Simulation of a Pressure Driven Droplet Generator

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Abstract: The present paper describes a 2D-axisymmetric simulation of a three-dimensional droplet generator driven by a gas pressure gradient. The software used here is COMSOL Multiphysics®, with the Microfluidics module to approach the topic of laminar two-phase flow with the phase field method. The aim of the process is to produce regular patterns of droplets.
Keywords: Microfluidics, droplet generator, flow focusing, phase field

1. Introduction

Droplet-based microfluidics constitutes a large field of research in new biotechnologies, aerosols or other 2D-Microfluidics devices. Several applications use droplets of immiscible fluids between two liquid phases, some others a coupling between liquid and gas phases. In this case, either bubbles of gas in the liquid phase or droplets of liquid in the gas can be produced. The process used here belongs to the last category and aims to generate droplets with a size of several microns.

Flow focusing have been and are still the object of a constant research, especially concerning drug encapsulation, synthesis of diverse materials, and is widely studied in two dimensions, for the processing of microsystems[1]. The liquid/liquid coupling is the subject of great interest and research concentrates on the droplets production mode and their properties[2].

Several researchers studied the 3D-liquid/gas configuration, to understand the theory underlying the physical processes[3], covering a wide range of experimental parameters like density or viscosity, for biomaterials processing purpose[4]. While some of them explored the way to combine it with electrospray[5], others preferred to stick to the liquid/gas flow, focusing on the instabilities occurring to produce droplets[6].

The final industrial application will be the atomization of a pharmaceutical active ingredient on a deposit, creating a patch used to cure food allergy.

2. Process studied

2.1 Industrial process

Here, we will focus on an industrial application of a 3D-Microfluidics device: the Pneumo-HydroDynamic Droplet Generator. The aim of the process is to produce mono-disperse, regular pattern of droplets, with a minimum size. To use it on an industrial-scale, one needs to control the physical phenomena involved. For this reason, a numerical model has been developed to predict the actual behaviour of the process.

The device used here consists in a cone-shaped nozzle with an inner diameter of 150 µm inserted in a gas-pressurized chamber, with an outlet orifice with diameter 200µm. See Figure 1 for a scheme of the device.

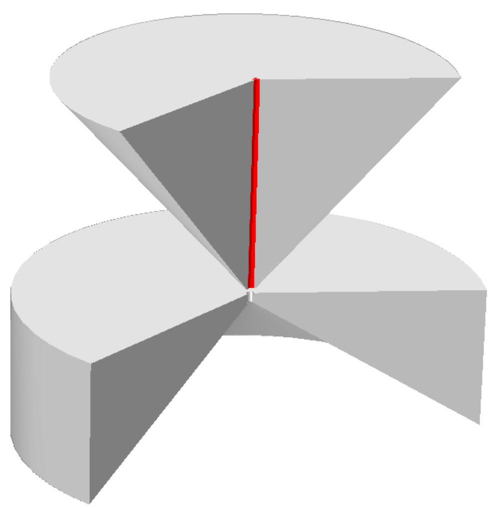

Figure 1 : Schematic representation of the inner parts of the device. At the top, a nozzle is the inlet of liquid and at the bottom the ejector, lower part of the gas chamber, is represented.

2.2 Flow regimes & modes

In this part the different flow regimes and droplets formation modes will be introduced.

There are two distinct behaviours in the process:

- The flow regime of the liquid volume at the nozzle exit (the shape of the meniscus),
- The droplet generation mode at the apex of the shape.

Let us consider two possibilities for the flow regimes in the range of parameters studied:

i) The shape of the volume is constant in time: this is the stationary dynamic flow regime, where the word "stationary" stands for the absence of motion of the global shape of the liquid, and "dynamic" recalls that there is a local motion of the fluid, a downward flow. The meniscus is stable, most often as a cone.

ii) The shape of the volume varies with time: this is the transient flow regime. At this point, the bibliography makes us assert that the flow is periodic: there are time patterns in the shape of the meniscus. Some call this regime the "cone shaking mode"[6].

For the lower part, we can distinguish several droplets formation modes:

a) The dripping mode: Regime in which droplets are produced from the pinching of the interface at a short distance from the emitting orifice. Within dripping mode, there is a window of operational parameters for which the satellites droplets disappear, giving a high monodispersity of droplets sizes. The dripping mode occurs in general for low liquid flow rate and applied pressure. Large single drop are emitted from the outlet of the orifice.

b) The jetting mode: A smooth and undisturbed jet appears near the outlet of the hole until it breaks up into droplets due to instabilities driven by the surface tension force. Both main droplet and satellites droplets are formed. However, depending on the operational parameters, it is possible to obtain droplets of the same size. Moreover, submodes/ transitional modes can be observed in jetting mode such as helical jetting mode, described by the spreading of a non-axisymmetric disturbance along the jet, with a whip-like effect and then breaks up into droplets.

3. Governing equations

3.1 Fluid motion

The Navier-Stokes equations are used to describe the incompressible flow of both liquid and gas in the entire domain. First, the condition of mass conservation stands for the flow:

$$\nabla . u = 0$$

where u is the velocity vector. Secondly, the momentum balance describes the transient evolution of the system.

$$\rho \frac{\partial u}{\partial t} + \rho(u.\nabla)u = \nabla.[-pI + \eta(\nabla u + \nabla u^T)] + \rho\vec{g} + F_{st}$$

where u is the velocity vector, which is continuous, p is the pressure, ρ is the density of the fluid concerned, η is the dynamic viscosity, and F_{st} is the surface tension force.

3.2 Phase field approach

A phase field method is used here to study the motion of the interface between the liquid and the gas. For this purpose, an Eulerian formulation is employed.

Due to the medium range of the Reynolds' numbers associated with both fluids, the flows are laminar, as is commonly the case in microfluidics. The Laminar Two-Phase Flow approach is used with the Phase Field method for the numerical modeling in COMSOL Multiphysics®.

In this method, the multiphase flow is described by a function ϕ. The liquid is described by $\phi = -1$ and the gas by $\phi = 1$. The interface between the fluids is associated with values in the range $-1 < \phi < 1$.

The Cahn-Hilliard equation governs this function; however, due to presence of a 4th order derivative in this equation, COMSOL Multiphysics® prefers to solve for two coupled equations:

$$\frac{\partial\phi}{\partial t}+u.\nabla\phi=\nabla.\frac{\gamma\lambda}{\epsilon^2}\nabla\psi$$
$$\psi=-\nabla.\epsilon^2\nabla\phi+(\phi^2-1)\phi$$

where u is the velocity vector, ϕ the phase field variable, γ the mobility, λ the mixing energy density, and ϵ the parameter of the interface thickness.

The mixing energy density λ, the interface thickness parameter ϵ and the surface tension coefficient σ are related by the formula:

$$\sigma=\frac{2\lambda\sqrt{2}}{3\epsilon}$$

One defines then the mobility rate χ, with $\chi=\gamma/\epsilon^2$. An adjustment of both phase field parameters χ and ϵ, along with the maximal size of mesh h, is essential in order to ensure a good convergence to the numerical model.

Remark: With the help of the ϕ function, one can define two variables reflecting the contribution of each fluid in the system studied:

$$V_{liq}=\frac{1-\phi}{2}$$

$$V_{gas}=\frac{1+\phi}{2}$$

which allows us to write the density ρ and the viscosity η as follows:

$$\rho=\rho_{liq}+\left(\rho_{gas}-\rho_{liq}\right)V_{gas}$$
$$\eta=\eta_{liq}+\left(\eta_{gas}-\eta_{liq}\right)V_{gas}$$

A more detailed theory related to the laminar phase field method can be found in the source reference paper[7].

4. Numerical Model

In this model, we have developed a 2D-axisymmetric approximation model thanks to a rotational symmetry. This simplifies the complexity of the problem and then reduces the runtime of the simulations compared to a full 3D description. The mesh used is refined in the center of the device, near the symmetry axis, where the interface can move during the computation.

The liquid used is similar to milk (DP), and the gas is N_2 (CP). The surface tension coefficient between the two fluid phases was set to $\sigma=35.6\ mN/m$, the contact angle was $\theta=\pi/2\,rad$ and the selected material properties are shown in Table 1.

Property	Milk (DP)	N_2 (CP)
Density (kg/m3)	957	1.225
Dynamic viscosity (mPa.s)	1.8	0.018

Table 1 : Fluid properties used in simulations

PARDISO was set as the direct solver for the resolution of the phase initialization. For the time-dependent study, an extra equation was added in order to compute the ratio between the current liquid volume in the system and the expected one (a method for the numerical validation concerning mass conservation). For this purpose, a segregated PARDISO solver was set for this second time-dependent study.

The resolution time ranges between 0 and several milliseconds and time steps are of the order of $10^{-5}-10^{-4}$ s.

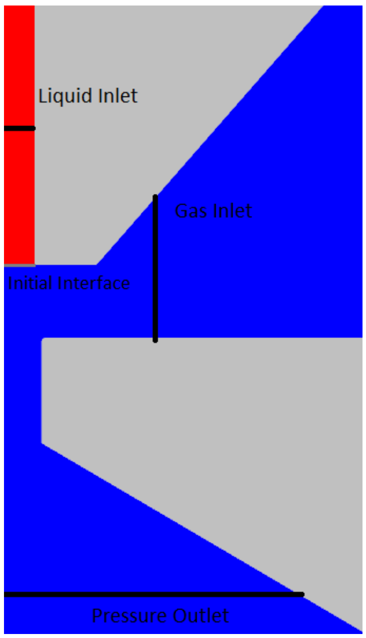

Figure 2: Boundary conditions defined for the droplet generator in the 2D axisymmetric model. The device has two inlets, one set with a constant liquid flow rate and the other with constant gas pressure. The outlet is set to a zero reference pressure.

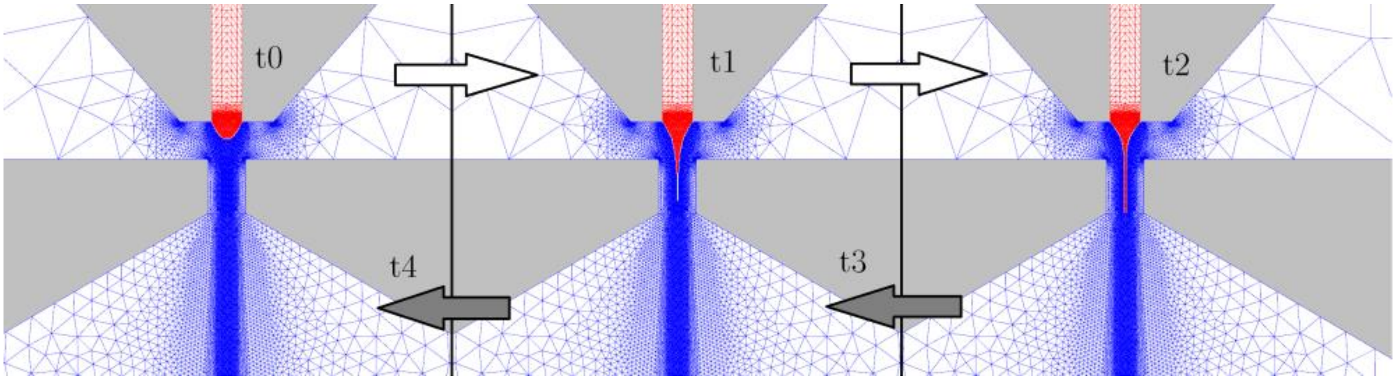

Figure 3: Typical time sequence for a transient flow regime: the gas pressure in the chamber is 0.2 bar, the liquid flow rate is 2 ml/h. This is a cycle of the behaviour of the liquid volume at five times t0, t1, t2, t3 and t4.

Boundary conditions are as specified in Figure 2, with the 2D view in COMSOL Multiphysics®.

5. Results and discussion

A typical time sequence for the transient flow regime is shown in Figure 3. We can decompose the occurring events as follows:

- First, a hanging droplet is formed at the nozzle outlet.
- Secondly, gas pressure gives the liquid a cone-like shape.
- Then, the liquid flows downward as a thread, and loses its kinetic energy
- Eventually, the surface tension makes the liquid return to a hanging droplet shape.

The period of such a cycle lasts around 0.7 ms.

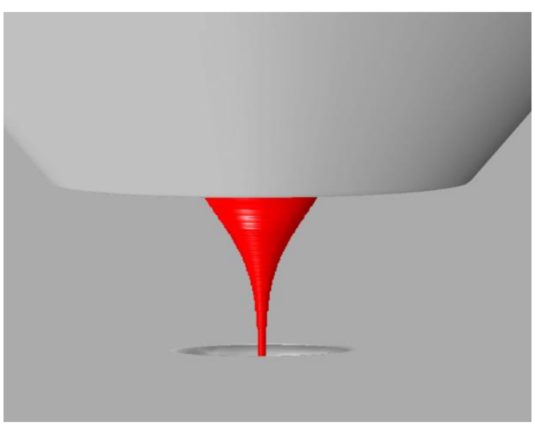

Figure 4: Clip showing the cone-shaped liquid volume in stationary dynamic flow regime.

One can see in Figure 4 the classical shape for the stationary dynamic flow regime, for a liquid flow rate inlet of 5 ml/h and for a gas pressure of 0.2 bar.

Simulations were run at different total liquid flow rates (1 to 10 ml/h) and gas pressures (0.02 to 0.8 bar). The flow regime configuration can be characterized by the two following non-dimensional numbers:

$$We_{liq} = \frac{\rho_{liq} u^2 R_{in}}{\sigma}$$

$$We_{gas} = \frac{2 P_{gas} R_{out}}{\sigma}$$

The distribution diagram of the different flow regimes is shown Figure 5

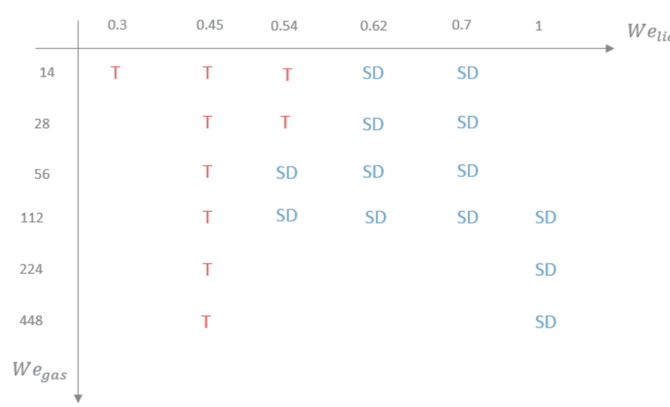

Figure 5: Diagram showing the flow regime as a function of the Weber numbers. The red "T" stands for transient and the blue "SD" means stationary dynamic.

This diagram has been validated under certain experimental results obtained at DBV Technologies.

6. Conclusions

In this work we have successfully simulated a pressure driven droplet generator. Taking advantage of the rotational symmetry of the device, the model was implemented in 2D, which significantly reduces the computational time (5 hours in average).

A characterization of the flow regimes have been made in order to further study, in a future work, the droplet formation mode. The goal of this study will be to produce at industrial scale droplets with minimum size, in a stationary dynamic flow regime jetting mode.

In a forthcoming study, we will look at the coupling between microfluidics and other physics, such as electricity, in order to see if an electric field in the system can change the atomization and the direction of the formed droplets.

7. References

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