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MODELLING OF CO-AXIAL AND TRI-AXIAL MILLI-FLUIDIC DEVICES FOR CO-EXTRUSION OF SEMI-SOLID SOLIDS

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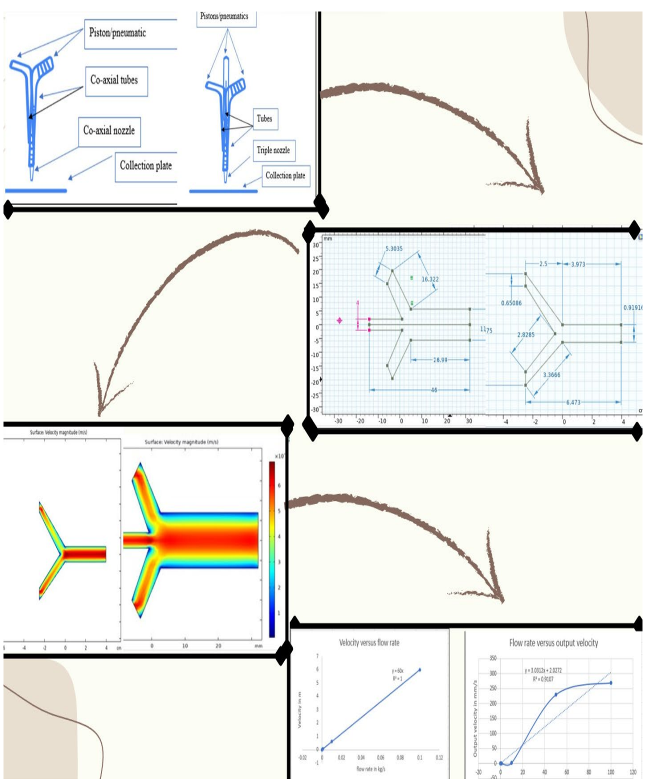
Graphical abstract



Abstract

With the use of a milli-fluidics device, it is possible to manipulate small amounts of fluid in the millimeter range with pinpoint accuracy. The milli-fluidics are currently lacking in studies of the relationship between fluid viscosity, output velocity and output pressure. Thus, this study examines the effects of viscosity on fluid dynamics in the co-axial and tri-axial milli-fluidics. This geometry of the co-axial and tri-axial milli-fluidics consist of single outlet, two inlets and three inlets, respectively. The tri-axial milli-fluidics is 46 mm long and 11.31 mm wide, while, the coaxial milli-fluidic is 64.73 mm long and 9.2 mm wide. The co-axial milli-fluidics constituted of 775 domain elements and 147 boundary elements, while, the tri-axial milli-fluidics mesh constituted of 1518 domain elements and 178 boundary elements. Laminar flow was observed for the flow of the materials through the channels. When the dynamic viscosity approaches 5 mPa.s, the simulation reveals that the flow rate is inversely proportional to the dynamic viscosity for co-axial milli-fluidics. It was difficult to combine fluids with different viscosities with small volume of water in a narrow boundary, thus the parallel flow of material was observed. When using the one outlet channel for the tri-axial milli-fluidics, the assemble pressure at the three inlets was decreased compared with co-axial milli-fluidic. Even when the dynamic velocity of the fluid at outlet 1 increased, its velocity remained consistent. An extruder using tri-axial milli-fluidics can be used if the interfacial tension for intake 1 is higher than for inlet 2 and the dynamic viscosity of fluid 1 is above 2 mPas, according to the volumetric fraction model. The tri-axial milli-fluidic was found to be suitable for producing cladding of material with the balanced pressure from the two side channels.

Keywords: Co-axial extruder, tri-axial extruder, milli-fluidics, laminar flow, micro-fluidic, computational fluid dynamic.

1.0 INTRODUCTION

The micro- or milli-fluidic technique is becoming more popular for materials' coatings in several industries. Some industries used this technique to coat hazardous materials.

Essentially, a microfluidic device in micrometres allows for the manipulation and processing of a tiny quantity of liquid in a space of many micrometres. In comparison to microfluidics, milli-fluidics in millimetres size enables a higher volume of fluid to be controlled and flow through [1]. The volume of fluids handled by milli-fluidics is still minimal compared with the manipulating of fluid in test tube. When employing milli-fluidics for fluid flow controlled, the advantages include rapid analysis, effective liquid extraction, and the ability to detect specimens with a low amount of test analytes needed [2]. A milli-fluidics technique may be used to replace a few of the larger liquid handling systems [3]. Modern microfluidic and milli-fluidic instruments may be found in a broad range of fields such as food safety testing, mixing chemicals, polymeric fibers fabrications cell culture, medicinal diagnostics, microbiology and pharmaceutical development [4].

The fluid flow in milli-fluidics is typically simplified and turbulence occurs if microstructures intended to create microturbulence are present in the flow path [5]. Due to the lack of an external driving force, the shape of the micro-channels is critical for fluid folding to facilitate liquid flow within the micro-channels for mixing [6]. A linear channel with an output and an input are the most basic features of the milli-fluidic device based on its specific functionalities [7]. Co-axial and tri-axial milli-fluidic devices may be used to provide co-linear extrusion and encapsulation of the fluids or the semi-solid solids for fluid mixing. Co-axial extrusion, as opposed to traditional tree-shaped systems, merely requires smaller mixing channels as well as a simpler structure to facilitate the mixing process [8]. Due to the Y-shaped connection, the system has two inlets and a single outlet[9]. Whilst the tri-axial milli-fluidic consists of three inlets and one outlet similar to the tree-shaped system. Before fabricating and testing the milli-fluidics designed for co-axial or tri-axial extrusions, computer simulation helps in estimating the fluid flow patterns of the milli-fluidics. In relation to the ratio of the fluid exit channel to the intake channel [10]. The objective of the current investigation is to determine the relationship between the viscosity, velocity and pressure of fluid to co-extrude carboxymethyl cellulose (CMC) and ammonia fertilizer. through mathematical simulation. Since fertilizers have negative impacts on environment such as harming the surrounding areas. Leached Ammonia fertilizer from soil can harm all quartic aspects in water channels, lakes, and rivers. So, co-extrusion is necessary for Ammonia fertilizer. This technique is used to coat the fertilizers and then reducing its degradation in soil. The carboxymethyl cellulose (CMC) is used as outer layer of fertilizer coating since this material has no negative impacts on the environment. Such a study has not been investigated extensively, despite several research reported on the flow patterns [11].

In a regard of co-axial microfluidic modelling, Chait, P. N. S., et al., (2022), created a computer model which made the assumption that the fluid at low viscosity flowing along a solid boundary with no slippage. In addition, poly-dimethyl siloxane (PDMS) was used to be the boundary material. The work assumed Newtonian liquids, which are independent of shear rate, for the two liquids which enter the inlet. The flow rate was set at 0.1 m/s in both inlets assuming the pressure as zero. In addition, this work used a multiphase flow in their simulation and found that the two fluid flows were divided side by side since the volume fraction simulation predicts that the fluid were not well mixed. The co-axial presented laminar flow that permits linear fluid flow. The tri-axial channel, however, offers changes of flow characteristics as the fluid's dynamic viscosity at the central inlet channel increases. [12]. However, this study and the finding was not applicable for flow material with high viscosity such gel or paste. Simulation of material with higher viscosity maybe characterized by different flow pattern that requires further investigation.

The aim of this paper is to study the effects of changing the viscosity to the milli-fluidic in co-axial and triaxial directions. The multifluidic channels are to be performed in COMSOL Multiphysics® in the form of 2D model, which can be used as triaxial and/or coaxial channels. The selected materials are used for each inlet and boundaries of non-slip condition was assumed. The fine-mesh triangular elements were used for solving the partial differential equations of the model.

2.0 METHODOLOGY

COMSOL Multiphysics® was used to create co-axial and tri-axial milli-fluidics models. In the establishment of the models in two-dimensional geometry, co-axial milli-fluidics were designed with two inlets whereas tri-axial milli-fluidics have three inlets and both milli-fluidics have single outlet. The width of the co-axial milli-fluidic outlet channel is 9.2 mm, each inlet is 6.5 mm wide, and the length of the inlet is 33.67 mm while the total length of the extruder is 64.73 mm length as shown in Figure 1a.

The outlet channel of the tri-axial milli-fluidic 11.312 mm. Inlets 1, 2 and 3 have same width which is 5.3 mm. The length of the inlet is 16.33 mm while the total length of the extruder is 46 mm length as shown in Figure 1b.

The user has a choice between meshing controlled by the user or by physics. When using user-controlled meshing, the user determines the mesh's scale factor and geometry, while the model determines the mesh's properties. Building a mesh is a technique used in computer simulation to break down a large model more efficiently into smaller, more manageable bits. The finer the element used, the longer is the simulation time.

The COMSOL Multiphysics applies the finite element technique or the partial differential equations (PDEs). Although the finite element approach is frequently used in electrochemical processes, this computational method differs in that it solves the PDE in an integral (weak) form, unlike the finite difference method. As a sum over a collection of basic functions specified on finite elements, unknowns may be discretized. The term "mesh" is used to describe the geometry in which the finite components are put together, such as 2D triangles or 3D tetrahedron tessellation.

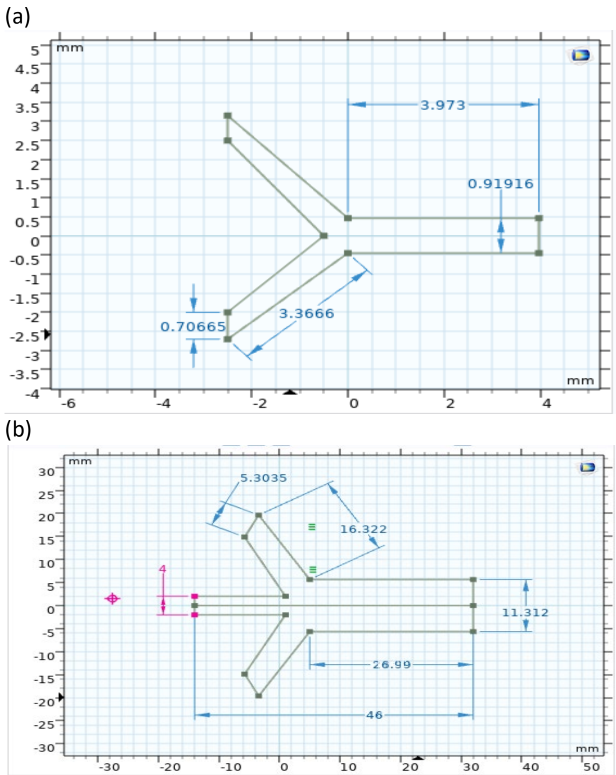


Figure 1 The constitutive two-dimensional models of the (a) co- and (b) tri-axial milli-fluidic designed for co-linear extrusions of fertilizer

Alternatively, in user-controlled meshing, the mesh's elements' sizes and shapes must be chosen by the user, but in physics-controlled meshing, the mesh's features are determined by the model. Creating a mesh will aid in breaking the model up into more manageable chunks for easier computational simulation solutions. This computer model was set with the no-slip condition that the fluid has zero velocity in relation to the boundary at a solid boundary of Poly-dimethyl siloxane (PDMS). Prior to doing the simulation, the velocity was fixed. Two liquids entering via the intake are converted to Newtonian liquids that are independent of the shear rate. There are two main equations are used which are eq (1) and eq (2).

$$\rho(\mathrm{d}v/\mathrm{d}t) + \rho(v.\nabla)v - \eta\nabla v + \nabla p = 0 \qquad (1)$$

$$\nabla. v = 0 \qquad (2)$$

Where,

V is the velocity vector (m/s),
P is the pressure (kN/m^3)
ρ is the density (kg/m^3)
η is the dynamic viscosity (Pa·s).

The co-axial milli-fluidics constituted of 775 domain elements and 147 boundary elements, whilst, the tr-axial milli-fluidics mesh constituted of 1518 domain elements and 178 boundary elements.

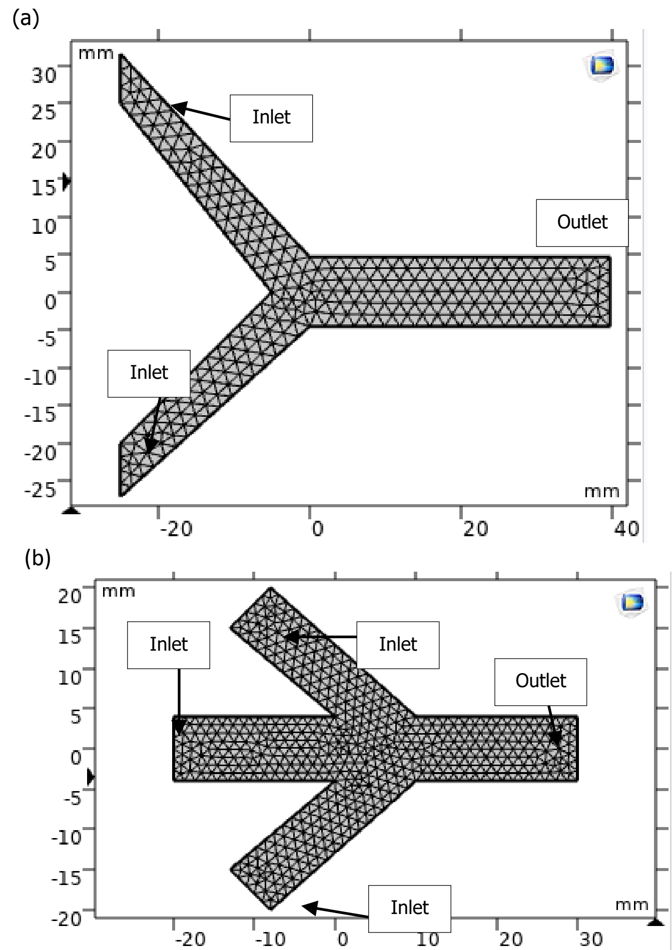


Figure 2 The finite elements mesh of (a) co- and (b) tri-axial milli-fluidics

Figure 2 shows the finite elements mesh in co-axial and tri-axial milli-fluidics channels. Both of them have different dimensions and scaling.

Table 1 Material Properties used for simulation

Parameter	Carboxymethyl cellulose (CMC)	Ammonia Fertilizer	References
Dynamic viscosity	800 to 1200 mPa.s	8.0 to 17.0 mPa.s	[13-14]
Density	1.6 g/cm^3	1.32 g/cm^3	[15-16]
Melting point	270 °C	133 °C	[17-18]
Degradation in water	7.27 mmol/L	31 to 53 mmol/L	[19-20]

The dynamic viscosity for CMC and ammonia fertilizer is 800 to 1200 mPa.s and 8.0 to 17.0 mPa.s respectively. While the density of the used CMC and ammonia fertilizer is 1.6 g/cm^3 and 1.32 g/cm^3 respectively. Bothe CMC has melting point at 270 °C and ammonia fertilizer has melting point at 133 °C. The degradation in water for CMC and ammonia fertilizer is 31 to 53 mmol/L and 7.27 mmol/L as it can be seen in Table 1.

The flow of materials is categorized into two types of flows such as laminar and turbulent [21]. In this research, the type of flow is selected to be laminar flow because it is smoother, while the turbulent flow is uncontrolled and chaotic. Turbulent flow is less likely to occur for semi-solid material compared with liquid due to the higher density of material [22]. When assessing the state of a fluid's flow, the viscosity or density of a material, is a crucial consideration; a greater viscosity improves the laminar flow of a material. The flow rate of materials is a directly proportional to the output velocity of the material flow. Therefore, the output velocity can be controlled by controlling the mass flow rate of materials.

$$Q = \frac{v}{t} \quad (3)$$

where,

- Q is the volumetric flow rate in the channel
- v is the volume of fluid
- t is the time of passing a material through an area.

The volumetric flow rate is direct proportion to the output velocity.

$$Q = \frac{\pi p r^2}{8 n L} \quad (4)$$

where,

- r is the radius of the channel.
- η is the viscosity of fluid in the channel.
- L is the channel's length.
- P is the pressure at the channel.

The velocity is determined by the Reynolds number, a dimensionless flow parameter that also depends on the fluid's viscosity, density, and channel size. No of the size of the fluid system, the Reynolds number measures how much the fluid is flowing relative to how viscous it is by comparing its inertial force to its shearing force. Laminar flow occurs when a fluid is extremely viscous or travels slowly. The Reynolds number is giving by:

$$\mathrm{Re} = \frac{\rho u D_{\mathrm{H}}}{\mu} \quad (4)$$

where,

DH is the hydraulic diameter of the pipe (m)
u is the mean speed of the fluid (m/s)
μ is the dynamic viscosity of the fluid (Pa·s)
ρ is the density of the fluid (kg/m^3).

In this study, the Reynolds number is obtained as 0.3534 for co-axial milli-fluidics channel and 0.3974 for tri-axial milli-fluidics channel. These values are affecting the flow of material which is laminar due to low Reynolds numbers. Table 2 shows the materials used in the milli-fluidic channel to be coated.

Table 2: Material assignment

Type of milli-fluidic	Channel	Semi-solid Material
Co-axial	Inlet 1	CMC
	Inlet 2	Fertilizer
Tri-axial	Inlet 1	CMC
	Inlet 2	Fertilizer
	Inlet 3	CMC

We have created similar model in experiments but the report on the validation experimental results is beyond the scope of this manuscript. However, in the experiment, we have successfully cladded the ammonia fertilizer with CMC using the model simulated. The results of experiment are similar to the modeling presented in our results in Figures 3, 4 and 5.

3.0 RESULTS AND DISCUSSION

After simulating the fluid mechanics of materials in the model designed, the output velocity and pressure of the co-axial milli-fluidic are as shown in Figure 3.

In Figure 3 (a), the flow rate of 0.001 g/s yielded lower output velocity at 23×10^{-7} m/s, and while, higher flow rate at 0.1 g/s yielded higher output velocity at 23×10^{-5} m/s as shown in Figure 3 (b). The relationship between flow rate and output velocity is as shown Figure 3(e) which illustrates how the output velocity is directly proportion to the flow rate. This means that, if the flow rate increases, the output velocity increases and vice versa. The viscosity of materials can affect the output velocity, where output velocity decreases due to high viscous materials, and increases when the viscosity of materials is lower. The flow starts to saturate when the input flow exceeding 60 g/s, as well as the output velocity starts to saturate when the input flow is 60 g/s.

Based on Figure 3 (c), the pressure is lower at 2.18×10^{-5} Pa when simulated with a lower flow rate at 0.001 g/s, and the pressure is higher at 2.19×10^{-3} Pa when simulated with a higher flow rate at 0.1 g/s. This relationship is as shown in Figure 3(e), where the pressure increases slightly when the flow rate increases and decreases when flow rate decreases. The pressure increased with the input flow rate, after exceeding the velocity at 60 g/s, the output pressure increases linearly with the input velocity. As in Figure 3 (c) and Figure 3 (d), the inlet for CMC shows high pressure, this is due to high viscosity of CMC, and the inlet for ammonia fertilizer shows low pressure due to low viscosity of ammonia fertilizer.

The results of fluid velocity in the co-axial extruder have been observed in different levels according to the mass flow rate and materials parameters. By increasing the mass flow rate, the output velocity increases.

The millifluidic pressure rises in direct proportion to the dynamic viscosity of input fluids [23]. From laminar to turbulent flow, a variety of cross-sectional geometries, and a large array of relative surface roughness are all accommodated by the extensive library of predefined expressions for Darcy friction

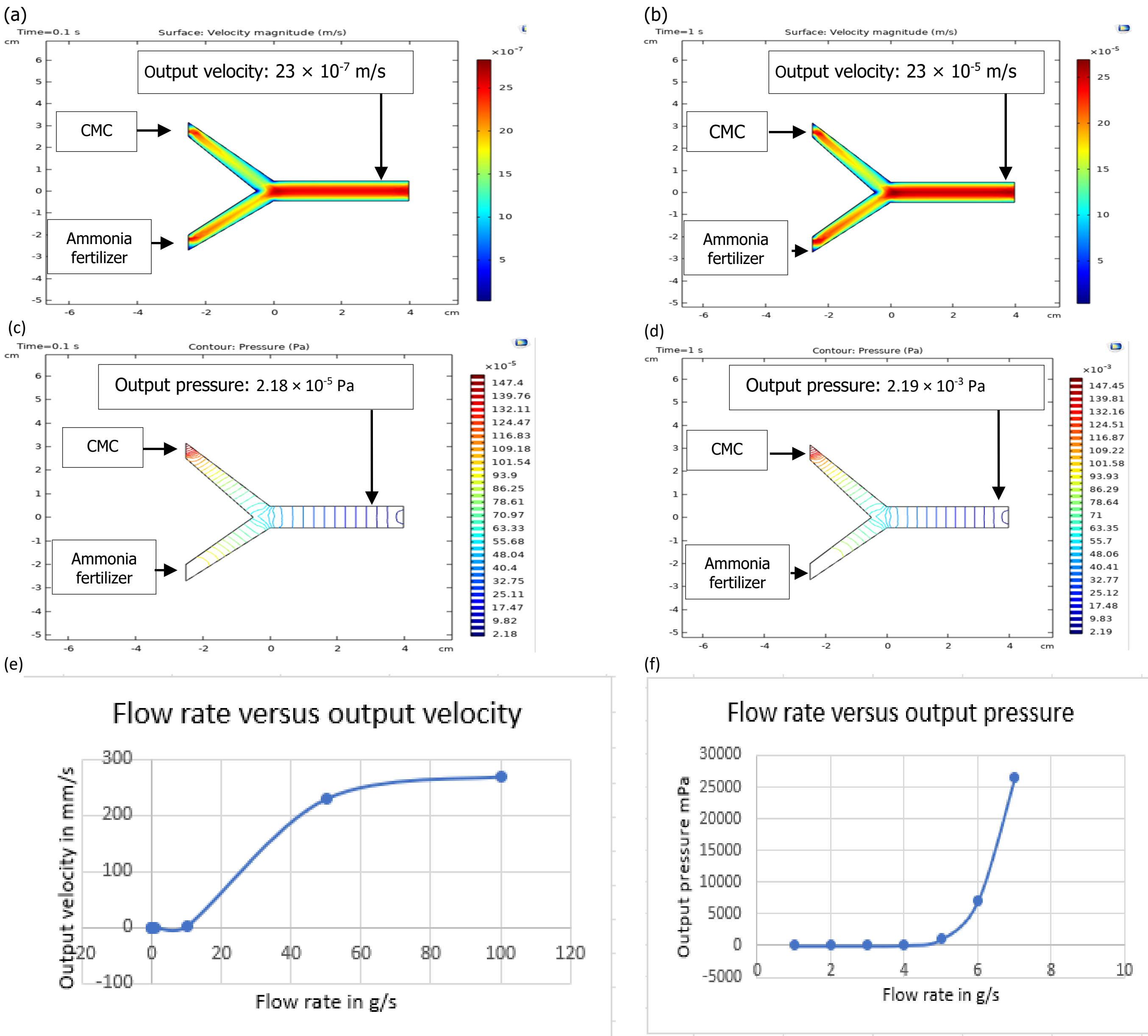


Figure 3 Output velocity for flow rate (a) 0.001 g/s , (b) 0.1 g/s , output pressure for flow rate (c)) 0.001 g/s, (d) 0.1 g/s and graph of flow rate versus (e) pressure and (f) velocity in co-axial milli-fluidic

factors. Additional pressure decreases occur as a result of momentum changes in elements such as bends, compression,

and expansions [24]. The pressure at the channel is a critical parameter to be considered to avoid leaking of fluids, once the millifluidics impacted with high pressure. The material used for boundary in the channel is poly-dimethylsiloxane (PDMS) which has the ability to overcome the generated pressure by fast flow in the channel. Poiseuille's law states that the velocity of a fluid is proportional to its pressure and conversely related to its dynamic viscosity [25]. The pressure rises because of the increment in dynamic viscosity [26].

For the tri-axial millifluidic, the output velocity reaches 0.06 m/s when the flow rate is 1 g/s as in Figure 4 (a). If the flow rate decreases to 0.1 g/s, the output velocity decreases to reach 6×10^{-3} m/s as in Figure 4 (b). Output velocity decreases to 6×10^{-4} m/s and 6×10^{-5} m/s when the flow rate decreases to 0.01 g/s and 0.001 as in Figure 4 (c) and Figure 4 (d) respectively. Based on the graph of velocity versus flow rate, the velocity increases by increasing the flow rate of fluidic materials in the tri-axial channel as in Figure 6 (a).

The output pressure reaches 0.18×10^{4} Pa as shown in Figure 5 (a). Based on Figure 5 (b), the output pressure for 0.1 g/s of flow rate is 0.18×10^{3} Pa , while the pressure for 0.01 g/s of flow rate is 51.98 Pa as in Figure 5 (c). According to the results in Figure 5 (d), the output pressure for 0.001 g/s of flow rate is 5.2 Pa. For the graph of pressure versus flow rate, the output pressure increases when the flow rate of the flow material increases in the tri-axial channel as in Figure 6 (b).

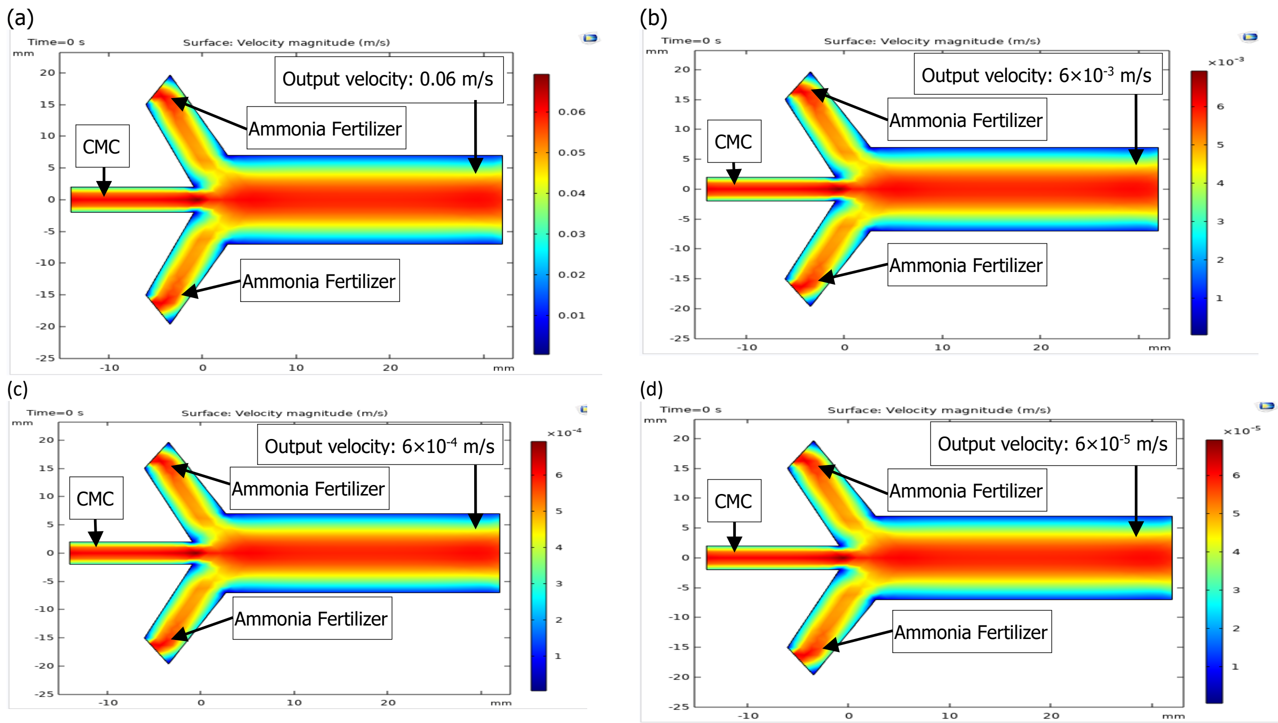


Figure 4 Output velocity for flow rate (a) 1 g/s , (b) 0.1 g/s , (c) 0.01 g/s and (d) 0.001 g/s in tri-axial milli-fluidic

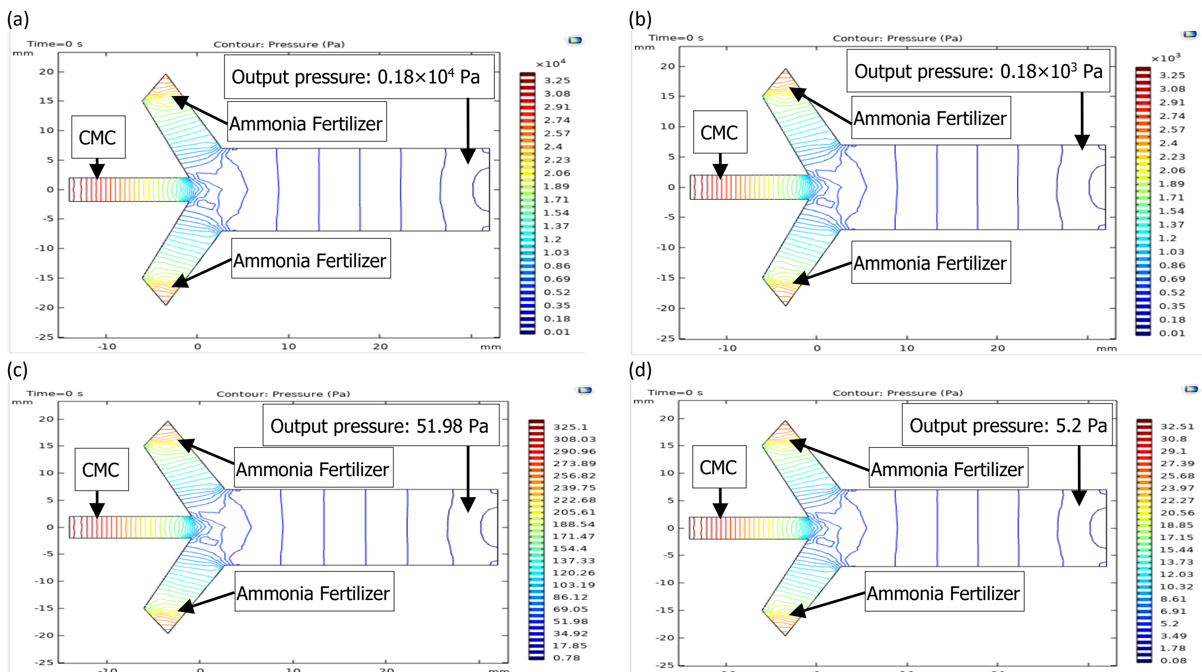


Figure 5 Output pressure for flow rate (a) 1 g/s , (b) 0.1 g/s , (c) 0.01 g/s and (d) 0.001 g/s in tri-axial milli-fluidic

As it can be seen in Figure 6, volumetric flow rate is directly related to pressure drop under laminar flow circumstances. When the flow rate is doubled, the pressure drop is also doubled. The square of the volumetric flow rate causes a pressure decrease in turbulent flow [27]. There is a four-fold increase in pressure drop when the flow rate is doubled [28]. Thus, the relationship between mass flow rate and output velocity is direct proportion. A fluid's shear strength is created by the inter - molecular friction that occurs when two layers of the fluid try to glide over one other.

If the viscosity of material is high, the flow of material will be slower and then the output pressure becomes very high. similarly, the density of materials increases its viscosity and velocity becomes slower [29].

Microfluidic devices are optimized based on fluid pressure and velocity using the equations of flow rate. It is possible to model the flow of fluid in microfluidic devices using the COMSOL Multiphysics software [30].

(a)

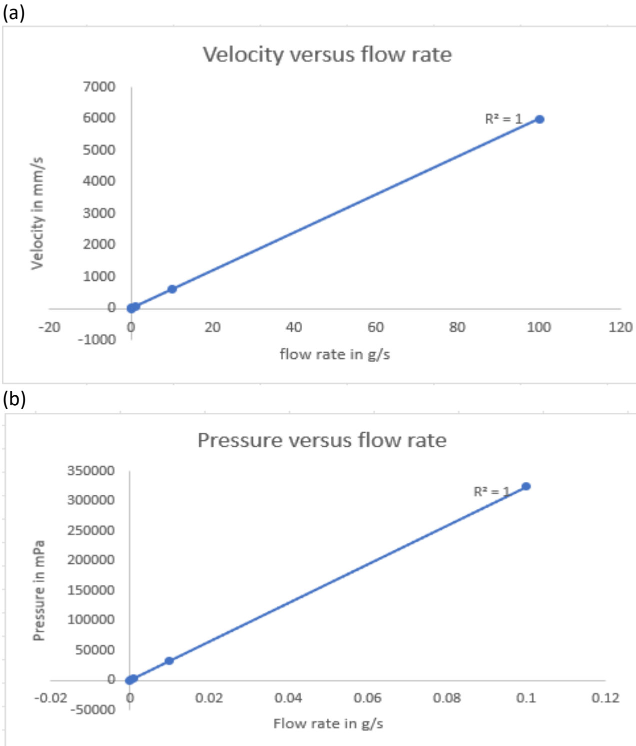


Figure 6 Graph of (a) velocity versus flow rate and (b) pressure versus flow rate in tri-axial extruder

Based on the study by Chait, P. N. S., et al., (2022) which simulated the flow and pressure of liquid in a bi-axial microfluidic, the fluid velocity remained stable at 0.2 m/s as the viscosity rose from 0.1 mPa·s to 10 mPa·s. The velocity is roughly 0.3 m/s although the dynamic viscosity of the fluid 1 increased from 0 to 10 mPa·s. In addition, the fluid velocity rose to 0.3 m/s after the intersection leading to the outflow channel. Nevertheless, the velocity remained unchanged despite the increased the velocity of the fluid at inlet 1 [12]. In comparison with the current study, the fluid velocity of previous work reported in [30] is much higher.

In this study that applies semi-solid material to the bi-axial millifludic, the velocity is much slower for semi-solids which is almost 23×10^{-5} m/s in co-axial milli-fluidic channel and 6×10^{-5} m/s in tri-axial milli-fluidic channel. This velocity is most suitable for the flow of semi-solid materials which can be extruded. In addtion, the viscosity observed in this study rose from 2180 mPa to 263800 Pa in co-axial milli-fluidic channel and from Output pressure: 5200 mPa to 32000 mPa in tri-axial milli-fluidic channel. With low pressure, materials can flow easily, unlike with high pressure, which impedes the flow of materials through the milli-fluidic channel.

The tri-axial millifluidic channel provides precise results as linear, while co-axial millifluidic channel prvides non-linear results which is not applicable for many semi-solid materials such as ammonia fertilizer and CMC. So, in this study, tri-axial millifluidic channel was used for modelling ammonia fertilizer coated with CMC.

4.0 CONCLUSION

The main objective of this paper is to study the effects of changing the viscosity to the milli-fluidic in co-axial and triaxial channels. This objective has been achieved by simulating co-axial and tri-axial milli-fluidic channels in COMSOL Multiphysics software with different range of flow rate values. The input values of flow rate delivered a different values of output velocity and pressure. These channels were designed to test the fluid of fertilizers and Carboxymethyl Cellulose (CMC) with different parameters and mass flow rate. The first objective of this research is modelling the flow of material in the co-axial extruder using COMSOL MUTLIPHYSICS simulation, which has been successfully done and the results obtained from the simulation show that the output velocity is proportional to mass flow rate. The tri-axial milli-fluidic channel was used in this study since it gave approximated outcomes. The pressure of the flow of materials can be distributed at the outlet channel to avoid damages to the channel.

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