An Investigative Study of Microfluidic Capabilities of Star-CCM+

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Abstract

Flow in microchannels studied using Star-CCM+ is presented. Firstly, single phase flow in prismatic channels of rectangular and circular cross section is modeled. The velocity profile is validated against the analytical profile for both the cases. Then, Droplet formation in microfluidic T-junction and microfluidic flow focusing device is study. The volume-of-fluid (VOF) method has been employed to model the devices. However, very high spurious currents and thick interface were observed, when a coarse mesh was used near the interface. These currents were found to be reducing as the mesh was refined. So, to minimize these currents and to sharpen the interface adaptive mesh refinement (AMR) technique was employed.

Introduction

Fluid flow in Microchannel (with characteristic dimension less than 1000 μm) has attracted a large amount of audience in past two decades because of its great potential and application in micro devices. Some of these applications include micro-scaled cooling of high power generating electronic micro-devices such as microchips. Another application of microfluidics is controlled droplet formation in Microchannels. Droplets at microscopic scales are useful in wide range of applications particularly when the size of the droplet and the frequency of the droplet formation can be controlled. Droplets in Microchannels form the centerpiece of many lab-on-a-chip devices. For example, droplets can be moved around as a means of pumping fluids. Another
application is the use of droplets as chemical reactors where the kinetics can be monitored and controlled precisely. Droplets have also been used as templates for producing micro-particles with specialized biological, chemical, and optical properties. Creation of mono-disperse emulsions requires microfluidic channels for droplet formation as traditional methods produce droplets of varying sizes [1].

However, many unexpected phenomena have been reported when dealing with micro-flows [2]. The limited available data show behavior that is either exactly same or significantly different from the macroscopic behavior and theory. The reason for this anomaly has been attributed to micro-effects, which become significant as the characteristic length scale decreases. Some of these micro-effects include high lateral momentum diffusion, surface forces etc. Also, the applicability of continuum hypothesis is questionable.

The present study investigates the ability of Star-CCM+ to model flows in Microchannels. Flows for low Knudsen number have been studied to eliminate inapplicability of continuum hypothesis. Firstly, flow characteristics (velocity profile and pressure gradient) of simple flow in Microchannels of rectangular and circular cross section were validated.

After validating the single phase flow model, multiphase flow in Microchannels was validated by modeling Droplet formation in a Microfluidic T-junction and a Microfluidic flow focusing device.

A schematic diagram of T-junction is shown in fig. 1. The T-junction geometry consists of a main channel and a dispersed channel that merge at a right angle. The main channel carries the continuous fluid (carrier fluid), while the dispersed channel carries the dispersed phase. The T-junction uses shearing action or pressure forces or both to form Droplets.
A schematic of the flow focusing device is shown in fig. 2. There are three inlets to the device out of which, the outer ones carry the continuous fluid and the inner one carry the dispersed fluid. The interface is disturbed by forcing the three liquid streams to move through an orifice placed at a certain distance from the inlet. Depending upon the flow parameters and geometrical parameters, the disturbance might lead to the breakup of the inner liquid stream into small droplets, which then flow downstream into the collection tube.

Both the geometries were modeled using Volume of fluid (VOF) because of its ability to accommodate large surface topology changes including surface rupture and coalescence. Star-CCM+ was successfully able to model the T-junction, however, very high spurious currents were observed at the interface and to reduce these currents, adaptive mesh refinement (AMR) technique was used to model the flow focusing device.

**Methodology**

**Single Phase Flow**

Incompressible laminar 3-D Navier-Stokes equations for pressure driven water flow were solved. Also, no slip at the wall, velocity inlet and pressure outlet were imposed. Periodic boundary condition was imposed for the rectangular channel, while for circular channel developed velocity profile for macroscopic channel was imposed at the inlet.

**Multiphase Flow and Droplet Formation**

Study of droplet formation through numerical modeling imposes a great challenge because of the complex interfacial dynamics and the formation of singularity at the time of interface breakup [1]. There have been plenty of methods of available to model droplet formation, which can be
categorized into two categories: Sharp interface methods and diffuse interface methods [1]. The problem of modeling past transition of Droplet formation arises in case of sharp interface methods because of the formation of singularity at the surface break-up. However, the surface breakup is implicitly modeled in case of diffuse interface methods, while solving the governing equations. One of such diffuse interface methods is Volume of fluid (VOF).

**Volume of Fluid (VOF)**

The VOF is well known for its ability to conserve the mass of the traced fluid and to accommodate great surface topology changes. This change is traced easily, so the interfaces can for example join, or break apart.

Mathematical formulation of VOF involves defining a color function $C$, which assumes a value of 1 in one phase, 0 in another and fractional value at the interface [3]. Fig. 3 demonstrates how ‘$C$’ varies with the volume fraction of the fluid.

The properties of the fluid in the domain are defined as the function of $C$. Any general property $\phi$ at any grid point is defined as:

$$\phi = C \phi_c + (1 - C) \phi_d$$

Where $\phi_c$ and $\phi_d$ are the properties of fluids ‘c’ and ‘d’ respectively.

VOF solver involves an additional advection equation along with the momentum equations and the continuity equation. The advection equation is as follows:

$$\frac{DC}{Dt} = \frac{\partial C}{\partial t} + u \cdot \nabla C$$
Since, every fluid parcel retains the color that it was assigned while the fluid parcel moves in the domain, the total derivative of the color is zero.

We used a second order discretization scheme for the convection term. Also, an antidiffusion step was added to sharpen the interface. An antidiffusion (or sharpening) factor of 0.7 was used.

**Adaptive Mesh Refinement (AMR)**

A dynamics mesh was used, which refines after every few computation time steps. The mesh was made to be very fine near the interface and coarse for far from the interface. The mesh base size at each point is decided by the volume of fraction of any of the fluid.

**Results**

**Single Phase Flow**

Flow characteristics (velocity profile and pressure distribution) for both the channels are in prediction of macroscopic theory. Velocity profiles for circular channel are shown in fig. 4. It can be seen that the velocity profile obtained matches with the analytical profile predicted from the macroscopic theory within an error of 3%. However, the velocity scalar scene in fig. 5 shows that the velocity profile imposed at the inlet does not exactly match with the actual developed profile.

Fig. 6 shows the velocity profile obtained in rectangular channel being compared with the analytical profile. It can be seen that the obtained velocity profile is within macroscopic prediction. Velocity scalar scene of the domain is shown in fig. 7.

**Multiphase Flow**
**Microfluidic T-junction**

The dimensions of microfluidic T-junction are taken as shown in fig. 8. The flow rate ratio $(Q_a/Q_c)$ and $\text{Ca} (\mu_c U_c/\sigma)$, where the subscripts ‘c’ and ‘d’ represent the continuous fluid and the dispersed fluid respectively, were taken to be 0.25 and $5 \times 10^{-3}$ respectively. Since, the capillary number was very small, the droplet formation for this case was surface forces dominated and the role of viscous forces in droplet formation was negligible.

Fig. 9 shows a timeline of droplet formation in microfluidic T-junction. The droplet size and the mechanism of break-up is exactly the same as predicted by Garstecki et al [4]. However, very high spurious currents were observed at the interface, because of which the time step was reduced to satisfy the CFL condition. Velocity scalar scenes for same interface location and different mesh sizes are shown in fig 10. It can be seen that the spurious currents tend to decrease as a finer mesh is taken.

**Microfluidic Flow Focusing Device**

Dimensions of the device are as same as the one taken by Shelly et al [5]. The flow rate ratio and Ca were taken to be 0.25 and $7.2 \times 10^{-3}$. Star-CCM+ successfully modeled the device within reasonable computation time.

Also, based on the observation of T-junction modeling, adaptive mesh refinement technique is applied. The mesh is made very fine near the interface and the mesh changes as the interface moves. Fig. 11 shows a series of snapshots of the mesh as the dispersed phase advances in the device. Because of a very fine dynamic mesh, a thin interface is obtained. Since, the mesh is very fine at the interface the spurious currents are minimized, which saves the computation time. So,
the adaptive mesh technique is an effective method of modeling interfacial flows and capturing very sharp interface.

REFERENCES

Figure 3 Variation of the color function in the domain with the volume fraction of the fluid

Figure 4 Validation of velocity profile with the analytical solution. Solid line represents the analytical velocity profile for macroscopic channels.

Figure 5 Velocity scalar scene of the circular channel
Figure 6 Validation of the velocity profile with the analytical solution. Here, H and W are the height and width of the channel, and X and Y are the coordinates along the width and the height measured from the mid-section of the channel. Solid line represents the analytical velocity profile for macroscopic channels.

Figure 7 Velocity scalar scene of the rectangular channel
Figure 8 Orthographic view of the T-junction geometry taken for computation modeling

Figure 9 Timeline of Droplet formation in Microfluidic T-junction
Figure 10 Velocity scalar scene of the T-junction for different mesh base size,

Figure 11 An illustration of adaptive mesh refinement
Figure 12 An illustration of droplet formation in microfluidic flow focusing device