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Numerical Simulation of Plasma Separation in a Backward facing Step Microchannel

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ABSTRACT

Current plasma separation techniques involve the separation of cell-free plasma from whole blood using large equipment, such as centrifuges. These equipment have mobility constraints and require the patients to be at the location of the separation facility. The present study involves the numerical simulation of blood flow in a microchannel using OpenFOAM. A backward-facing step design of the microchannel is considered and the plasma separation efficiency of different configurations of the backward-facing step microchannel is estimated. Two different models for blood flow are considered in this study. The Newtonian model is used for the single-phase simulations. The multiphase simulation, however, considers the two-phase model for the blood flow, consisting of cell-free plasma and red blood cells (RBCs). The phases are assumed to be separated and stratified at the inlet of the microchannel in the multiphase simulation. The effect of inlet velocity, hematocrit or RBC volume fraction and, the configuration of the microchannel on the efficiency of plasma separation process is analyzed in the numerical simulations. To simplify the simulations, properties of water are considered in the single-phase simulation and properties of air and water are considered for plasma and RBCs respectively in the multiphase simulations.

Keywords: plasma separation, multiphase flow, OpenFOAM, microchannel, backward facing step.

1. INTRODUCTION

Blood plasma is made up of a variety of components which play a vital role in regulating cell function. Therefore, it is important to efficiently separate plasma and blood cells. This separation process is also known as plasmapheresis.

The most commonly used medical practice of plasma separation is using a centrifuge. The lack of mobility of such facility has resulted in a demand for compact, efficient, inexpensive and easy-to-use clinical plasma separation devices. With the help of research in microfluidics, which has burgeoned in the 21st century, microfluidic chips are developed to replace the classic centrifuges. These microfluidic chips use the hydrodynamic mechanism of bifurcation law, or plasma-skimming effect, and the centrifugal forces induced by the microchannel design. In this study, we will be studying plasma separation in microchannels using the CFD tool OpenFOAM.

2. LITERATURE REVIEW AND OBJECTIVE

Identifying the suitable model for the blood flow is an essential component of any hemodynamic study. Both Newtonian and non-Newtonian models of blood are studied extensively. Furthermore, these models are coupled with one of single-phase, two-phase or multiphase models. One of the simplest models studied was in Morimoto et al. (2010) [3]. It considers a quasi-two-phase model to study the efficiency of the plasma separation in a branched microchannel. The numerical study considers a non-Newtonian rheological model with spatially varying viscosity. The study investigates the effect of flow rate in a branched channel on the efficiency of plasma extraction process using a multi-layer model. The layers, differentiated by their viscosity, were plasma, blood cells and a transition layer. An inflow layer, called plasma layer, was determined for varying flow rates and this in turn pointed to the size of the particles that could be efficiently separated through the plasma separation process.

Further, a Newtonian, single-phase model was used by Huang et al. (2010) [4]. The process of plasma separation in a microchannel was optimized using a backward facing step instead of a simple bifurcation in [3]. In addition to the measure of inflow layer used in [3], the study measures the volumetric flow rate in the branch to quantify the efficiency of the plasma separation process. The study investigates flow through the following microchannels: a straight, bent and converging channels. The bent microchannel was incorporated to induce centrifugal effect in the flow before the separation at the branch. The goal was to identify the microchannel design which can extract particles of least size at the highest flow rate ratio (α) through the branch for given inlet conditions. The flow rate ratio is the ratio of volumetric flow rate in the side channel (Q_1) to the inlet flow rate (Q_0). The flow rate ratio is given by

$$\alpha = Q_1/Q_0 \tag{1}$$

To simplify the study, a Newtonian, single phase model with properties of water was used. The results of the numerical simulation confirmed that microchannel with both converging and bending channels had the highest plasma separation efficiency.

A variation of the curved microchannels from [4] were employed to study plasma separation by Zhang et al. (2008) [5]. The study considers a two-phase model of blood flowing through a curved microchannel. The entire system is also in rotation which results in three forces on the blood flow: two centrifugal forces and Coriolis force. The problem was simulated using the Eulerian multiphase model of the commercial software Fluent. The study was conducted for different inlet hematocrit and it was found that the separation efficiency monotonically increases as the hematocrit decreases.

The present study is an extension of [4] using OpenFOAM, an open source CFD code for flow simulations. The study starts with the validation of the numerical results in [4] using the simpleFoam solver of OpenFOAM. The properties of water are considered to simplify the simulation. The study is then extended to the two-phase model using the multiphaseEulerFoam solver. Other than the two microchannel models used in [4], the present study considers a microchannel with bent inlet, which is also converging uniformly until reaches the backward-facing step. It is to be noted here that, water and air have been used in the simulations instead of RBCs and plasma respectively, to simplify the simulations.

3. MATERIALS AND METHODS

For a low Reynolds number flow, lateral migration of the blood cells take place in the microchannel. Therefore, a plasma layer is observed adjacent to channel wall. However, this layer is too thin to extract plasma from the blood sample. A basic bifurcation structure, therefore will not be enough to extract the cell-free plasma. Keeping this in mind, a microchannel with a backward facing step is employed in this study. Flow over a backward facing step results in a pressure drop on the step edge due to the sudden expansion. It also induces vortices at the step edge, creating a recirculation region. Since the side channel is located at the step edge, the presence of the recirculation region limits the particles entering the side channel as the inertia of the particles is expected to keep them in the recirculation region [4]. The authors believe that this phenomenon can be extrapolated to the air-water model, just like the plasma- RBC model.

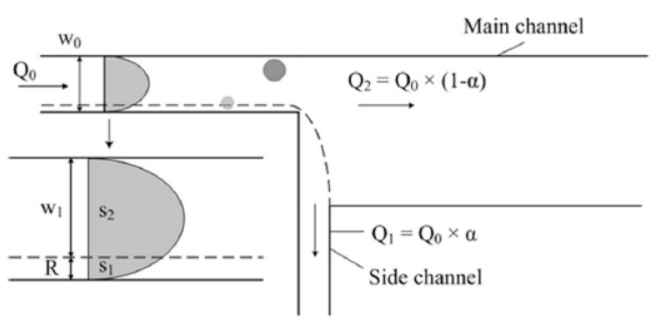
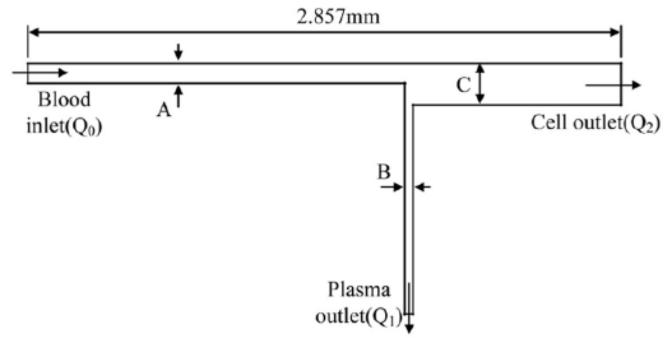


Figure 1: Schematic of the plasma separation process [4].

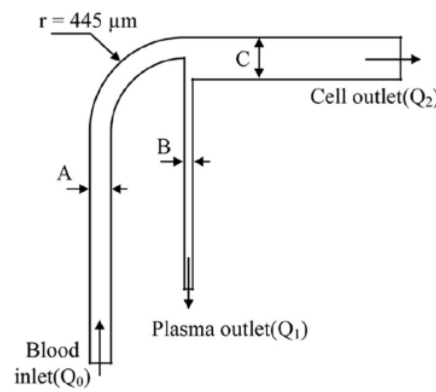
The basic principle of the backward facing step microchannel is shown in fig. 1. It is assumed that the velocity fields inside the channel follow Poiseuille's law. The dashed line shows the streamline extended from the edge of the side channel to the inlet. Of all the streamlines in the inlet, only the ones below the dashed line will enter the side channel. Therefore, the any particle with a radius larger than R will not be entering side channel. The goal, along with to obtain highest flow rate ratio (α), is also to minimize R enabling the microchannel to separate smaller particles.

The layout of two microchannels used in this study is shown in fig. 2. The Type I microchannel has a straight inlet while Type II employs a bent microchannel to induce centrifugal effects. The inlet width if the channel is 100 μm and at the outlet both channels are 204 μm wide. The radius of curvature of the bending microchannel is 445 μm.

In this study, a novel Type III microchannel was used. The uniform bent in Type II microchannel is replaced by a gradually converging bent inlet. The bent inlet of Type III microchannel is illustrated in fig. 3.



(a)



(b)

Figure 2: Layout of the microchannels: Type I (a) and II (b). The bent inlet in Type II induces centrifugal effect (A = 100 μm; B = 40 μm; C = 204 μm; D = 50 μm; depth of the microchannel is 40 μm) [4].

Unlike the circular arc of the outer walls of the curved section, the inner walls follow an elliptical shape.

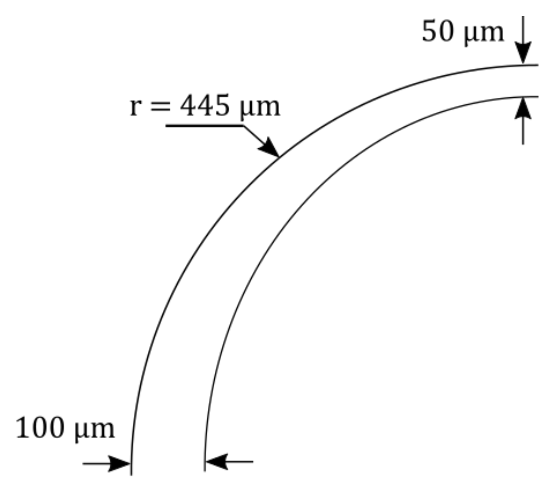


Figure 3: The bent section of the inlet of Type III microchannel. [4].

3.1 Single-phase Numerical Simulation

To validate the results from [4], the single-phase simulation is carried out by considering the properties of water for the whole blood. The density and viscosity of blood-plasma is therefore assumed to be 997 kg/m^3 and 8.55×10^{-4} kg/m-s respectively. Also, a Reynolds number of 5, which corresponds to an inlet velocity of 7.5×10^{-2} m/s is considered for the simulation.

Simulations were performed using OpenFOAM 7 on a personal computer. The finite volume method and a two-dimensional structured grid was used to solve the governing equations. For the steady, incompressible, laminar flow, the OpenFOAM solver simpleFoam was used to solve the continuity equation:

$$\nabla \cdot \mathbf{u} = 0 \tag{2}$$

and the momentum equation:

$$\nabla \cdot (\mathbf{u} \otimes \mathbf{u}) - \nabla \cdot \mathbf{T} = -\nabla p + \mathbf{S}_u \tag{3}$$

where $\mathbf{u}$ is the velocity, p is the kinematic pressure, $\mathbf{T}$ is the stress tensor and $\mathbf{S}_u$ is the momentum source.

At the inlets, the velocity was kept at a fixed velocity and the outlets were set to a fixed pressure. The boundary conditions are summarised in table 1.

Table 1: Boundary conditions for single-phase simulation

Boundary	p (m^2/s^2)	$\mathbf{u}$ (m/s)
Inlet	Zero Gradient	0.075
Outlets	0	Zero Gradient
Walls	Zero Gradient	No slip

The total number of elements were approximately 670,000 for Type I microchannel. For Type II and III microchannels, 756,000 mesh elements were considered in the mesh.

3.2 Multiphase Numerical Simulation

For the multiphase simulations, the OpenFOAM solver multiphaseEulerFoam was used. To simplify the simulation, the properties of plasma and RBCs are taken to be the same as that of air and water respectively. The multiphaseEulerFoam uses the Euler-Euler multiphase model. The geometry of the microchannels of Type I and II are retained in this study. The inlet boundary, however, is split into two section. The bottom section of the inlet face is the air inlet and the top section for RBCs, which are air and water inlets respectively in this simulation.

The inlet and wall boundary conditions are maintained the same as that in case of the single-phase simulations. The only additions being the volume fraction (f) for each phase and an extra boundary due to spit inlet. At the outlets, flow rate velocity boundary conditions are imposed and its values are specified keeping the inlet flow rates of both air and water, satisfying the mass conservation. The boundary conditions are summarised in table 2. ZG in the table stands for zero gradient.

Table 1: Boundary conditions for single-phase simulation

Boundary	P (Pa)	$\mathbf{u}$ (m/s)	f_{air}	f_{water}
Air Inlet	ZG	0.075	1	0
Water Inlet	ZG	0.075	0	1
Outlets	0	Flow rate	ZG	ZG
Walls	ZG	No slip	ZG	ZG

The total number of elements were approximately 4,000. The number of elements were kept low as the multiphase solver, multiphaseEulerFoam is computationally, a very expensive solver.

4. RESULTS AND DISCUSSION

The two microchannel designs described earlier were investigated using the OpenFOAM solvers simpleFoam and multiphaseEulerFoam. The results from the single-phase solver simpleFoam were compared to results obtained using the SIMPLEC method in CFD-ACE in [4].

4.1 Single-phase Numerical Simulation

A flow of Reynolds number 5 is simulated and the results are compared with ones from [4]. To calculate the flow rates, centerline velocity at the outlets are considered. To calculate the minimum radius (R) of the particles which can be excluded from the side channel, the vertical distance of the last streamline entering the side channel from the bottom wall of the inlet is measured. The steady-state streamlines for the single-phase simulation of flow through the bent microchannel is shown in fig. 4. The large concentration of streamlines near the inner walls of the curved section indicates the centrifugal effects in the microchannel.

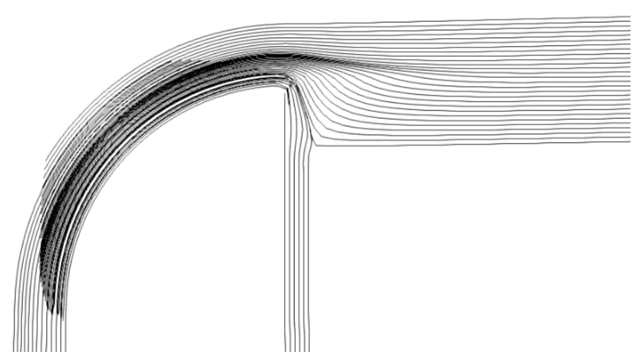


Figure 4: Steady-state streamlines for Type II microchannel at a Reynolds number of 5.

The flow rate ratio (α) from the simulation is compared with the results from [4] in table 3.

The results from the simulation agree well with the results from [4]. The increased flow rate ratio in Type II microchannel also verifies the trend in [4] which indicated that bent microchannels induce centrifugal effect and aids plasma separation from whole blood at higher flow rates, compared to Type I microchannel.

However, the flow rate ratio is the highest in Type III microchannel.

Table 3: Comparison of the flow rate ratio (α) with literature [4]

Microchannel Type	α (%)	α (%)[4]
Type I	6.4	7.2
Type II	7.1	7.3
Type III	8.8	–

The minimum radius (R) of the particles which can be excluded from the side channel from the simulation is compared with the results from [4] in table 4. The vertical distance of the last streamline entering the side channel from the bottom wall of the inlet is measured using the Ruler tool in ParaView.

Table 4: Comparison of the minimum radius (R) of the particles which can be excluded from the side channel with literature [4]

Microchannel Type	R (μm)	R (μm)[4]
Type I	12	9
Type II	11.5	8.5
Type III	7	–

The results from the simulation are comparable with the results from [4]. The simulation agrees with the trend in [4] that Type II microchannel can separate larger particles and hence thicker layer plasma layers injected through the inlet can be separated more efficiently.

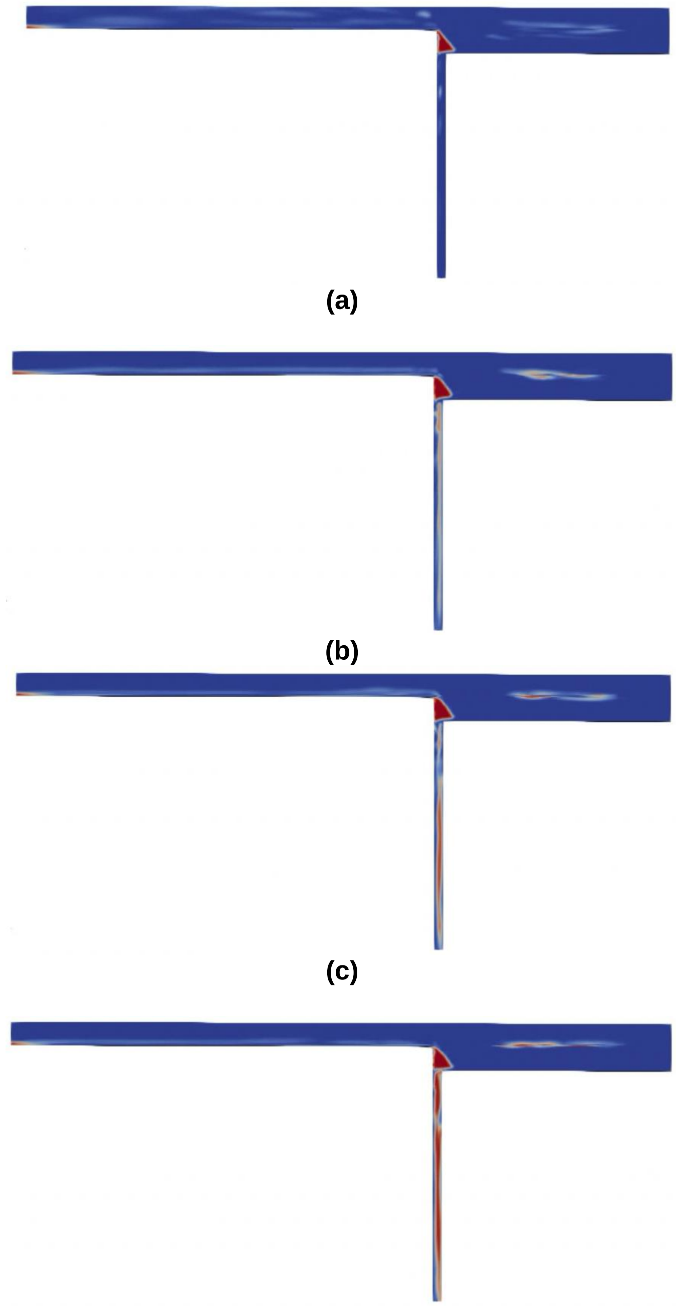
However, the minimum radius (R) of the particles which can be excluded from the side is least in Type III microchannel.

4.2 Multiphase Numerical Simulation

To extend the single-phase simulations to multiphase, air and water are assumed to enter the microchannel in the form of stratified layers, with air being the bottom layer. This assumption is based on the plasma skimming effect which results in a plasma layer formation adjacent to the channel wall in blood flow with low Reynolds number. Based on the results from the single-phase simulations, the thickness of air layer at the inlet is fixed to 10 μm for a flow of Reynolds number 5.

The simulations were carried out for Type I microchannel using multiphase OpenFOAM solver multiphaseEulerFoam and the simulations were run for 50 seconds. The volume fraction of air (f_{air}) at 5, 15, 25 and 30 seconds in shown in fig. 5. The red indicates the air in the plots.

The results from the simulation shows that with inlet air thickness of 10 μm for a flow of Reynolds number 5, the air can be separated through the side channel of Type I microchannel with high efficiency. The flow rate of air, at the two outlets, is monitored from 35 to 50 seconds and it is found that approximately 80% of the air flows through the side channel.



(a)

(b)

(c)

(d)

Figure 5: Contour plots of volume fraction of air (f_{air}) at (a) 5 seconds, (b) 15 seconds, (b) 25 seconds, and (b) 35 seconds for inlet air thickness of 10 μm for a flow of Reynolds number 5 in Type I microchannel

5. CONCLUSIONS

In this study, microchannels of different structures were employed to analyse the efficiency of plasma separation using the CFD tool OpenFOAM. A straight and bent microchannels were taken from [4] for validation using the single-phase OpenFOAM solver simpleFoam. A novel microchannel design was also proposed, utilizing the backward-step geometry, the centrifugal force and converging inlet to extract plasma from whole blood. The single-phase simulations showed that the novel microchannel design could extract plasma at flow rate ratio (α) of 8.8%, which 1.7% more than the bent inlet Type II microchannel. It was also found that of the minimum radius (R) of the particles which can be excluded from the side channel is the least in the newly proposed microchannel. The authors believe the same can be extrapolated to whole blood and Type III microchannel to be the more efficient structure for plasma separation. The simulations were then extended to multiphase simulation using the Euler-Euler model. The OpenFOAM solver multiphaseEulerFoam was employed to study stratified air and water flow through the microchannels. The thickness of the air layer considered the minimum radius (R) of the particles which can be excluded from the side channel found using the single-phase simulations. The multiphase models showed that the inlet air thickness of the order of R from the single-phase simulation aided in high-efficiency separation of air. The multiphase simulations were carried out only for the straight microchannel. The multiphase study is underway for the other two microchannel structures, namely, bent inlet Type II and the bent inlet with converging width Type III microchannels, to identify the amount of air extracted, averaged over time, to verify the α trend predicted by the single-phase simulations.

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NOMENCLATURE

f	Volume fraction	--
p	Kinematic pressure	[m^2/s^2]
P	Pressure	[$kg/m\text{-}s^2$]
Q_0	Inlet flow rate	[m^3/s]
Q_1	Flow rate in the side channel	[m^3/s]
R	Radius of the particle	[m]
S_u	Momentum source	[m/s^2]
T	Stress tensor	[m^2/s^2]
u	Velocity	[m/s]
α	Flow rate ratio	--

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