A MODEL OF 2 DIMENSIONAL FLOW IN A TWIN SCREW MIX-EXTRUDER KNEADING DISC USING A FULL 2 DIMENSIONAL SOLUTION OF THE FLOW EQUATIONS

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A method of modelling 2 dimensional flow in a kneading disc of a screw mix-extruder (SME) has been developed which involves solving the differential equations for flow directly, without the approximation used previously which effectively reduced the flow to 1 dimension. The pressure and velocity distributions obtained appear to be realistic, and agree reasonably well with results obtained previously. The model should be able to be readily expanded to 3 dimensions.
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A Model of 2 Dimensional Flow in a Twin Screw Mix-Extruder Kneading Disc Using a Full 2 Dimensional Solution of the Flow Equations

1 Introduction

The study of the flow behaviour of propellant materials in twin screw mix-extruders (SMEs) continues to be a subject of considerable interest in the international propellant community. Modelling of the flow with a computer offers the possibility of estimating the effect of various processing parameters without the need for many expensive experimental trials. Recent work in computer modelling of flow in SMEs has been reviewed in reference 1, which also presented a simplified model of flow in a 2 dimensional kneading disc. The basis of the model was the FAN approach of Tadmor [2], which essentially reduces the dimensionality of the model by 1, so that the flow in the 2 dimensional kneading disc was modelled by 1 dimensional flow, and flow in a 3 dimensional screw channel would be modelled as 2 dimensional flow. While the FAN approach has the advantage of reducing the size of the computational problem, it ignores the circulating component of the flow which is important in determining degree of mixing. Hence for the study of mixing in 3 dimensional screw channels a fully 3 dimensional model is required.

This paper presents a model of flow which does not involve an artificial reduction of the dimensionality of the flow. The model is evaluated for the case of full 2 dimensional flow in a 2 dimensional kneading disc as a first step, and in future it is expected that the model will be expanded to handle 3 dimensional problems.
2. Theory

2.1 Derivation of Flow Equations

The flow in the 2 dimensional kneading disc is illustrated in Figure 1. As was done previously with the FAN based model [1], the flow channel between the extruder wall and the kneading disc has been flattened out, with the barrel wall becoming a straight line moving to the right with velocity $V$. Since in future the model is to be extended to 3 dimensions, where the 1 direction will be along the flow channel, the cross channel directions considered here will be taken to be the 2 and 3 directions. In the 3 direction the flow is solely pressure generated, as there are no external applied velocities at the boundaries in the 3 direction. However, in the 2 direction a velocity is applied to the top surface of the fluid, and hence the velocity in the 2 direction of the fluid in the interior of the channel is, in general, a complex function of drag and pressure flow. However, the flow will be assumed to be locally Newtonian, and therefore linear, so the effect of the applied velocity can be simplified by considering the flow to be a linear combination of pressure driven flow and imposed shear flow.

![Diagram](image)

*Figure 1: Geometry of the flow channel and mesh of cells used in solution of flow equations.*
The basis of the model is to divide the flow region into rectangular cells. Within each cell the flow will be assumed to be locally Newtonian with a constant viscosity in the cell, but a different viscosity in each cell which depends on the average shear rate in the cell. The rheological behaviour of the fluid in the flow channel will be modelled using a generalised Newtonian equation:-

$$\tau = \mu \gamma$$

Where $\tau$ is the shear stress, $\mu$ is the generalised viscosity, and $\gamma$ is the shear rate.

The viscosity will be given by a power law equation:-

$$\mu = k \gamma^{n-1}$$

The equations of motion for 2 dimensional creeping flow of an incompressible fluid in the 2 and 3 directions are:-

$$0 = -\frac{\partial P}{\partial x_2} + \frac{\partial}{\partial x_2} \left( \mu \frac{\partial v_2}{\partial x_2} \right) + \frac{\partial}{\partial x_3} \left( \mu \frac{\partial v_2}{\partial x_3} \right)$$

$$0 = -\frac{\partial P}{\partial x_3} + \frac{\partial}{\partial x_2} \left( \mu \frac{\partial v_3}{\partial x_2} \right) + \frac{\partial}{\partial x_3} \left( \mu \frac{\partial v_3}{\partial x_3} \right)$$

These are coupled partial differential equations which cannot be solved directly.

The equations are solved by producing an estimate of the pressure, and then using the pressure distribution to calculate the velocity distribution. The velocities so obtained are used to produce a new estimate of pressure, and the process is repeated until convergence is obtained. The details of the solution methods will be different for pressure and velocity.

The method for solving for pressure is based on a generalisation of the FAN method used previously [2]. The flow in each cell can be considered to be made up of pressure driven flow in the interior of the cell with superposed shear flow from moving boundaries, as illustrated for flow in the 2 direction in Figure 2. The values of $v_2$ and $v_3$ are calculated from the total flow in the channel. It is important to note that in the model the pressure will be evaluated at the centre of the cell.

Within the cell the viscosity is assumed to be constant, and so in evaluating the double derivatives

$$\frac{\partial}{\partial x_3} \left( \mu \frac{\partial v_2}{\partial x_3} \right) \cdot \frac{\partial}{\partial x_2} \left( \mu \frac{\partial v_3}{\partial x_2} \right)$$

the viscosity can be taken outside the derivative. However, the derivatives

$$\frac{\partial}{\partial x_2} \left( \mu \frac{\partial v_2}{\partial x_2} \right) \cdot \frac{\partial}{\partial x_3} \left( \mu \frac{\partial v_3}{\partial x_3} \right)$$

will be evaluated between adjacent cells, and so the viscosity has to be treated as a variable when expanding these derivatives.
Using these assumptions, equations 1 and 2 can be rearranged to give:

\[
\frac{\partial^2 v_2}{\partial x_3^2} = \frac{1}{\mu} \frac{\partial P}{\partial x_3} - \frac{1}{\mu} \frac{\partial}{\partial x_3} \left( \frac{\mu}{\partial x_3} \right) \frac{\partial v_2}{\partial x_2} \tag{3}
\]

\[
\frac{\partial^2 v_3}{\partial x_2^2} = \frac{1}{\mu} \frac{\partial P}{\partial x_2} - \frac{1}{\mu} \frac{\partial}{\partial x_2} \left( \frac{\mu}{\partial x_2} \right) \frac{\partial v_3}{\partial x_3} \tag{4}
\]

A simple way to solve these equations is by an iterative procedure where the velocity field from the previous iteration is used to calculate the derivatives:

\[
\frac{\partial}{\partial x_2} \left( \frac{\partial v_2}{\partial x_2} \right), \frac{\partial}{\partial x_3} \left( \frac{\partial v_3}{\partial x_3} \right)
\]

These derivatives can then be treated as constants and be lumped with the pressure derivatives, and the equations integrated directly.
For the geometry illustrated in Figure 1, the equations can be integrated to give

\[ v_2(x_3) = v_{2b} \left( \frac{x_3}{\Delta X_3} + \left( 1 - \frac{x_3}{\Delta X_3} \right) \right) v_{2l} \]

\[ -\frac{\Delta X_3^2}{2\mu} \left( \frac{\partial P}{\partial x_2} - \frac{\partial}{\partial x_2} \left( \mu \frac{\partial v_2}{\partial x_2} \right) \right) \left( \frac{x_3}{\Delta X_3} - \frac{x_3^2}{\Delta X_3^2} \right) \]

\[ v_3(x_2) = v_{3b} \left( \frac{x_2}{\Delta X_2} + \left( 1 - \frac{x_2}{\Delta X_2} \right) \right) v_{3l} \]

\[ -\frac{\Delta X_2^2}{2\mu} \left( \frac{\partial P}{\partial x_3} - \frac{\partial}{\partial x_3} \left( \mu \frac{\partial v_3}{\partial x_3} \right) \right) \left( \frac{x_2}{\Delta X_2} - \frac{x_2^2}{\Delta X_2^2} \right) \]

where \( \Delta X_2 \) and \( \Delta X_3 \) are the cell dimensions in the 2 and 3 directions.

The flows through the boundaries of the cell in each direction are obtained by integrating equations 5 and 6 to give:

\[ Q_2 = \frac{v_{2b} + v_{2l}}{2} \cdot \Delta X_3 - \frac{\Delta X_3^3}{12\mu} \left( \frac{\partial P}{\partial x_2} - \frac{\partial}{\partial x_2} \left( \mu \frac{\partial v_2}{\partial x_2} \right) \right) \]

\[ Q_3 = \frac{v_{3b} + v_{3l}}{2} \cdot \Delta X_2 - \frac{\Delta X_2^3}{12\mu} \left( \frac{\partial P}{\partial x_3} - \frac{\partial}{\partial x_3} \left( \mu \frac{\partial v_3}{\partial x_3} \right) \right) \]

If the flow in the positive 2 direction out of cell \((J,K)\) is given by \(Q_2(J,K)\), and the flow into the cell by \(Q_2(J-1,K)\), and in the 3 direction by \(Q_3(J,K)\) and \(Q_3(J,K-1)\), then conservation of mass requires that

\[ Q_2(J,K) + Q_3(J,K) - Q_2(J-1,K) - Q_3(J,K-1) = 0 \]

If equations 7 and 8 for the appropriate cells are substituted into 9, the pressure in the cell is given in terms of the flow velocities and viscosities. If values of the velocities and viscosities are available from a previous iteration, they can be substituted into conservation equation to give an equation for the pressure in each cell in terms of the pressures in the surrounding cells. The method of solving this set of equations for the pressures in each of the cells will be discussed in the next section.

Once an estimate of the pressure distribution is known, it can be used to calculate an estimate of the velocity distribution from equations 3 and 4.

The method of solution of these equations will be discussed in a subsequent section. This procedure can be iterated until the values of pressure and velocity converge to constant values.
2.2 Method of Solution of Equations for Pressure Distribution

The pressure distribution is calculated by converting the differential equations 7 and 8 into finite difference equations, and substituting them into equation 9. The finite difference equation for $Q_2$ is:

\[
Q_2(j, k) = \frac{V_2(j, k) + V_2(j, k-1)}{2} \frac{Dx^3}{12 \mu_2(j, k)} \left[ \frac{P(j + 1, k) - P(j, k)}{DX} \right] + \frac{DX^3}{12 \mu_2(j, k)} \left[ \frac{\mu_3(j + 1, k)}{2 \cdot DX^2} \left( \frac{V_2(j + 1, k) - V_2(j, k)}{DX} \right) \right] - \mu_3(j, k) \frac{V_2(j, k) - V_2(j - 1, k)}{DX} - \mu_3(j, k - 1) \frac{V_2(j, k - 1) - V_2(j - 1, k - 1)}{DX} \right]
\]

(10)

where $V_2(j, k)$ is the velocity in the 2 direction at the lower right corner of cell $(j, k)$ and the subscripted viscosity terms are the averages of viscosity at the centre points of the walls dividing the cells in the 2 and 3 directions respectively. The second derivative in the 2 direction can only be evaluated at the cell walls because that is where the velocities are defined. The required value is at the cell centre, so the average of the wall values is used. If equation 10 is substituted into equation 9 and rearranged to put the pressure terms on the left hand side and other terms on the right hand side, then the contribution from $Q_2(j, k)$ is given by:
\[
\frac{DX_3^3}{12\mu_2(J,K)} \frac{P(J,K)}{DX_2} - \frac{DX_3^3}{12\mu_2(J,K)} \frac{P(J+1,K)}{DX_2} = \\
\frac{DX_3}{2} \left( V_2(J,K) + V_2(J,K-1) \right)
\]

\[
\frac{DX_3^3}{12\mu_2(J,K)} \frac{1}{2.DX_2^2} \left( \mu_3(J+1,K).V_2(J+1,K) - (\mu_3(J+1,K)+\mu_3(J,K)).V_2(J,K)+\mu_3(J,K).V_2(J-1,K) \right)
\]

\[
\frac{DX_3^3}{-12\mu_2(J,K)} \frac{1}{2.DX_2^2} \left( \mu_3(J+1,K-1).V_2(J+1,K-1) - (\mu_3(J+1,K-1)+\mu_3(J,K-1)).V_2(J,K-1)+\mu_3(J,K-1).V_2(J-1,K-1) \right)
\]

A similar equation is obtained for Q_3(J,K):

\[
\frac{DX_2^3}{12\mu_3(J,K)} \frac{P(J,K)}{DX_3} - \frac{DX_2^3}{12\mu_3(J,K)} \frac{P(J,K+1)}{DX_3} = \\
\frac{DX_2}{2} \left( V_3(J,K) + V_3(J-1,K) \right)
\]

\[
\frac{DX_2^3}{12\mu_3(J,K)} \frac{1}{2.DX_3^2} \left[ \mu_2(J,K+1).V_3(J,K+1) - (\mu_2(J,K+1)+\mu_2(J,K)).V_3(J,K)+\mu_2(J,K).V_3(J,K-1) \right]
\]

\[
\frac{DX_2^3}{12\mu_3(J,K)} \frac{1}{2.DX_3^2} \left[ \mu_2(J-1,K+1).V_3(J-1,K+1) - (\mu_2(J-1,K+1)+\mu_2(J-1,K)).V_3(J-1,K)+\mu_2(J-1,K).V_3(J-1,K-1) \right]
\]

The pressure term P(J,K+1) has been put on the right hand side so that the left hand side only contains variable terms in K, and not K-1 or K+1.

Similar equations are obtained for the flows Q_2(J-1,K) and Q_3(J,K-1).

Substituting into equation 13 gives an equation of the form

\[
\]

The A, B and C terms contain only DX_2, DX_3, and \mu(J,K), and the G term contains velocities, viscosities, and pressures for cells J,K+1 and J,K-1. Similar equations are obtained for all the other cells, giving a set of equations of a tridiagonal form which can easily be solved by standard methods.
In the particular iterative solution method used here the pressures are solved for each row of constant K in turn. The velocities, viscosities, and pressures for values of K different from the value under consideration are taken from the previous iteration.

2.3 Method of Solution of Equations for Velocity Distribution.

There are 2 methods of deriving the velocity distribution based on the model proposed in Section 2.1. The velocity distribution within a cell is parabolic, as given by equations 3 and 4. For the sake of discussion, the velocity in the 2 direction will be considered. At the boundaries of the cells in the 3 direction the shear stresses in each cell have to be equal. The shear stress is given by:

\[ \tau = \mu \frac{\partial v_2}{\partial x_3} \]

where the lower case "v" denotes the continuously variable velocity in the cell. For the boundary between cells \((J,K)\) and \((J,K-1)\) the equality of shear stresses gives:

\[ \mu(J,K) \frac{\partial v_{2z}(J,K)}{\partial x_3} = \mu(J,K-1) \frac{\partial v_{2b}(J,K-1)}{\partial x_3} \]  

where \(v_{2z}(J,K)\) is the value of the velocity at the upper right hand corner of the \((J,K)\) cell, and \(v_{2b}(J,K-1)\) is the velocity at the lower right hand corner of cell \((J,K-1)\), see figure 2. The derivatives of velocity are obtained by integrating equation 3. For all values of K in a vertical column of cells in the channel, equation 13 leads to a set of simultaneous equations in the velocities at the cell corners. The values of the velocities at the channel walls are known from the boundary conditions, so the equations can be solved by direct substitution methods to give the velocity distribution.

The same equations for the velocity distributions can also be obtained in a more formal manner by converting equations 1 and 2 into finite difference equations. To calculate the velocities in the 2 direction, equation 1 can be rearranged and converted to finite differences to give:
\[\frac{1}{DX3} \left( \mu_2(J,K+1) \cdot \frac{V2(J,K+1) - V2(J,K)}{DX3} \right) - \mu_2(J,K) \cdot \frac{V2(J,K) - V2(J,K-1)}{DX3} = \]
\[\frac{P(J+1,K) + P(J+1,K+1) - P(J,K) - P(J,K+1)}{DX2.2} \]
\[\frac{1}{DX2} \left( \mu_3(J+1,K) \cdot \frac{V2(J+1,K) - V2(J,K)}{DX2} - \mu_3(J,K) \cdot \frac{V2(J,K) - V2(J-1,K)}{DX2} \right) \]

where \(V2(J,K)\) is the velocity at the lower right hand corner of cell \((J,K)\). This method of differencing the equations was chosen because the viscosity has been assumed constant in each cell, so the local spatial derivatives of the viscosity are zero. Hence the derivative of the product of the viscosity and the first derivative of velocity can be approximated by the difference of the product between 2 cells, and so equation 13 should be a good approximation to the true equation.

Multiplying by \(DX3 \cdot DX3\) and rearranging equation 14 gives:

\[\begin{align*}
\mu_2(J,K+1).V2(J,K+1) - (\mu_2(J,K+1) + \mu_2(J,K)) & \cdot V2(J,K) \\
+ \mu_2(J,K) \cdot V2(J,K-1) &= \\
\frac{DX3^2}{DX2} \cdot P(J+1,K) + P(J+1,K+1) - P(J,K) - P(J,K+1) \\
- \frac{DX3^2}{DX2} \left[ \mu_3(J+1,K) \cdot V2(J+1,K) - (\mu_3(J+1,K) + \mu_3(J,K)) \cdot V2(J,K) \\
+ \mu_3(J,K) \cdot V2(J-1,K) \right]
\end{align*}\n
Rearranging gives

\[\begin{align*}
\mu_2(J,K+1).V2(J,K+1) - (\mu_2(J,K+1) + \mu_2(J,K)) & \cdot V2(J,K) \\
- \frac{DX3^2}{DX2} \cdot (\mu_3(J+1,K) + \mu_3(J,K)) & \cdot V2(J,K) + \mu_2(J,K) \cdot V2(J,K-1) = \\
\frac{DX3^2}{DX2} \cdot P(J+1,K) + P(J+1,K+1) - P(J,K) - P(J,K+1) \\
- \frac{DX3^2}{DX2} \cdot (\mu_3(J+1,K) \cdot V2(J+1,K) + \mu_3(J,K) \cdot V2(J-1,K))
\end{align*}\n
\[(16)\]
Similar equations are obtained for the other cells and together they form a system of equations of the form:


with the variables to be solved \( V_2(J,K+1), V_2(J,K), V_2(J,K-1) \). The equations can be solved stripwise for constant values of \( J \). In this case the viscosities, pressures, and \( V_2(J+1) \) and \( V_2(J-1,K) \) are evaluated from values from the previous iteration. The equations for each \( J \) are then solved by a direct substitution method, and the process iterated until the values of velocity converge.

A similar procedure is used to solve the velocities in the 3 direction.

### 3. Results and Discussion

A computer program to implement the model described above has been written in BASIC. The kneading disc modelled had a flight clearance of 1 mm, a depth in the centre of the channel of 8 mm and a total length of 67.5 mm. This channel was represented on a grid of cells numbering 25 by 16 of dimension 2.7 mm by 0.5 mm (see Fig. 1). The power law viscosity parameters were \( k = 5000 \text{ Pa.s} \) and \( n = 0.5 \).

Calculated values of the pressures at the cell centres are given in Table 1. Only the left half of the channel is shown because the flow is symmetrical. The positive 2 direction is from left to right and the positive 3 direction is down the page. The pressure is defined to be zero at the centre of the flight tip and at the centre of the channel. The values are negative in the rest of the region because the flow is out of left half into the right half of the channel, where the pressure is positive. The pressure increases with increasing distance in the 2 and 3 directions in the main part of the channel as would be expected.

Values of the velocity in the 2 and 3 directions at the right hand corner of the cells are given in Tables 2 and 3. The velocities are symmetrical about the cells in columns 0 and 12. The pressure gradient in the 3 direction causes the upward velocity in the 3 direction in the left hand part of the channel which leads to a circulating flow. The circulation can be seen in Tables 4 and 5 which give the magnitude and direction of the total flow.

The FAN model, which was used previously to calculate flow in a similar channel, was essentially only a 1 dimensional model, and only the variation of pressure and velocity in the 2 direction were calculated [1]. To compare the models, the FAN model was used with the geometry and viscosity parameters of the current model. The results of the 2 models are compared in figures 3 and 4. Figure 3 shows the variation of pressure in the 2 direction, and the FAN values are about 10 to 15% lower than the full 2 dimensional values. Given the approximations involved, particularly in the FAN model, the agreement is acceptable.

A comparison of the calculated values of the components of velocity in the 2 direction is given in Figure 4. The velocities are evaluated along the vertical line of symmetry in the centre of the channel. It can be seen that the agreement is very good.
The model has been constructed with the aim of future expansion to 3 dimensions. The results obtained confirm the reliability of the model in 2 dimensions and do not indicate any impediment to further expansion.

Figure 3: Comparison of calculated pressure profile in the 2 direction from the current 2 dimensional model and the previous FAN model.
Figure 4: Comparison of the 2 component of velocity in the 3 direction from the current 2 dimensional model and the previous FAN model.
**Table 1: Pressure distribution (kPa)**

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**Table 2: Velocity distribution (mm/s) - 2 direction**

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4. Conclusions

A model of flow in a 2 dimensional channel has been developed which explicitly calculates the distribution of pressure and velocity in 2 dimensions. The pressure and velocity distributions obtained appear to be realistic, and compare well to distributions obtained with the simpler FAN method.

The model should be capable of being readily expandable to model 3 dimensional flows.

5. References


A model of 2 dimensional flow in a twin screw mix-extruder kneading disc using a full 2 dimensional solution of the flow equations.

A method of modelling 2 dimensional flow in a kneading disc of a screw mix-extruder (SME) has been developed which involves solving the differential equations for flow directly, without the approximation used previously which effectively reduced the flow to 1 dimension. The pressure and velocity distributions obtained appear to be realistic, and agree reasonably well with results obtained previously. The model should be able to be readily expanded to 3 dimensions.
A Model of 2 Dimensional Flow in a Twin Screw Mix-Extruder
Kneading Disc Using a Full 2 Dimensional Solution of the Flow Equations

R.C. Warren

(MRL-TN-636)

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