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Application of Analytical Technique to Resolving the Flow Dynamics in Self-wiping Co-rotating Twin Screw Extruders

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Abstract- In this paper, a method by which the fluid velocity profile and the net flow rate in self-wiping co-rotating twin screw extruders can be estimated without determining the pressure gradient has been proposed. The method involves using analytical technique to determine the fluid velocity in the local zones of the extruder such as the down channel and axial velocity and subsequently, the net flow rate in the extruder, based on the simplified flow theory for isothermal Newtonian channel flow. It is shown that the velocity distribution is highly dependent on the helix angle, channel height and the ratio of the pressure to drag flow rate. The velocity profile in the down channel direction is shown to have positive values for pressure to drag flow ratio $\leq 1/3$, valid for helix angle $0 \leq 90$, whereas it has both positive and negative values for pressure to drag flow ratio $> 1/3$. The reverse is the case for helix angle > 90, with negative values for the pressure to drag flow rate $\leq 1/3$ and the presence of backflow, having positive and negative values for pressure to drag flow rate $> 1/3$. In the axial direction, the axial velocity is always positive for helix angles between $0 \leq 90$. The purpose of this technique is to aid theoretical estimation of several important parameters in twin screw extruders which are directly or indirectly related to the velocity profile such as the degree of fill in conveying zones, the effective mean residence time, mean time delay and also the residence time distribution, with the goal of avoiding the use empirical method of estimation. The approach has been validated by carrying out experimental investigation.

***Keywords*:** Velocity, drag flow rate, pressure flow rate, net flow rate, degree of fill.

1. Introduction

Twin screw extruders are continuous flow systems employed particularly in the food and polymer processing industry for mixing, blending, de-volatilization, compounding and/or reactive extrusion. Of the available types, the self-wiping co-rotating twin screw extruder is widely used especially in the polymer industry due to its capability for good mixing (Kohlgrubber, 2008).

Due to the complexity of the screw configuration in self-wiping co-rotating twin screw extruder, where screws of different geometrical structures such as helical screws, forward and reverse kneading blocks; are combined in a modular form to suit the specific extrusion task, it is quite difficult to accurately model the fluid flow dynamics in the extruder based on the fact that the changing screw structure influences the flow dynamics (Tadmor et al., 2006). As a result, simplified approaches are often used to model the flow profile. As has been established in the well-known isothermal Newtonian extrusion theory, the flow in a self-wiping co-rotating twin screw extruder is usually a combination of drag and pressure flow (Meijer and Elemans, 1988). Thus it is desired to be able, to a great extent of accuracy, determine the net flow rate so as to be able to estimate important parameters that influence the extrusion process such as the degree of fill and the mean time delay. To determine the net flow rate, one must be able to determine the drag flow rate and the pressure flow rate. But it is quite difficult to determine the pressure flow rate as it occurs simultaneously with and also opposes at the same, the drag flow rate in the pressure build up zones of the extruder. Hence the reason simplified approaches are applied.

Several models have been presented in the literature to model the flow dynamics. Tadmor et al. (2006) presented a mathematical model of isothermal flow of a Newtonian fluid in shallow-screw channels resulting in a simple design equation, giving enormous understanding of the flow mechanism which is very useful for first order calculations. This model represents the standard classic pumping model for single screw extrusion. The development of the model starts by reversing the conceptual synthetic process. The space between a tightly fitting screw and the barrel was shown to be a helical channel. When the channel is unwound from the screw and laid on a flat surface, the result is a rectangular straight channel.

Vergnes et al. (1998) proposed a global computational flow model for self-wiping co-rotating twin screw extruders considering the local zones. The flow in the screw zone was modeled using cylindrical coordinates in which the channel section is considered to be perpendicular to the screw flights, with special interest on flow in the peripheral direction. A pressure flow rate relationship was then developed for these two categories of flows. In a simplified one-dimensional approach, the section of the channel was considered to be rectangular, with a constant width. They assumed that the flow is locally Newtonian and isothermal. Using this assumption, the longitudinal volumetric flow rate along the C-shaped chamber was given. Flow in the kneading disc zone was modeled based on a one-dimensional lubrication approximation approach.

Booy (1980) derived a mathematical model of isothermal flow of a Newtonian liquid through co-rotating twin screw extruder. Two flow regimes were studied. In the first, equations were given for drag flow rate, pressure flow rate and flow through the nip zone in section of the twin screw extruder where the channels are completely filled with liquid, generated a pressure gradient and provided a discharge pressure at the metering zone. In the second regime in which the channels are partly full, it was shown how the degree of fill changes with the flow rate, speed and dimensions of the screw. Screws were shown to generate pressure only when the flow rate is smaller than the drag flow rate. A pressure gradient will occur in the discharge zone in the length of the screw needed to provide the required discharge pressure. It was shown that upstream of that filled zone, the channels will be partially full and transport is by drag flow only.

Meijer and Elemans (1988) developed a simple model for hot melt closely intermeshing co-rotating twin-screw extruder, analogous to the analysis of a single-screw. In their approach, the flow was modelled based on the behaviour of the local zones and configuration obtainable in the industry. Three functional zones were distinguished: the partially filled zone having a degree of fill $f \quad (0 < f < 1)$, the completely filled, pressure generating zone and the completely filled, pressure consuming zone. It was stated that in the partially filled zone, there is no pressure development and thus maximum drag flow rate occurred. They stated that the real throughput was always less than the drag flow rate and thus gave the degree of fill as the ratio between the throughput and the drag flow rate. They noted the relevance of developing a model that can be directly used other than emphasizing the flow in complex geometries.

Potente et al. (1994) developed composite models for the calculation of the filling level profiles, the pressure profiles, the melting profiles, the residence time distribution, the temperature profiles, the shear stress profiles, and the power consumption in modular tightly intermeshing co-rotating twin screw extruders. A complex systematic design procedure was compiled. Their simulation of the intermeshing co-rotating machine involved both screw and kneading disc elements, including left- and right-handed sections. Kneading blocks were approximated by a screw of "equivalent pitch", making allowance for the leakage flow across the flights from one channel to the adjacent channel. The mathematical treatment of co-rotating twin screw extruders was carried out based on the theory of single screw extruders. For the flow modelling part, it was observed that contrary to single-screw extruders, the self-wiping co-rotating twin screw extruders are generally not operated from a full hopper but through a metering unit. They proposed that to correctly calculate the overall conveying system of a co-rotating twin screw, it is necessary to have physico-mathematical models that make allowance for the three mechanisms of:

feeding and conveying of solid material, melting and conveying of melt, whilst simultaneously taking into account the filling in the local zones. They used the groove model to form the basis of all the models. In the groove model, the screws are pictured as being fixed and the screw barrel surface as rotating around the screws (kinematic reversal). The screw channels and the screw barrel surface are taken as being laid out flat and projected in a single plane. They stated that for co-rotating twin screws, this gives a physical substitute model with a defined number of parallel channels over which a plate moves with a velocity known as the rotational velocity of the screw barrel.

Though extensive work has been done in modelling the flow in the self-wiping co-rotating twin screw extruder, there is still a great challenge in determining all the parameters needed to calculate the net flow rate in sections where drag flow and pressure flow co-exist. While it is quite easy to determine readily, the drag flow parameters, it is very difficult to readily determine the pressure flow parameters such as the pressure gradient and the viscosity to be able to determine the net flow rate. This challenge has resulted in over simplifying the model estimation or where available, using software packages to try to determine these parameters.

The main target of this paper is to propose a method by which the analytical technique of isothermal Newtonian flow in shallow channels can be applied to resolving the flow dynamics in self-wiping co-rotating twin screw extruder and to obtain the net flow rate without necessarily determining the parameters for the pressure flow rate. To achieve this, the velocity profile in the extruder was first analysed from which the net flow rate was determined, showing how it is influenced by the screw geometry. Thereafter, it was shown how important parameters such as the degree of fill and the time delay can be determined from the net flow rate. Validation was made against results obtained experimentally.

2. The Analytical Technique

The flow in a self-wiping co-rotating twin-screw extruder without a die can be described as an open shallow channel flow (Tadmor et al., 2006). As has been established in the well-known isothermal Newtonian extrusion theory, a fluid particle starting at the feed zone of the extruder advances in the down channel direction (z axis) in the screw channel. Thus the volumetric flow rate Q_v is obtained by integrating the z-component of the fluid velocity vector over the cross-section of the channel perpendicular to the z-axis. Mathematically, this is given as

$$Q_v = \int_0^h \int_0^W v_z dxdy \tag{1}$$

The continuity equation (Katz, 2010) of the rectangular coordinate in the z-axis or the z component of the momentum equation for steady isothermal flow of an incompressible Newtonian fluid is given as

$$\rho\left[v_x\left(\frac{\partial v_x}{\partial x}\right)+v_y\left(\frac{\partial v_z}{\partial y}\right)+v_z\left(\frac{\partial v_z}{\partial z}\right)\right]=-\left(\frac{\partial P}{\partial z}\right)+\mu\left[\frac{\partial^2 v_z}{\partial x^2}+\frac{\partial^2 v_z}{\partial y^2}+\frac{\partial^2 v_z}{\partial z^2}\right] \tag{2}$$

The left hand side of eq. 2 above represents the acceleration terms and can be neglected for the slow flow of highly viscous fluids. Furthermore, if the channel cross section is not a function of the z coordinate, then v_z does not change with z. Thus eq. 2 reduces to

$$\frac{1}{\mu}\left(\frac{\partial P}{\partial z}\right)=\left[\frac{\partial^2 v_z}{\partial x^2}+\frac{\partial^2 v_z}{\partial y^2}\right] \tag{3}$$

Assuming that there is no clearance between the top of the screw flight and the barrel surface and that we have a single screw channel ($m = 1$), the boundary conditions obtainable are given as

$$v_z(0, y) = 0 \tag{4}$$

$$v_z(x, 0) = 0 \quad (5)$$

$$v_z(w, y) = 0 \quad (6)$$

$$v_z(x, h) = V_z \quad (7)$$

Where V_z is the maximum velocity in the down channel direction (z component) occurring at the surface of the rotating screw. The channel in self-wiping co-rotating twin screw extruder has a small radial clearance through which leakage or loss of pumping capacity can occur, but this can be neglected. It can also be assumed that the variation of v_z with respect to x is small enough so that the derivative $\frac{\partial^2 v_z}{\partial x^2}$ can be ignored. Equation 3 thus reduces to

$$\frac{1}{\mu}\left(\frac{\partial P}{\partial z}\right) = \frac{d^2 v_z}{dy^2} \quad (8)$$

The boundary conditions for the flow become

$$v_z(0) = 0 \quad (9)$$

$$v_z(h) = V_z \quad (10)$$

Thus the solution of equation (8) above satisfying the boundary conditions can be written as

$$v_z = y(\frac{V_z}{h} - \frac{y(h-y)}{2\mu}\left(\frac{\partial P}{\partial z}\right) \quad (11)$$

For the simplified flow theory, the integral of equation (1) reduces to

$$Q_v = w \int_0^h v_z dy \quad (12)$$

The volumetric flow rate after introducing equation (11) into (12) and integrating gives

$$Q_v = \frac{V_z w h}{2} F_d + \frac{w h^3}{12\mu}\left(-\frac{dP}{dz}\right) F_p \quad (13)$$

Where the first term is the drag flow rate and the second term is the pressure flow rate. This can be written as

$$Q_v = Q_d + Q_p \quad (14)$$

Where

$$Q_d = \frac{V_z w h}{2} F_d \quad (15)$$

and

$$Q_p = \frac{w h^3}{12\mu}\left(-\frac{dP}{dz}\right) F_p \quad (16)$$

Where Q_d is the drag flow rate, Q_p is the pressure flow rate, F_d and F_p are shape factors for the drag and pressure flow respectively, V_z is the maximum down channel velocity, w and h are the width and height of the channel respectively, μ is the viscosity of the fluid and $\frac{dP}{dz}$ is the down channel pressure gradient.

To be able to determine the axial velocity, it is necessary to consider the motion of the fluid in the xy axis. Thus both the v_x and the v_y components of the velocity have to be determined. If the assumptions that the flow is steady, incompressible with constant viscosity are made and that the acceleration terms are neglected for the x and y components, the momentum equation reduces to

$$\frac{1}{\mu}\left(\frac{\partial P}{\partial x}\right) = \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} \quad (17)$$

$$\frac{1}{\mu}\left(\frac{\partial P}{\partial y}\right) = \frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} \quad (18)$$

To derive a solution to equations (17) and (18) above, a simplifying assumption has to be made that

$$\frac{\partial^2 v_x}{\partial x^2} \ll \frac{\partial^2 v_x}{\partial y^2} \quad (19)$$

This condition could be satisfied for screws having shallow, wide channels. Applying this simplification, equation (17) reduces to

$$\frac{1}{\mu}\left(\frac{\partial P}{\partial x}\right) = \frac{\partial^2 v_x}{\partial y^2} \quad (20)$$

The solution of equation (20) satisfying the boundary conditions

$$v_x(0) = 0 \quad (21)$$

$$v_x(h) = -V_x \quad (22)$$

is given as

$$v_x = -y\left(\frac{V_x}{h}\right) - \frac{y(h-y)}{2\mu}\left(\frac{\partial P}{\partial x}\right) \quad (23)$$

It is necessary to note that the v_x component of the velocity only causes circulation. Thus,

$$\int_0^h v_x dy = 0 \quad (24)$$

The pressure gradient is determined by introducing equation (20) into equation (24) to give

$$\frac{\partial P}{\partial x} = -\left(\frac{6\mu V_x}{h^2}\right) \quad (25)$$

The expression for v_x can now be determined by putting equation (25) into equation (23) to give

$$v_x = y\left(\frac{V_x}{h}\right)\left[2 - \left(\frac{3y}{h}\right)\right] \quad (26)$$

The net flow rate can be determined by analytical solution of the two flow rates Q_d and Q_p, if they both exist mutually within a local zone of the extruder. Recall from above that the volumetric flow rate in the down channel direction is given as

$$Q_v = \frac{V_z wh}{2} F_d - \frac{wh^3}{12\mu}\left(\frac{dP}{dz}\right) F_p \tag{27}$$

$$Q_v = Q_d - Q_p \tag{28}$$

If we divide equation (29) by Q_d, it becomes

$$\frac{Q_v}{Q_d} = 1 - \frac{Q_p}{Q_d} \tag{29}$$

Let $\beta = \frac{Q_p}{Q_d}$, and referring to the velocity equations above, let $a = \frac{y}{h}$, then,

$$\frac{Q_v}{Q_d} = 1 - \beta \tag{30}$$

Bringing a and β into equation (11) above, the down channel velocity profile can be written as

$$\frac{v_z}{V_z} = a(1 - 3\beta + 3a\beta) \tag{31}$$

Furthermore, the maximum value of β occurs when the pressure gradient reaches its maximum value. This only occurs when the end of the channel is blocked (closed discharge). In this case, since there is no advancement of fluid down the channel, the condition

$$\int_0^1 v_z da = 0 \tag{32}$$

is valid. Introducing equation (31) into (32), we obtain

$$\int_0^1 a(1 - 3\beta + 3a\beta) V_z da = 0 \tag{33}$$

$$\frac{1}{2} - \frac{3\beta}{2} + \beta = 0 \tag{34}$$

Which shows from equation (34) that the maximum value of β is unity. Considering positive pressure gradient, the minimum value of β is zero, because μ, h and V_z are positive quantities. A plot of a against $\frac{v_z}{V_z}$ at various β values between 0 and unity can be done to determine the variation of the velocity in the channel. The maximum velocity V_z and thus the maximum drag flow rate Q_D are given as

$$V_z = \pi D_s N cos\theta \tag{35}$$

$$Q_D = \pi D_s N wh cos\theta \tag{36}$$

Where θ is the helix or pitch angle. The x −component of the fluid velocity vector given by equation (26) can now be written as

$$\frac{v_x}{V_x} = a(2 - 3a) \tag{37}$$

The axial fluid velocity v_l can thus be determined by resolving the v_x and v_z components which gives

$$v_l = v_x cos\theta + v_z sin\theta \tag{38}$$

Introducing equations (31) and (37) into equation (38), the axial velocity can then be given as

$$\frac{v_l}{V} = 3a(1-a)(1-\beta)sin\theta cos\theta \tag{39}$$

Where

$$V = \pi D_s N \tag{40}$$

$$V_x = V sin\theta \tag{41}$$

$$V_z = V cos\theta \tag{42}$$

3. Results and Discussion

With reference to the velocity equations above and from figures (1) and (2) below, it can be deduced that for a screw element having a helix or pitch angle between 0 and 90, shear rates in the yz plane are reseanably greater than those in the xy or ly planes. The axial velocity is always positive as can be seen in figure (2), which means that there cannot be any backflow. The axial velocity profile is seen to be parabolic with the maximum at the mid – plane.

The velocity at any point in the channel height a is a function of the helix angle. As the helix angle is increased, shear rates in the xy plane increases and attains its maximum at $\theta = 90°$. As the helix angle is decreased, shear in the yz plane increases and reaches a maximum when $\theta = 0°$. Note that shear pattern in the xy is independent of the flow ratio β whereas in the yz, it is greatly dependent on β. This is quite an important parameter to consider since transport occurs mainly in the down channel direction i.e., the yz plane. Velocity vectors in the z – plane has positive values only for $\beta \leq 1/3$ whereas for $\beta > 1/3$, it has both positive and negative values as can be seen in figure 1. This indicates that pressure will continue to rise for helix angle between 0° and 90° and attains its maximum at $\beta = 1/3$. Note that screw elements with helix angle between 0° and 90° are forward conveying elements such as the 30° and 60° forward kneading disc. This indicates that since the flow attains its maximum at $\beta = 1/3$, it means that the forward kneading disc reaches its inherent throughput at $\beta = 1/3$. The inherent throughput is the point at which the local conveying zone is fully filled. Any further increase in β (i.e. $\beta > 1/3$) will result in backflow in the down channel direction as can be seen in figure (1) below until it attains its maximum at $\beta = 1$. Since at $\beta = 1/3$, a forward conveying local zone is fully filled, we can write that

$$\beta = \frac{Q_p}{Q_D} \tag{43}$$

$$\frac{Q_p}{Q_D} = 1/3 \tag{44}$$

$$Q_p = \frac{Q_D}{3} \tag{45}$$

$$Q_d = \frac{Q_D}{2} \tag{46}$$

Putting equations (45) and (46) into (28),

$$Q_v = \frac{Q_D}{2} - \frac{Q_D}{3} \tag{47}$$

Thus,

$$Q_v = \frac{Q_D}{6} \tag{48}$$

The reverse can be said to be the case for helix angle $\theta > 90°$, since the cosine of the angle greater than 90° gives negative values. As such the curves shown in figure 1 will be the reverse, the situation obtainable in reverse kneading discs. From equation (48) above, it can be inferred that at fully filled state for the forward conveying zone with pressure gradient, the net flow rate will be one sixth of the maximum drag flow rate at a specific screw speed. If the local zone is not fully filled yet, then the degree of fill can be given as the ratio between the feed volumetric flow rate Q_v and net flow rate, shown mathematically as

$$f = \frac{Q_v}{Q_d - Q_p} \tag{49}$$

Thus,

$$f = \frac{Q_v}{Q_D/6} \tag{50}$$

it is possible to determine the mean time delay once the degree of fill has been estimated. The mean time delay is basically the time the fluid spends in the unfilled portion of the local conveying zone (Poulesquen and Vergnes, 2003). If the total mean residence time is given as

$$t_m = \frac{V}{Q_v} \tag{51}$$

then the mean time delay can then be defined as

$$t_d = (1 - f)t_m \tag{52}$$

where V is the free volume in the local zone of the extruder and $(f t_m)$ is the effective mean residence time.

3.1. Model Validation

Experiments were carried out to validate the theoretical model in a laboratory scale twin screw extruder with length to diameter (L/D) ratio of 25:1 with a screw diameter of 23.25mm, barrel diameter of 24mm and a center-line distance C_l of 18.6mm using the pulse tracer technique. The mean residence time and mean time delay for both the theoretical model and the experiment were determined and shown in table 1. Feed rates (Q) of 10, 15 and 20kg/h and screw speed (N) of 200 and 400rpm were investigated.

Table 1. Validation of Experimental and Theoretical Mean Residence Time and Time Delay.

$\boldsymbol{N}$(rpm)	$\boldsymbol{Q}$(kg/h)	$\boldsymbol{t_m}$(s)Experimental	$\boldsymbol{t_m}$(s)Theoretical	$\boldsymbol{t_d}$(s)Experimental	$\boldsymbol{t_d}$(s)Theoretical
200	10	42	43.19	26	25.53
200	15	27	28.80	15	15.15
200	20	20	21.60	10.5	10.2
400	10	42	43.19	28	28.50
400	15	27	28.80	18	18.12
400	20	20	21.60	13	12.93

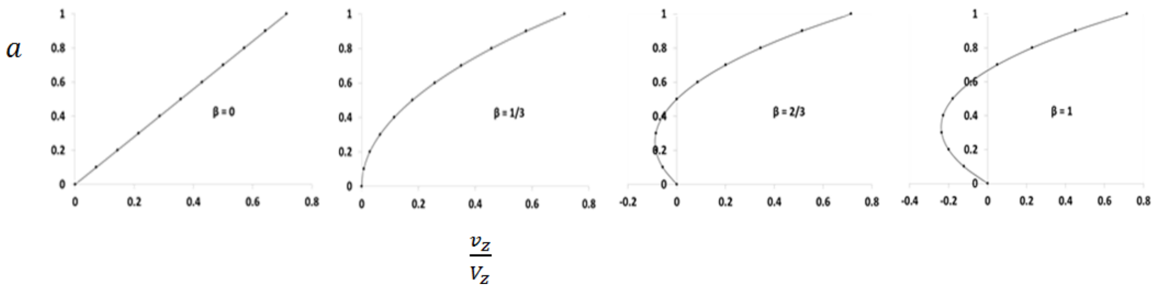

Fig. 1. The down channel velocity profile for various values of β.

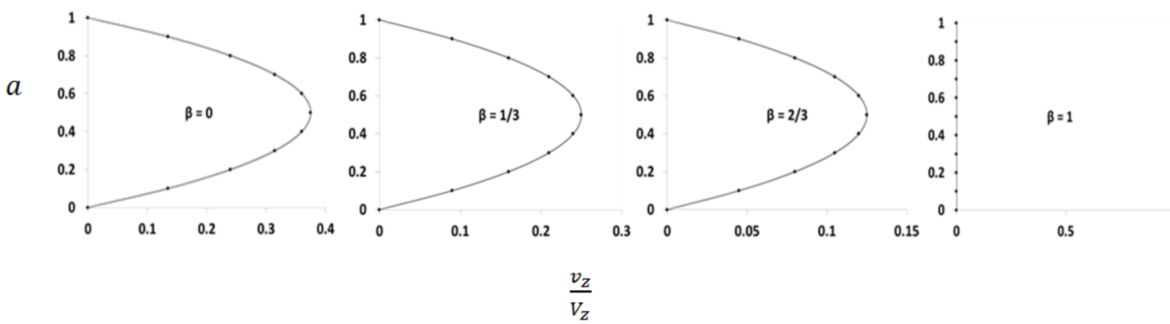

Fig. 2. The axial velocity profile for various values of β.

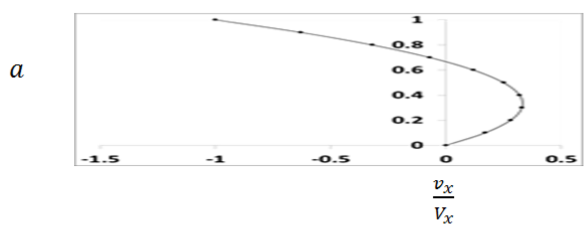

Fig. 3. Cross channel velocity profile.

In the axial direction, the velocity vector is positive for all values of β. This means that all fluid particles in the axial direction of the channel advance towards the exit with no "backflow", though some fluid particles can travel faster than others. For closed discharge ($\beta = 1$), the fluid particles make no advance in the axial direction clearly shown in figure 2. It simply advances and retreats in the x and z directions and in one plane. As the fluid particle approaches the screw flight, it is turned under and due to the presence of the pressure gradient, it then flows back to the opposite side of the channel, where it is eventually turned up by the flight. On the other hand, at $\beta = 0$, a fluid particle will exhibit a flattened helix as it flows towards the discharge port. The advancement of the particle results in circulation in the xy plane but will always advance in the down channel and axial directions. It could be deduced in a sense that increasing β results in slowing down the advancement of the fluid particles towards the exit of the channel. This is so because a fluid particle must make more turns on its helix as β increases.

4. Conclusion

The analytical technique for resolving the flow dynamics in self-wiping co-rotating twin screw extruder proposed in this paper offers immense potential to enable the determination of important parameters in the extruder such as the degree of fill needed in determining the effective mean residence time and the mean time delay. It is of the view that better approximation can be made of these parameters without resorting to empirical methods or software prediction which can be time consuming and expensive.

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