to relax the stability constraint

- semi-implicit treatment of surface tension term, cf. Hysing 2006

Numerical confirmation

Existence of the constant : $c_2 = 8$ (left) et $c_2 = 9$ (right)



Another approach to reduce numerical cost 1/2

Observation :

Microfluidics : in straight channel, asymptotical interfaces are obtained fastly and exist on “long” time

Idea :

Make the most of stationary shape of droplets

How ?

By working in the drop’s frame of reference, with a splitting

Another approach to reduce numerical cost 2/2

Splitting : work in the drop's frame of reference

Algorithm :

(a) Find the speed of translation of the droplet : u^d

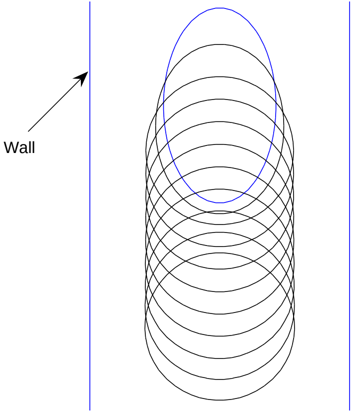
(b) Iterative step : shape correction of the interface

$$\begin{cases} \text{Stokes} \Rightarrow u_{tot} \\ \text{Transport} : \phi_t + (u_{tot} - u_d\, U)\,.\,\nabla\phi = 0 \text{ with } \Delta t = \min(\Delta t_\sigma, \Delta t_c) \end{cases}$$

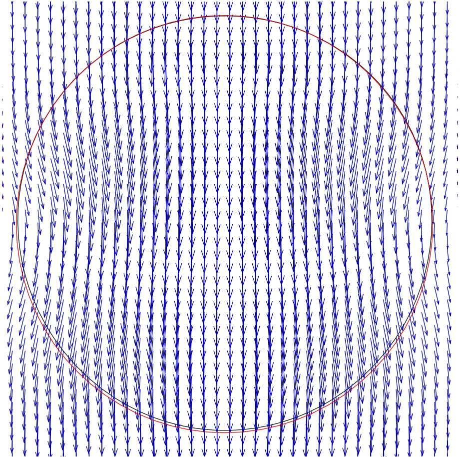
(c) "One shot" step : translation of the droplet

$$\phi_t + u_d\, U\,.\,\nabla\phi = 0 \text{ with } \Delta t_{inj} = \Delta x / \max(u_{inj})$$

Numerical results

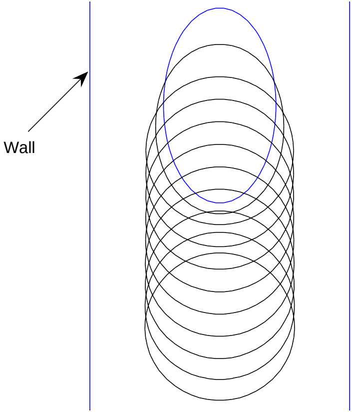


movie : No instability

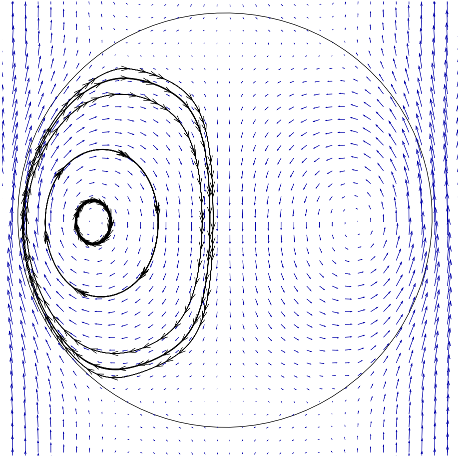


Global flow

Numerical results



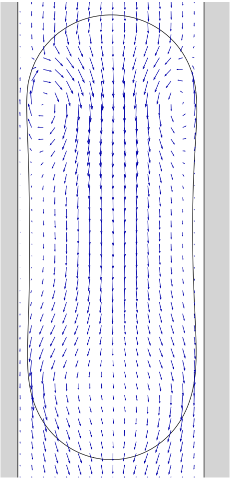
movie : No instability

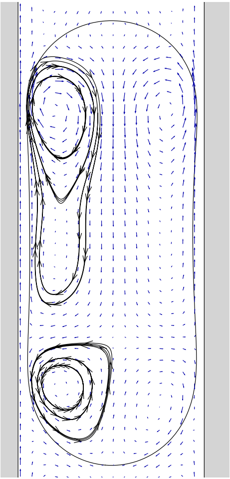


Drop's frame of reference

Various mixing states : confined, slow

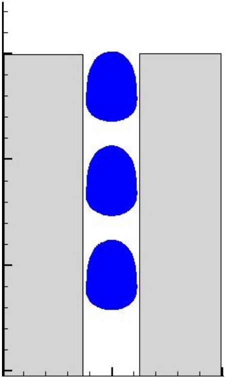
Frame OR : global, ... | ... droplet



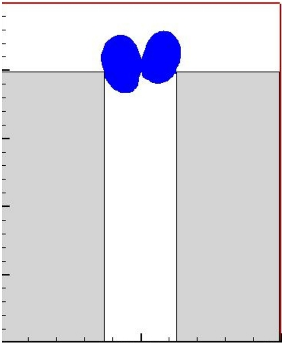


Trains of droplets & collision

Train



Collision



Conclusions

- Level Set method : well adapted to Microfluidics where surface tension is predominant
- **Proposition of a new stability condition**
- Agreement between simulations and physical experiments
  ➜ study of mixing inside the droplets

Current and future work

- full axisymetric 3D
- study near the channel's wall
  - which fluid dynamics ?
  - other boundary condition ?

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