

Flow Simulation of a Microfluidic Analog of the Four-Roll Mill

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ABSTRACT¹

The fluid dynamics of channel geometries for liquid state materials characterization in microfluidic devices are investigated using finite element flow simulation and flow classification criteria. A pressure driven microchannel device is sought that has an adjustable flow type, approximating the function of the four-roll mill. Channel flow geometries are investigated in which the full range of linear flows (extension, shear and rotation) can be approximated in the neighborhood surrounding a stagnation point. A class of flow geometries is identified which makes use of opposing, laterally offset fluid streams that produce a stagnation point in the center of the geometry.

Keywords: microfluidics, four-roll mill, flow classification, finite element analysis, linear flow

1 INTRODUCTION

Fluid flow in microfluidic devices is becoming more and more common, driven by the miniaturization of many technologies [1-3]. Such devices afford a number of advantages over conventional methods, including greater speed, replacement of multiple manual steps, conservation of expensive and/or limited quantity reagents, and reduced human error.

The goal in this study is to develop a microfluidic device for liquid state materials characterization. This goal requires first and foremost, a flow geometry capable of generating flows suitable for materials characterization. The ideal types of flow for the characterization of fluids are linear flows which are described by the stream function and corresponding velocity vector

$$\psi = \frac{1}{2}(\xi\gamma x^2 - \gamma y^2) \quad (1.1)$$

$$\underline{v} = (\gamma y, \xi\gamma x) \quad (1.2)$$

The nature of these kinematics are characterized by the constants ξ and γ [4]. The quantity ξ is the flow type, and indicates the nature of the deformation experience by the fluid; the flow is extensional for $\xi = 1$, shear for $\xi = 0$, and pure rigid body rotation for $\xi = -1$. The quantity γ is the flow

strength, and indicates the magnitude of the velocity gradient relative to the flow type.

In a linear flow, the velocity gradient tensor is constant and the flow type is uniform, which makes measurement of flow properties as a function of deformation rate unambiguous. In addition, linear flows contain a stagnation point at the origin point (0,0). The stagnation point serves a number of beneficial purposes in the present context. First, the material residence time in the neighborhood of the stagnation point is high, giving the material adequate time to respond to the applied deformation. Residence time is in effect, a third type of flow classification criteria [4]. In addition, the long residence time also provides a stable environment for material observation and measurement, and it allows one to ignore the inhomogeneities present in a complex flow, provided that the stagnation region is reasonably broad, and the flow gradients are suitably uniform.

A number of devices that approximate particular modes of linear flows at the macroscale are available [5-14]. The device that comes closest to the desired functionality is the four roll mill. While this is primarily thought of as a device for producing planar extension ($\xi = 1$), it can also be used to provide mixed flows with $0.2 < \xi < 1$ [7-8], and rotational flows where $\xi \sim -1$ [9]. However, the four roll geometry cannot produce simple shear ($\xi = 0$), and difficulties can be anticipated in trying to produce and control a miniature device with moving parts. This leads us to seek a solution based on channel flow.

In this study, a pressure driven microchannel device is sought that has an adjustable flow type, approximating the function of a four roll mill. In particular, we investigate classes of channel flows in which the full range of linear flows can be approximated in the neighborhood surrounding a stagnation point. To evaluate candidate geometries, finite element flow simulations in the zero Reynolds number limit were undertaken. Flow classification criteria [4] were then used to delineate combinations of geometry and boundary conditions for which the flow type can be adjusted between shear and extension in the neighborhood surrounding the stagnation point, while providing adequate flow strength. A class of flow geometries is identified which makes use of opposing, laterally offset fluid streams. Opposing fluid streams are

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necessary to produce a stagnation point. Lateral offset is necessary in order to produce shear.

2 MODELING

2.1 Flow Simulation

To evaluate candidate geometries, flow was simulated using the finite element method. All flows were assumed to be steady, two-dimensional, and at the zero Reynolds number limit. Modeling was carried out using the commercial finite element packages² FIDAP [15] and FlexPDE [16]. The governing equations solved by FIDAP are the Navier-Stokes equations with the incompressible condition

$$-\nabla p + \eta \nabla^2 \underline{u} = 0 \quad (1.3)$$

$$\nabla \cdot \underline{u} = 0 \quad (1.4)$$

FlexPDE makes use of the alternative incompressible formulation

$$\nabla^2 p = -\nabla \cdot \nabla \cdot (\rho \underline{u} \underline{u}) + \beta (\nabla \cdot \underline{u}) \quad (1.5)$$

where β is a large value chosen such that $\nabla \cdot \underline{u}$ is sufficiently small.

2.2 Flow Classification

A suitable objective criterion for classifying the flow type in complex flows has been developed by Astarita [4]. For steady two-dimensional flows, where $\underline{u} = [u, v]$ and

$$\underline{D} = \begin{bmatrix} \varepsilon & \gamma \\ \gamma & -\varepsilon \end{bmatrix}, \text{ the flow type } \Xi \text{ is given by the expression}$$

$$\Xi = \frac{\varepsilon^2 + \gamma^2 - W^2}{\varepsilon^2 + \gamma^2 + W^2} \quad (1.6)$$

where $W = \omega - \Omega$, ω is the vorticity and

$$\Omega = \frac{\gamma \left(u \frac{\partial \varepsilon}{\partial x} + v \frac{\partial \varepsilon}{\partial y} \right) - \varepsilon \left(u \frac{\partial \gamma}{\partial x} + v \frac{\partial \gamma}{\partial y} \right)}{2\sqrt{\varepsilon^2 + \gamma^2}} \quad (1.7)$$

Like the constant ξ in linear flows, the variable Ξ has a value equal to 1 in purely extensional flows, 0 in shear flows, and -1 in a pure rigid body rotation.

For classifying flow strength, a relative flow strength can be defined as

$$S_r = \frac{\lambda}{\lambda_{ref}} \quad (1.8)$$

where $\lambda = \sqrt{\varepsilon^2 + \gamma^2}$ is an absolute measure of flow strength equal to the maximum eigenvalue of the stretching tensor,

and λ_{ref} is the flow strength at a reference point in the flow. In what follows, we classify different flow fields using Eqs. (1.6) and (1.8), taking the reference flow strength to be an average flow strength at the inlet or outlet of a channel geometry. This enables comparison of the strength of deformation in the stagnation region with the deformation in the pressure driven channels that drive the flow.

3 SIMULATION RESULTS

In determining the parameters of a flow device that could be used to generate a range of approximately linear flows in the region surrounding a stagnation point, it was recognized that creating a flow with a stagnation point requires the use of oppositely directed fluid streams. While this is generally a means to produce extensional flow, by creating lateral offset between the opposing streams, shear and even rotation can be produced as well. We make use of this principle in our investigation.

The geometry together with boundary conditions studied here is depicted in Figure 1. Overall the geometry represents a modification of the basic cross flow device. Two important modifications are evident. First, the flow channels in the vertical direction are asymmetrically offset from the center of the channel on the top and bottom of the geometry by distances of $\pm H_2 / 2$, respectively. Second, the horizontal channels are split by a spacer plate of thickness h_{fin} . This provides two extra flow channels in the horizontal direction. The upper and lower spacer plates are offset horizontally by a distance d_{off} .

The flow geometry has three different boundary pressures, P_{in} , P_1 , and P_2 . The pressure P_{in} represents a pressure that remained fixed during a simulation, while the values of P_1 and P_2 represent pressures that were allowed to vary. Simulation results showed that the flow type at the stagnation point in this geometry is solely a function of the ratio $P_{rat} = \frac{\Delta P_1}{\Delta P_2}$, where $\Delta P_i = P_{in} - P_i$. By specifying values for P_{in} , P_{rat} and $P_{mag} = \Delta P_2$, values for P_1 , and P_2 were set as $P_1 = P_{in} - P_{mag} \cdot P_{rat}$ and $P_2 = P_{in} - P_{mag}$. The relevant geometric and boundary condition parameters used in the simulations to be presented are listed in Table 1.

Plots of flow type and relative flow strength at the stagnation point as a function of P_{rat} are shown in Figures 2-3. Figure 2 shows that by cycling through values of P_{rat} , the entire range of flow types can be

² Identification of a commercial product is made only to facilitate reproducibility and to adequately describe procedure. In no case does it imply endorsement by NIST or imply that it is necessarily the best product for the procedure.

reached. For highly negative pressure ratios the flow type has a value that is negative, indicating a high degree of rotation. As P_{rat} decreases towards zero, the amount of rotation is continually reduced and the extensional flow type value of unity (extension) is reached at a pressure ratio of approximately -1. As the pressure ratio further increases and becomes positive, a shear flow type of zero at the stagnation point is eventually realized for a pressure ratio value of approximately 2. The relative flow strength depicted in Figure 3 is taken relative to the average flow strength at the inlet of the flow. The plot shows the flow strength continually rises (almost linearly) with increase in the pressure ratio. Thus, the flow strength value is relatively higher for shear (0.6), than for extension (0.23). Values are tabulated in Table 2.

4 DISCUSSION

In developing a microfluidic device for liquid state materials characterization, the most basic need is to have a suitable flow geometry for deforming the fluid in a controlled manner. We have sought to investigate classes of channel flows in which the full range of linear flows can be approximated in the neighborhood surrounding a stagnation point. Using a combination of finite element simulation and flow classification theory, a class of flow geometries that fit the above criteria has been determined. The full range of linear flow kinematics can be produced at the stagnation point, with varying, but in all cases acceptable degree of flow strength.

In the results presented, complete optimization of the flow geometry parameters has not been attempted as our primary goal in this initial study was simply to identify geometry and boundary condition combinations that allow us to achieve the basic goal of generating a full range of flow types. This, in coordination with experimental testing, is part of our ongoing work. There are a number of other items that will need to be examined in future work. First, our initial results presented here have considered the system to be 2-D in nature, as is done for example with the four roll mill. However, shear in the third direction is likely to have some effect and will be taken into account by means of 3-D flow simulation. In addition, non-Newtonian flow behavior will have to be addressed when working with polymer systems.

5 SUMMARY AND CONCLUSIONS

In this study, the fluid dynamics of pressure driven flow in microchannels was studied for the purpose of designing a liquid state, materials characterization device. A class of flow geometries was identified in which a full range of linear flows could be approximated in the neighborhood surrounding a stagnation point. The flow geometry that was identified makes use of opposing, laterally offset fluid streams. The opposing fluid streams are necessary to produce a stagnation point, and the lateral offset is necessary

in order to introduce rotation into the flow to produce shear. Geometry optimization in coordination with experimental testing is underway.

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Inlet Width (H_{in})	Inlet/Outlet Width 1 (H_1)	Inlet/Outlet Width 2 (H_2)	Fin Width (H_{fin})	Channel Length (L)	Offset Distance	Pressure Magnitude (P_{mag})	Inlet Pressure (P_{in})
2	1	2	0.05	5	0.5	1.0	0

Table 1. Geometry parameters and boundary conditions used for the parallel, laterally offset, channel geometry, with transverse flow channels. All units are relative.

Case	Pressure Ratio (P_{rat})	Pressure 1 (P_1)	Pressure 2 (P_2)	Flow Type	Relative Flow Strength
Extension	-0.9	0.9	-1	0.9995	0.233
Shear	2.2	2.2	-1	-0.0044	0.596

Table 2. Values for flow type and flow strength at the stagnation point for the parallel, laterally offset, channel geometry, with transverse flow channels, at offset distances mostly closely corresponding to the cases of extension and shear.

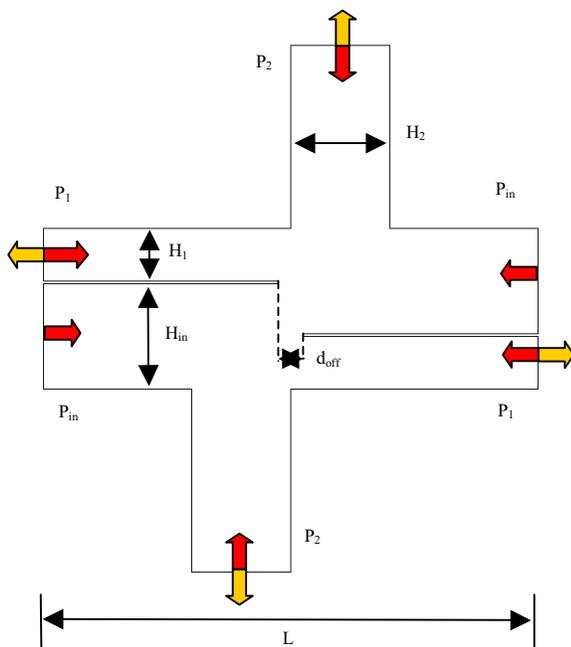


Figure 1. Flow geometry, parameters and boundary conditions. Geometry values used in the simulations are listed in Table 1.

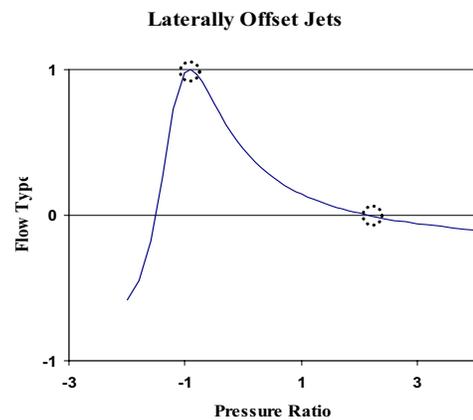


Figure 2. Flow type as a function of the pressure ratio.

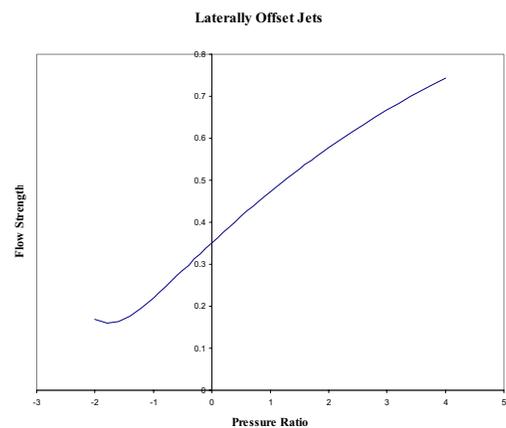


Figure 3. Relative flow strength as a function of pressure ratio.