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**A METHOD OF MODELLING THE FLOW OF A PROPELLANT
DOUGH IN A SINGLE KNEADING DISC OF A TWIN
SCREW MIX-EXTRUDER**

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R.C. WARREN

**ORDNANCE SYSTEMS DIVISION
WEAPONS SYSTEMS RESEARCH LABORATORY**

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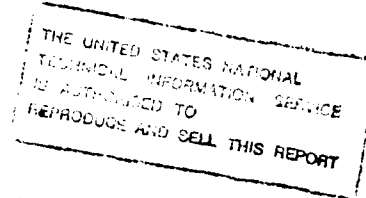
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TECHNICAL MEMORANDUM
WSRL-TM-10/90

**A METHOD OF MODELLING THE FLOW OF A PROPELLANT DOUGH
IN A SINGLE KNEADING DISC OF A TWIN SCREW MIX-EXTRUDER**

R.C. Warren

S U M M A R Y (U)

A simplified method of modelling 2 dimensional flow of propellant doughs in a kneading disc of a twin screw mix-extruder (SME) has been developed. The 2 dimensional model is a first step in the development of a full 3 dimensional model of flow in screws and kneading blocks in SMEs. The model is based on the FAN method of Tadmor as modified by Szydlowski et al, and it aims to use less computational effort than alternative models based on finite element analyses. Apart from one model for non-Newtonian fluids, which has several serious flaws, the existing models have assumed that the viscosity of the fluid was Newtonian. The model presented here gives a better method of calculating the flow of non-Newtonian fluids than the previous method, and it produces more realistic flow velocity profiles.

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Author's address:
Ordnance Systems Division
Weapons Systems Research Laboratory
PO Box 1700, Salisbury
South Australia

Requests to: Chief, Ordnance Systems Division

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1. INTRODUCTION

The study of the flow behaviour of propellant materials in twin screw mix-extruders (SMEs) has recently received considerable attention in the USA. Much of this work has been done by a group headed by D. Kalyon at the Stevens Institute, NJ, and also by R. Armstrong at MIT. Some of this work has been reported to the Continuous Mixer and Extruder Users Group Meetings held annually in the US(ref.1,2), as well as in the open literature(ref.3,4). The work was aimed at producing detailed and accurate descriptions of the flow in SMEs of a limited range of materials, usually inert composite propellant analogues. The computer models used in the analyses were fully 3 dimensional and used complex constitutive equations. The models were of such complexity that they had to be run on supercomputers and graphics processors. These facilities are not available for flow modelling at WSRL, where studies are being undertaken on the manufacture of nitrocellulose propellants by SME.

A need exists for the development of modelling methods which can be used with ordinary mainframe computers, or preferably, with the new generation desktop computers. These simplified models would not provide the same degree of detail as the complex models, but they could be used as an aid in experimental design by providing a guide to the likely effect of changes of various parameters on processing behaviour.

An approximate 2 dimensional finite element analysis of flow of Newtonian fluids in a screw channel was developed by Denson and Hwang(ref.5), and a similar approach to modelling non-Newtonian fluids was taken by Lai-Fook et al(ref.6). However, these finite element approaches are too complex and consume too much computer time to be useful in modelling propellant flow in SMEs. A simplified model of Newtonian flow in a kneading disc was described by Werner and Eise(ref.7), but no details of the solution method were given.

Simple models of flow in SMEs based on the FAN method of Tadmor(ref.8) have been developed by Szydłowski, Brzoskowski and White(ref.9). A basic approximation of these models is the reduction in the dimensionality of flow from 3 to 2, which results in a considerable reduction in complexity and computing time without a large loss of accuracy in the calculation of gross flow characteristics.

A more drastic approximation from the viewpoint of propellant processing was the assumption of a Newtonian viscosity. The assumption of a Newtonian viscosity implies that the viscosity is a constant independent of the shear rate, and hence it is independent of the velocity distribution. This assumption considerably reduces the complexity of the equations describing flow, because they are transformed from non-linear to linear equations. One important consequence of linear behaviour is that solutions of the equations remain solutions when multiplied by constant factors, and the sum of two or more solutions is a solution. This allows a wide variety of situations to be analysed by the solution of only a few equations.

Unfortunately, strong non-Newtonian behaviour is shown by most polymeric materials, including nitrocellulose (NC) based propellants(ref.10), and the assumption of a Newtonian viscosity is not acceptable. Some modelling of the flow of non-Newtonian fluids has been done by Szydłowski and White(ref.11) using the so-called power law equation for viscosity. This equation gives a reasonably accurate description of viscosity in many cases, but the way the equation was applied in the model does not appear to give the full accuracy possible (this matter is discussed later).

The aim of the present program of work is to build on the results of Szydłowski and White to produce a more realistic model which is applicable to the flow of nitrocellulose propellant materials in SMEs. This paper describes a first step in this direction, viz, the modelling of 2 dimensional flow in a single kneading disc. There are two reasons for starting with this simplified approach. Firstly, it is more efficient to develop the required numerical procedures using a simplified problem, and secondly it is easier to explore various more accurate approximation procedures which will be used in more complex models.

2. THEORY

A typical pair of kneading blocks made up of a staggered series of specially shaped discs for a co-rotating twin screw extruder is illustrated in figure 1. In an actual extruder these blocks are set-up in intermeshing pairs along parallel shafts inside a figure 8 shaped barrel. However, for the purposes of modelling, only the behaviour of a single kneading block in a cylindrical barrel will be considered. The main consequence of this assumption is that the effect of flow in the intermeshing region between the pairs of blocks is ignored.

The analysis of the simplified screw geometry is similar to the method of analysis of a single screw extruder(ref.12). The main assumption in the analysis is that (conceptually) the screw channel is opened out so that the barrel wall becomes flat, and the channel in the kneading block resembles the shape in figure 2. A further assumption is that the kneading block remains stationary and the barrel wall moves in the direction opposite to the screw shaft rotation.

The analysis of twin screw SMEs also involves some differences from the analysis of single screw extruders. The flow channels in single screws are relatively shallow and can be approximated by flat plates, but in the case of self-wiping twin screws, the channels are relatively deep and have a complex shape, and hence a more sophisticated modelling method must be used.

An extra simplifying assumption is made in modelling flow in screws or kneading blocks, viz, that the flow is essentially 2 dimensional. Obviously there will be some circulating flow in the channel, and near the tips there will be flow in the x_2 direction, see figure 3. Neglect of this flow may reduce the accuracy of the model slightly, and also it may contribute to the convergence problems at small flight tip gaps (to be described later).

For the modelling of flow in a single kneading disc considered in this paper, the dimensionality of the flow can be further reduced to 1. It is assumed that motion in the radial direction is negligible and that the circumferential velocity does not vary rapidly in the circumferential direction. These assumptions are summarised as

$$v_1 = v_2 = 0, \text{ and } \frac{\partial v_3}{\partial x_3} = 0 \quad (1)$$

The general equations of motion for a viscous fluid can be reduced for the geometry of figure 2 and the assumptions in equation (1) to

$$0 = -\frac{\partial P}{\partial x_3} + \frac{\partial \sigma_{32}}{\partial x_2} \quad (2)$$

For common fluids the shear stress, σ_{32} , can be written in terms of a generalised viscosity, μ , and the shear rate, $\partial v_3 / \partial x_2$, as

$$\sigma_{32} = \mu \frac{\partial v_3}{\partial x_2} \quad (3)$$

For the case where μ is a constant, equation (2) becomes

$$\frac{\partial P}{\partial x_3} = \mu \cdot \frac{\partial^2 v_3}{\partial x_2^2} \quad (4)$$

This equation provides the basis of the description of flow of the material, and the general method of solution of it is based on the FAN method of Tadmor(ref.8), as modified by Szydlowski et al(ref.9). The channel is divided into series of N elements in the x_3 direction, indexed with the variable I, as illustrated in figure 4. The pressure depends only on x_3 , and it is assumed to be constant within each element and vary only between elements. There are no sources or sinks for flow in the channel, so the total flow into any element must equal the flow out of that element. In particular for the I'th element the flow in, $Q(I-1)$, must equal the flow out, $Q(I)$. The solution is achieved by deriving equations for the magnitudes of the flows in terms of the pressures, and then solving the equations to give the pressure distribution. Once the pressure distribution has been determined, it can be used to calculate the velocity distribution.

Details of the methods of modelling the flow are given below in order of improving approximation and increasing expected accuracy.

2.1 Approximation #1. Newtonian viscosity

The simplest equations result when the viscosity, μ , is taken to be a constant which is independent of shear rate. This approximation was made by Szydlowski et al in reference 9. In this case equation (4) is linear, and can be integrated directly to give the velocity as

$$v_3(x_2) = V_3 \cdot \frac{x_2}{H} - \frac{H^2}{2\mu} \cdot \frac{\partial P}{\partial x_3} \cdot [(x_2/H) - (x_2/H)^2] \quad (5)$$

where H is the channel depth and V_3 is the velocity of the wall. Integrating over the cross-section gives the volumetric flow rate:

$$Q = V_3 \cdot \frac{H}{2} \cdot \frac{H^3}{12\mu} \cdot \frac{\partial P}{\partial x_3} \quad (6)$$

Equation (6) can be applied to each element in the flow channel to give a series of equations for the pressure profile. Details of the equations and the method of solution are given in Appendix I. Once the pressure distribution has been determined, it can be substituted into equation (5) to calculate the velocity distribution.

2.2 Approximation #2. Averaged power law viscosity: velocities calculated from Newtonian viscosity

The assumption of a shear rate independent viscosity is not realistic for propellant materials, which are known to show considerable shear thinning behaviour(ref.10). An adequate description of the viscosity of propellants is given by the power law,

$$\mu = k \cdot \left\{ \frac{\partial v_3}{\partial x_2} \right\}^{(n-1)} \quad (7)$$

where k is the consistency index, and n is the power law exponent with a typical value of 0.4 for propellants. Since the viscosity varies with the shear rate, which in turn varies with depth in the channel, the viscosity is a function of x_2 , ie $\mu = \mu(x_2)$.

Because μ is no longer a constant, equation (4) is not valid. For variable values of μ , substituting equation (3) into equation (2) gives

$$\frac{\partial P}{\partial x_3} = \frac{\partial \mu}{\partial x_2} \frac{\partial v_3}{\partial x_2} + \mu \cdot \frac{\partial^2 v_3}{\partial x_2^2} \quad (8)$$

Substituting equation (7) into equation (8) gives, after some manipulation

$$\begin{aligned} \frac{\partial P}{\partial x_3} &= n \cdot \mu \cdot \frac{\partial^2 v_3}{\partial x_2^2} \\ &= n \cdot k \cdot \left\{ \frac{\partial v_3}{\partial x_2} \right\}^{(n-1)} \cdot \frac{\partial^2 v_3}{\partial x_2^2} \end{aligned} \quad (9)$$

Hence for the particular case of a power law dependence of viscosity, the Newtonian equation is modified by only a multiplicative factor. In the model the value of k was multiplied by n and the equations solved in the same way as equation (4). It appears that this factor was not taken into account by Szydlowski and White(ref.9), which further reduces the accuracy of their results.

The simplest way to take account of the variable viscosity is to calculate an average viscosity for each element of the channel, see figure 2, and substitute this value in the equation for flow rate(ref.6). The average viscosity is calculated by dividing the channel depth into a series of M levels, indexed with the variable J , and calculating the viscosity at each level, then averaging. There are a number of types of average which could be used. Szydlowski and White in reference 9 calculate an average shear rate and then substituted it into equation (7). A second possibility is to calculate the mean viscosity from the values in each layer, but this method was found to cause the iterative procedures in the model to diverge. A third method, which was found to be the most accurate, is to take the reciprocal of the mean of the reciprocals of the individual viscosities, ie

$$\mu_{av} = \frac{1}{\text{average } (1/\mu_i)}$$

This form of average was suggested by the fact that the viscosity appears in the denominator of equation (6).

The shear rate in layer J is determined from the calculated Newtonian velocity profile. This approach was used by Szydlowski and White(ref.11).

2.3 Approximation #3. Averaged power law viscosity: velocities calculated from power law velocity profile

In reverse pitch kneading blocks and screws there will be considerable backflows and correspondingly large velocity gradients. The velocity profile calculated from the above procedure, and the corresponding viscosities, are unlikely to be related to the true values. Hence a superior method from that used by Szydlowski and White is required.

As a first step, a better approximation to the real velocity profile can be calculated from equation (9), using the already calculated viscosity and pressure profiles from Approximation #2, see a flow diagram of the solution process given in figure 5. The method of solution of equation (9) is given in Appendix I.

2.4 Approximation #4. Full solution

The pressures and volume flow rates obtained in Approximation #3 are not correct, as they were calculated using averaged viscosities. The full solution to equation (9) must be obtained by an iterative procedure involving adjusting the pressure profile to balance the actual inflow and outflow

of each element with the volume flow rates calculated from the most recently calculated velocity profile. The calculation of the true velocity profile must also use the individual viscosities from each level, and the process is illustrated in the flow diagram, figure 5.

The computer program developed in this study contains an algorithm for varying the pressure profile in an iterative process until the values of the pressure, velocity and viscosity converge. As a check that the solution had converged to the correct values, the pressures were also calculated directly from equation (9), using the final values of velocity and viscosity. Details of the calculation are given in Appendix I. The agreement was found to be better than 1%.

3. RESULTS AND DISCUSSION

The analysis described above is applied to modelling the flow in a kneading disc in the Werner-Pfleiderer ZSK 40 SME at WSRL. The barrel diameter is 40.3 mm, and the distance between screw shafts is 33.4 mm. The nominal screw element diameter is 40.0 mm, which gives a screw tip-barrel clearance of 0.15 mm. Because of numerical instability problems the minimum tip clearance modelled was 0.2 mm. The shape of the disc, and hence the flow channel, was calculated by the method of Booy(ref.13).

The power law parameters for viscosity (see equation (7)) used in the model were $k = 12500$ Pa and $n = 0.4$. These values are typical of solvent processed double base doughs(ref.10). These doughs usually show a yield stress when extruded in the batch process, but it is felt that the structure responsible for the yield stress would be broken down in the SME, and so the yield stress would be negligible.

The calculated velocity and pressure profiles for a screw speed of 120 RPM and a flight tip gap of 0.2 mm, for the various approximations, are given in figures 6 to 9. The bottom part of the figures is a scaled representation of the shape of the flow channel, with the first horizontal line representing the barrel wall. The middle part of the figures shows the velocity profiles at various positions along the length of the flow channel. The dashed lines are zero velocity for the appropriate profile. The top part of the figures is the pressure profile in the channel.

Only the leading half of the flow channel is shown in the figures, as the profiles are symmetrical about the centre of the channel. The pressure profile shows that the pressure built up by the flow in the channel drops linearly across the flight tip to the maximum negative level, and then builds up again in the channel. In the trailing half of the channel (not shown) the pressure reaches the maximum positive pressure just before the flight tip.

The calculated pressure profiles are qualitatively similar to the profiles obtained by Szydlowski and White(ref.9), and also Werner and Eise(ref.7).

The velocity profiles are complex, and show the effect of the interaction of drag flow and pressure flow. For pure drag flow between parallel plates the velocity profile is linear, and for pure pressure flow it is parabolic. The addition of pressure flows to drag flows produces composite profiles due to the presence of

backflows, see figure 10. It can be seen from figures 6 to 9 that the velocity profile in the gap is convex due to the pressure gradient forcing the material forward through the gap. In the body of the channel the direction of the pressure gradient is reversed, and there is backflow near the channel root.

The Newtonian profiles are given in figure 6. The maximum pressure is 30.8 MPa, and the velocity profiles in the channel are strongly curved. The non-Newtonian Approximation #2, see figure 7, shows a much smaller value of maximum pressure of 1.17 MPa, because the viscosity is greatly reduced. The velocity profiles are unchanged in this approximation. This case corresponds to the approximation used by Szydlowski and White(ref.11).

In Approximation #3, see figure 8, the pressures have still been calculated using the Newtonian formula for flow rate, but the velocity profiles have been calculated using a variable viscosity profile, and it can be seen that the velocity profiles are considerably flattened.

The full solution is given in figure 9. There are significant differences in pressure and velocity profile from the previous approximations. The pressure is increased by about 50% to 1.65 MPa, the velocity profiles are further flattened, and the backflow is considerably increased.

The calculated flow rates in the flight tip gap region were fairly independent of the approximation used, because the flow is almost totally due to drag. However, in the centre of the flow channel, the calculated flow rates varied considerably depending on the method of calculation, see Table 1. It is readily apparent that the total flow rate from the central elements is only a small fraction of the flow occurring inside the central elements, and the total flow is the difference between large forward and reverse flows.

For the Newtonian case the flow rates were calculated directly from equation (6), and also by integrating the calculated velocity profile using Simpson's Rule. No difference could be found between the two results. The change in calculated flow rates between Approximations #1 and #2 was relatively small

However there was a significant difference between the calculated flow rates using Approximation #3. In this approximation the pressure profile is calculated from flow rates given by equation (6) by substituting an average viscosity, and these values of the flow rate in each element are all equal to each other. However, the true value of the flow rate in each element was calculated from the actual velocity profile, and these values vary between $2.79 \times 10^{-5} \text{ m}^3/\text{s}$ in the flight tip gap to $1.51 \times 10^{-4} \text{ m}^3/\text{s}$ in the centre of the channel. This indicates that Approximation #3 does not give a very accurate estimate of the pressures or flow rates, and it is not usable as an improved approximation over Approximation #2.

It was possible that the poor results from Approximation #3 were due to the method of averaging the viscosity. Szydlowski and White used an average viscosity obtained by substituting the mean shear rate into the power law equation (7). Running the model with this form for the average viscosity gave a flow rate for the centre element of $2.40 \times 10^{-4} \text{ m}^3/\text{s}$, which is considerably more in error than the method used in this work. The corresponding pressure and velocity profiles are given in figure 11, and comparing with figures 8 and 9, it can be seen that the velocity profiles are further from the true profiles. For Approximation #2, the difference in flow rates calculated from the different averages were not significant, but the pressure calculated from viscosities using the mean shear rate was about 7% lower.

Comparing the results for Approximations #2 and #4 in Table 1, it can be seen that the difference in total flow rate is only of the order of 5%. However, there is a significant difference in the magnitudes of the forward and reverse flows, and the maximum pressures vary by about 50%. The velocity profiles in figures 6 and 9 show a large difference in flow patterns and hence mixing effectiveness. These results indicate that in the geometry considered in this work the extra computational effort required by the full solution is probably justified.

The effect of varying the flight tip gap can be seen in figures 9 and 12 to 13. As the gap widens, the maximum pressure decreases because of the smaller resistance to flow over the flight tip. The lower pressure reduces the amount of flattening of the velocity profiles. The curvature of the second velocity profile changes from convex to concave. The flow rates in the centre elements for different tip gaps calculated from approximation #4 are given in Table 1. The total flow rate increases by a factor of 4 for an increase in tip gap of a factor of 5. Both the forward flow increases and the back flow decreases with increasing tip gap.

TABLE 1. FLOW RATES AND AVERAGE VISCOSITIES IN THE CENTRE ELEMENTS OF THE FLOW CHANNEL AND MAXIMUM PRESSURES

Approximation	Flow ($\text{m}^3/\text{s} \times 10^5$)			Viscosity (Pa)	Max Pressure (MPa)
	Total	Forward	Reverse		
#1	2.62	26.40	23.80	5000	30.80
#2	2.79	26.40	23.80	466	1.17
#3	15.10	23.20	8.03	625	1.52
#4	2.90	19.40	16.50	577	1.65
#3 (Average μ from average shear rate)	24.00	27.30	3.34	511	1.31
Tip Gap 0.5 mm					
#4	8.22	21.70	13.50	611	0.96
Tip Gap 1.0 mm					
#4	11.80	26.40	8.36	670	0.56

Study of the velocity profiles calculated using Approximation #4 indicates where the maximum stresses are developed, and where viscous heat generation would be greatest. In the flight tip gap the site of maximum shear and heating is near the tip and away from the wall. In the channel the shear is highest near the barrel, and this has a shorter path to the barrel wall, and so should aid heat transfer from the propellant material to the circulating coolant in the barrel.

It can be seen that plug flow occurs in the lower part of the channel, and mixing is confined to the upper layers in the channel. This type of flow has been seen in flow visualisation studies of kneading blocks(ref.3). Forward and reverse kneading blocks with a staggering angle of 30° showed unmixed areas in the centre of the flow. Flow in these blocks would resemble the situation modelled here, where the staggering angle is effectively 0° .

4. CONCLUSIONS

A simplified method of modelling the 2 dimensional flow of propellant materials in a kneading disc of a SME has been developed. The model uses more accurate approximation methods than used previously for calculating the non-Newtonian flow shown by propellant materials. The model also includes a multiplicative factor which was omitted from previous work. The method should be applicable to modelling the 3 dimensional flow in kneading blocks and conveying screws.

5. ACKNOWLEDGMENTS

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APPENDIX I

DERIVATION OF FINITE DIFFERENCE EQUATIONS

I.1 Pressure profile in the Newtonian approximation

The flow rate Q in the x_2 direction of a Newtonian fluid with viscosity μ between 2 parallel plates a distance H apart and moving with a relative velocity V_3 is given by

$$Q = V_3 \cdot \frac{H}{2} - \frac{H^3}{12\mu} \cdot \frac{\partial P}{\partial x_3} \quad (6)$$

where $\partial P / \partial x_2$ is an applied pressure gradient.

In the flow channel defined by figure 2 there are no sources or sinks for flow, so the total flow into any element must equal the flow out of the element. In particular for the l 'th element the flow in, $Q(l-1)$, must equal the flow out, $Q(l)$, see figure 4. The flows are evaluated at the edges of the elements, so the variables associated with the flow must be evaluated at the same points. These variables include $H(l)$, $v_3(l)$.

The differential equation (6) is solved by converting it to a finite difference equation. Separate equations are set up for flows into and out of each element, and these are equated. Hence

$$Q(l-1) = Q(l) \quad (1.1)$$

and

$$V_3(l-1) \cdot \frac{H(l-1)}{2} - \frac{H(l-1)^3}{12\mu} \cdot \frac{\partial P(l-1)}{\partial x_2} = V_3(l) \cdot \frac{H(l)}{2} - \frac{H(l)^3}{12\mu} \cdot \frac{\partial P(l)}{\partial x_2}$$

Converting this equation to a difference equation gives

$$\begin{aligned} & \frac{(H(l) + H(l-1))}{2} \cdot \frac{V_3}{2} - \frac{((H(l) + H(l-1))/2)^3}{12\mu(l)} \cdot \frac{(P(l) - P(l-1))}{DX(l) + DX(l-1)} \cdot 2 \\ &= \frac{(H(l+1) + H(l))}{2} \cdot \frac{V_3}{2} - \frac{((H(l+1) + H(l))/2)^3}{12\mu(l+1)} \cdot \frac{(P(l+1) - P(l))}{DX(l+1) + DX(l)} \cdot 2 \end{aligned}$$

where $DX(I)$ is the length of the I 'th element. Variable element lengths are used for modelling the 2 dimensional disc to help overcome convergence problems near the flight tips. This complication should not be necessary in modelling 3 dimensional kneading blocks because the flow gradients near the flight tips should not be as great.

Multiplying through gives,

$$\begin{aligned} & \left\{ \frac{((H(I+1) + H(I))/2)^3}{6\mu(I+1) \cdot (DX(I+1) + DX(I))} \right\} \cdot P(I+1) \\ & - \left\{ \frac{((H(I+1) + H(I))/2)^3}{6\mu(I+1) \cdot (DX(I+1) + DX(I))} + \frac{((H(I) + H(I-1))/2)^3}{6\mu(I) \cdot (DX(I) + DX(I-1))} \right\} \cdot P(I) \\ & + \left\{ \frac{((H(I) + H(I-1))/2)^3}{6\mu(I) \cdot (DX(I) + DX(I-1))} \right\} \cdot P(I-1) = \frac{(H(I+1) - H(I-1))}{4} \cdot V_3 \end{aligned}$$

and hence,

$$\begin{aligned} & \left\{ \frac{(H(I+1) + H(I))^3}{12\mu(I+1) \cdot (DX(I+1) + DX(I))} \right\} \cdot P(I+1) \\ & - \left\{ \frac{(H(I+1) + H(I))^3}{12\mu(I+1) \cdot (DX(I+1) + DX(I))} + \frac{(H(I) + H(I-1))^3}{12\mu(I) \cdot (DX(I) + DX(I-1))} \right\} \cdot P(I) \\ & + \left\{ \frac{(H(I) + H(I-1))^3}{12\mu(I) \cdot (DX(I) + DX(I-1))} \right\} \cdot P(I-1) = [H(I+1) - H(I-1)] \cdot V_3 \end{aligned} \quad (1.2)$$

This set of N equations for all the elements has a tridiagonal form, viz:

$$A(I) \cdot P(I-1) + B(I) \cdot P(I) + C(I) \cdot P(I+1) = G(I), \quad I = 1, N \quad (1.3)$$

Since the number of equations is relatively small, they can be solved by an efficient direct substitution technique(ref.14). The boundary conditions are determined by the cyclic nature of the geometry. The value of the pressure in the 0'th element is the same as for the $N + 1$ st element, and when these

conditions are fed into the equations, a solution is possible. However the absolute magnitude of the pressure is not determined, and so a constant is added to the calculated pressures to give zero pressure in the center of the flight tip.

1.2 Solution of the differential equation for velocity

The velocity profile can be calculated from the differential equation describing flow,

$$\frac{\partial P}{\partial x_3} = n \cdot k \cdot \left\{ \frac{\partial v_3}{\partial x_2} \right\}^{(n-1)} \cdot \frac{\partial^2 v_3}{\partial x_2^2} \quad (9)$$

where $\partial p / \partial x_3$ is known. This equation is a second order differential equation, and can be readily solved by finite difference methods.

The difference equation is derived in the following way. The first derivatives are given by

$$\frac{\partial v_3(x_2)}{\partial x_2} \approx \frac{v_3(j+1) - v_3(j)}{dx_2} \quad \text{for } x_2 > x_2(j)$$

and

$$\frac{\partial v_3(x_2)}{\partial x_2} \approx \frac{v_3(j) - v_3(j-1)}{dx_2} \quad \text{for } x_2 < x_2(j)$$

where dx_2 is the step in the x_2 direction between $x_2 = (j+1)/H$ and $x_2 = j/H$. The step size is uniform in this case. The second derivative of v_3 is the derivative of the first derivatives,

$$\begin{aligned} \frac{\partial^2 v_3(x_2)}{\partial x_2^2} &\approx \left\{ \frac{v_3(j+1) - v_3(j)}{dx_2} - \frac{v_3(j) - v_3(j-1)}{dx_2} \right\} \\ &= [v_3(j+1) - 2v_3(j) + v_3(j-1)] / dx_2^2 \end{aligned} \quad (1.4)$$

For the j 'th level in the i 'th element equation (9) becomes

$$v_3(j+1) - 2v_3(j) + v_3(j-1) = dx_2^2 \cdot \frac{1}{\mu(l,j)} \cdot \frac{[P(l+1) - P(l)]}{[DX(l+1) + DX(l)]/2} \quad (1.5)$$

These equations have the tridiagonal form of equations (1.6), and they are solved in the same way.

1.3 Calculation of the pressure profile from the velocity profile

Equation (9) is used to calculate the pressure profile, ie,

$$\frac{\partial P}{\partial x_3} = n \cdot k \cdot \left\{ \frac{\partial v_3}{\partial x_2} \right\}^{(n-1)} \cdot \frac{\partial^2 v_3}{\partial x_2^2} \quad (9)$$

The corresponding difference equation is a rewritten form of equation (1.6)

$$P(l+1) - P(l) = \frac{[v_3(j+1) - 2v_3(j) + v_3(j-1)]}{dx_2^2} \cdot \mu(l,j) \cdot [DX(l+1) + DX(l)]/2$$

Since the values of velocity $v_3(l)$ and viscosity $\mu(l)$ are known from the previous iteration, the values of the pressure increments between elements, $P(l+1) - P(l)$, can be calculated. The pressure profile $P(x_3)$ is obtained by successively adding $P(l+1) - P(l)$ to the previously calculated pressure $P(l)$ to give the ordinate, and adding $(DX(l+1) + DX(l))/2$ to the previously calculated x_3 to give the abscissa. The starting point is

$$(P(0), x_3(0)) = (0,0).$$

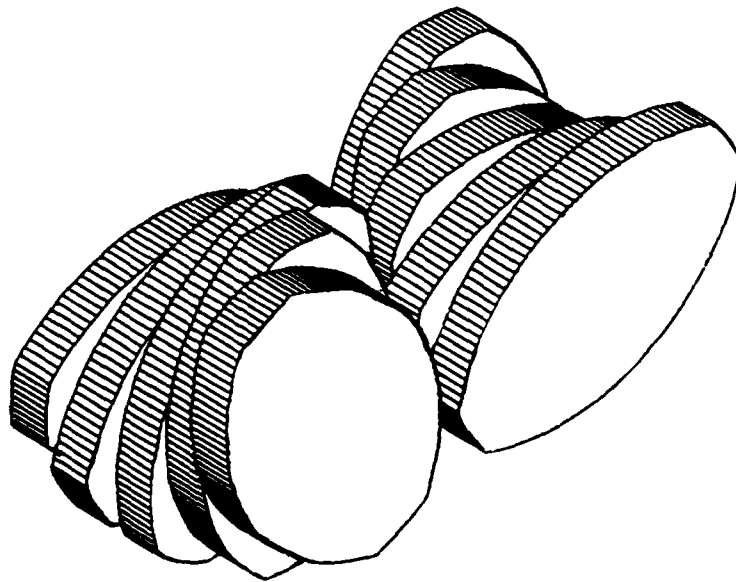


Figure 1. Intermeshing kneading blocks

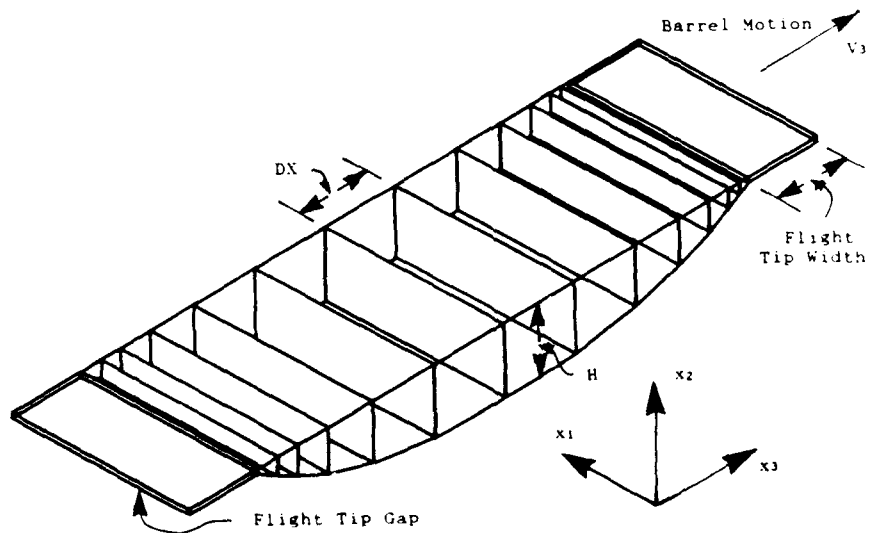


Figure 2. Geometry of opened out flow channel for modelling

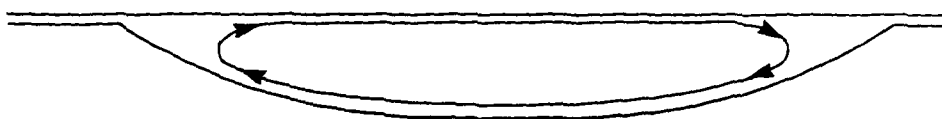


Figure 3. Circulating flow in the channel

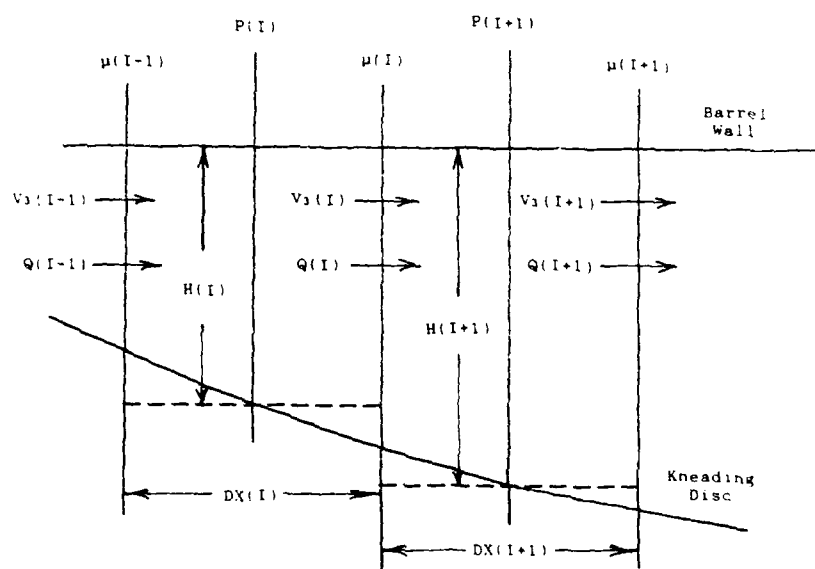


Figure 4. Quantities involved in flow in elements I and I+1

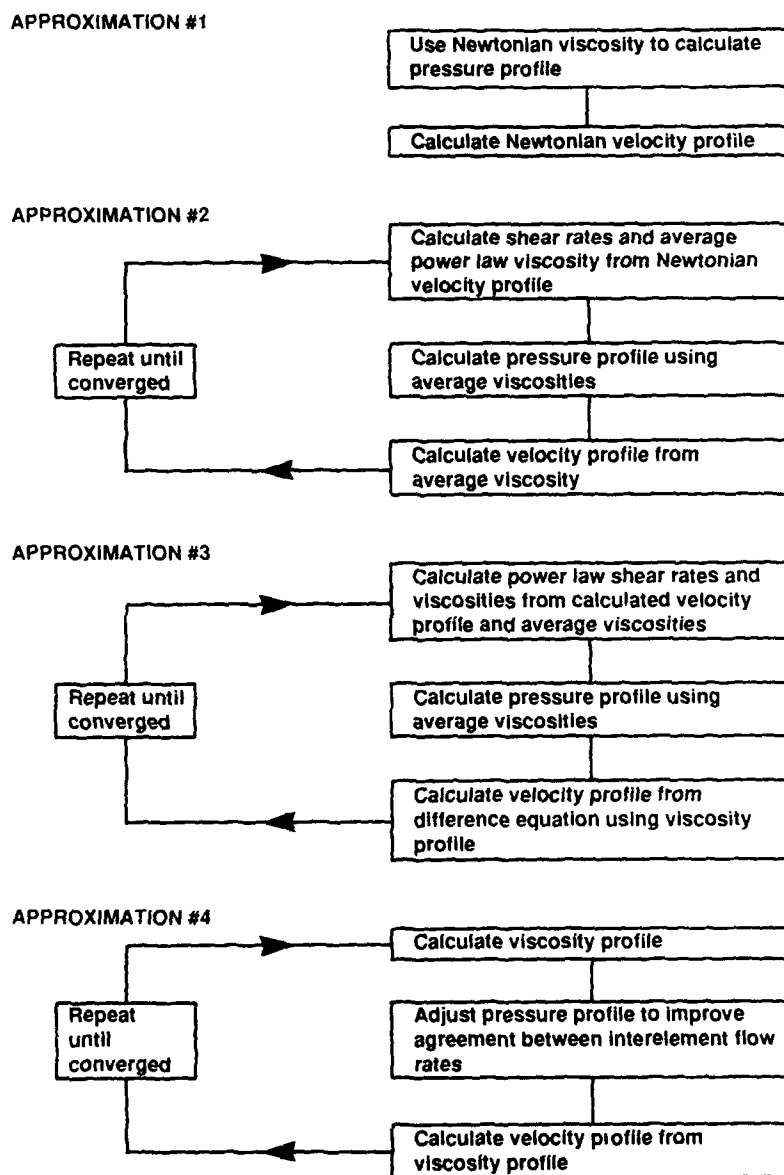


Figure 5. Flow diagram of the solution process for the equations of flow

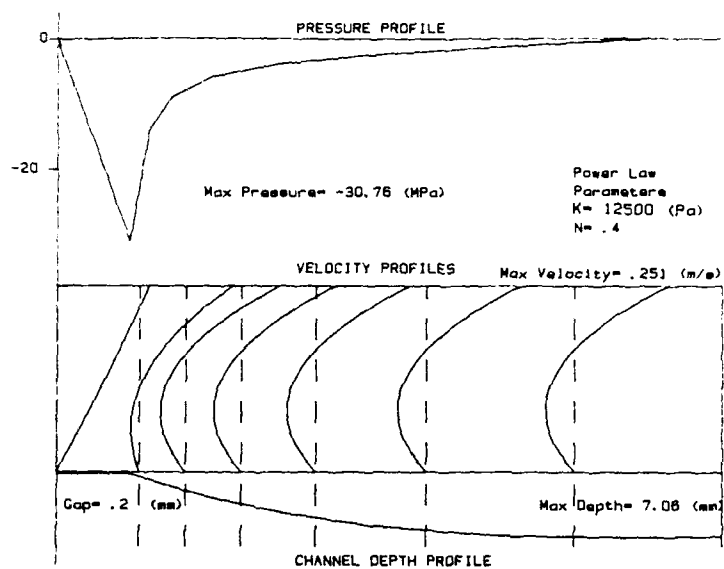


Figure 6. Pressure, velocity and channel profiles calculated from Approximation #1

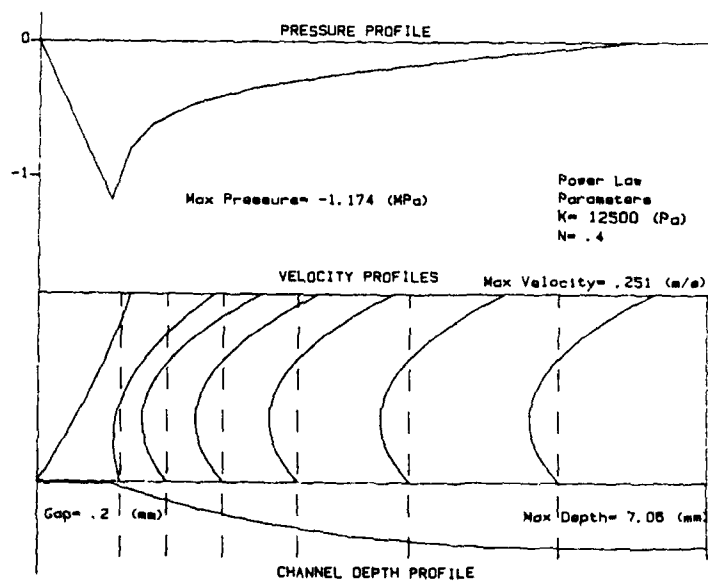


Figure 7. Pressure, velocity and channel profiles calculated from Approximation #2

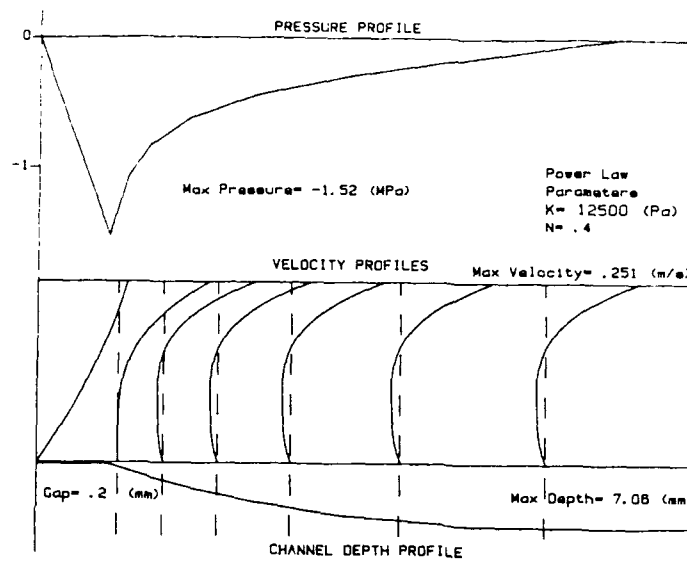


Figure 8. Pressure, velocity and channel profiles calculated from Approximation #3

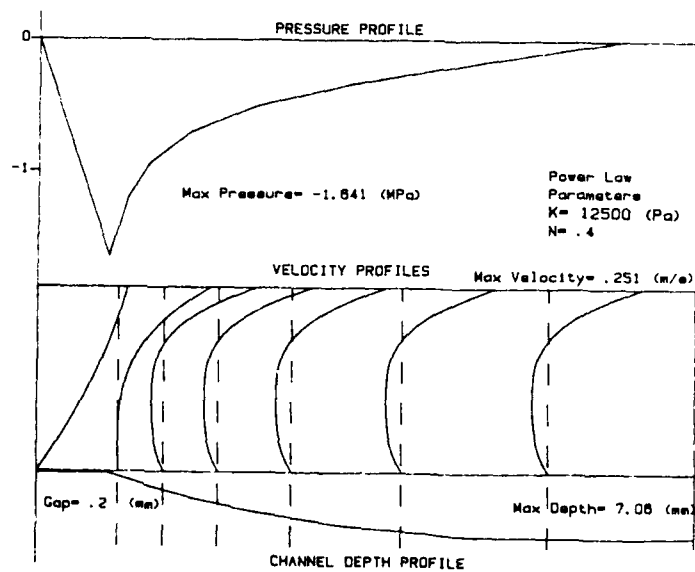


Figure 9. Pressure, velocity and channel profiles calculated from Approximation #4

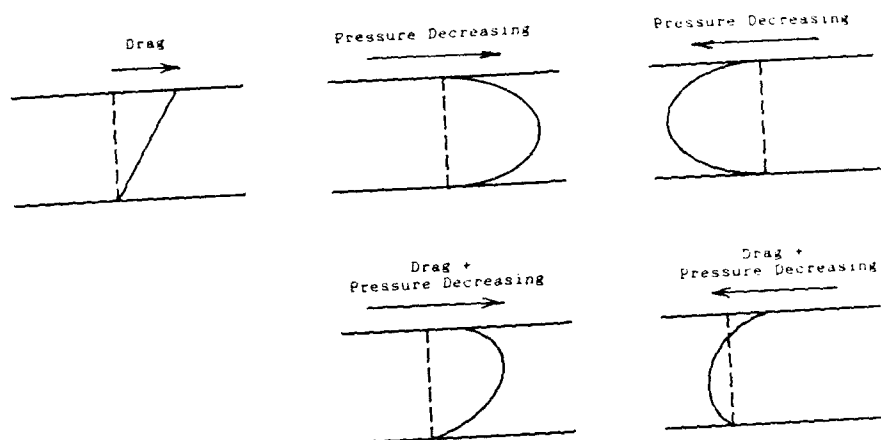


Figure 10. Schematic representation of the combination of drag and pressure flows

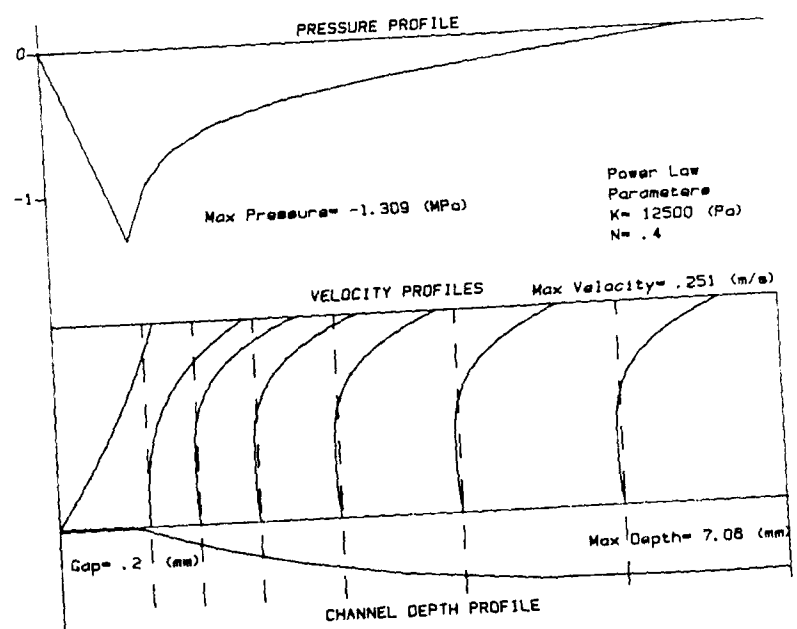


Figure 11. Pressure, velocity and channel profiles calculated from Approximation #1 with the average viscosity calculated from the mean shear rate

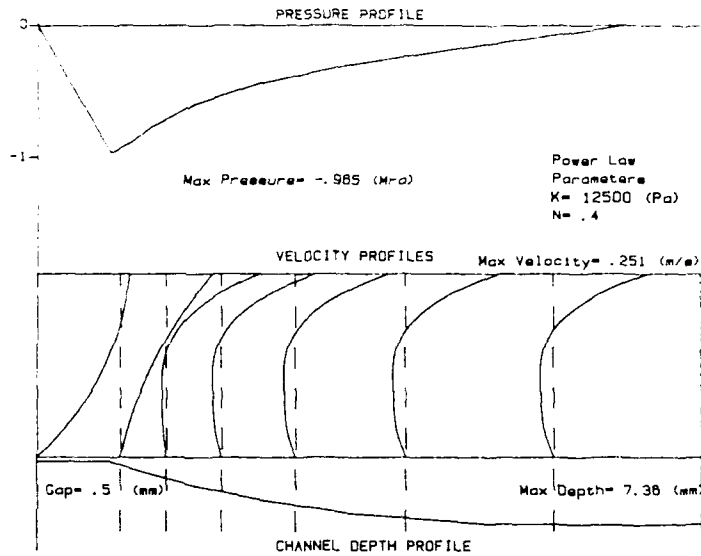


Figure 12. Pressure, velocity and channel profiles calculated from Approximation #4 with a flight tip gap of 0.5 mm

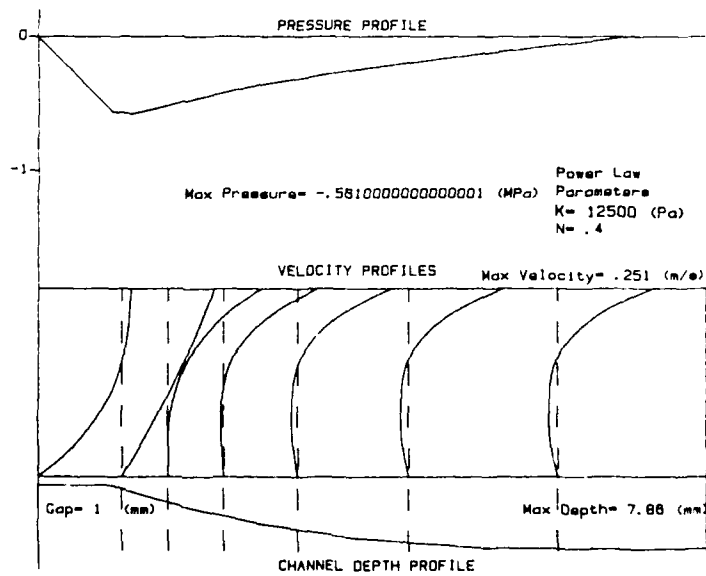


Figure 13. Pressure, velocity and channel profiles calculated from Approximation #4 with a flight tip gap of 1.00 mm

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15 DESCRIPTORS

a. EJC Thesaurus
Terms

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Non-Newtonian fluids

b. Non - Thesaurus
Terms

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16 COSATI CODES

2005

17 SUMMARY OR ABSTRACT

(if this is security classified, the announcement of this report will be similarly classified)

(U) A simplified method of modelling 2 dimensional flow of propellant doughs in a kneading disc of a twin screw mix-extruder (SME) has been developed. The 2 dimensional model is a first step in the development of a full 3 dimensional model of flow in screws and kneading blocks in SMEs. The model is based on the FAN method of Tadmor as modified by Szydlowski et al, and it aims to use less computational effort than alternative models based on finite element analyses. Apart from one model for non-Newtonian fluids, which has several serious flaws, the existing models have assumed that the viscosity of the fluid was Newtonian. The model presented here gives a better method of calculating the flow of non-Newtonian fluids than the previous method, and it produces more realistic flow velocity profiles.

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