3-D Comsol Analysis of Extruder Dies

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Abstract: Three-dimensional flow analysis was performed by using COMSOL Multiphysics chemical module for the propose of analyzing the flow properties and finding out the operating points of a test domain. The test domain chosen was the exact replica of the die within the Arcada laboratory where the maximum output of the extruder screw was predetermined. Using material property table for an exemplary melt of LDPE obtained from borealis Ltd., the logarithmic viscosity-shear rate graph was plotted and fitted to the 4-constant modified Careau constitutive flow model for numerical analysis of the viscosity. The parametric solving method was chosen with reasonable pressure values to help with the convergence of the iteration. The resulting velocity, pressure and shear rate profiles within several cross-sections of the die were obtained as a contour plots. These computed results were then compared to both the theoretical and experimental findings. The comparison suggested that the software is able to estimate the flow domain effectively and can be used to compute operational points for any profile die flow domain.

Keywords: COMSOL, Die design, Zero shear viscosity

1. Introduction
The design procedure of dies, unlike other parts of machine components, was considered as an art rather than science. The usual traditional methods of design depends on numerous trial-and error loops, mainly relying on the designer’s experience. However, the advancements in fields like mechanical, chemical and material engineering have made it easier to visualize the flow and set the parameters required in such a complex design. The recently developed software packages for mathematical modelling of polymer flows, makes the trial-and-error procedure a lot shorter. [1] The main objective of this study is to achieve efficient design modelling method that predicts the operational variables of the melt flow through the cavities of the die.

2. Governing Equations

2.1 Continuity equation
The mathematical flow analysis is obtained from the general equations for conservation of mass, momentum and energy. These equations combined with the material equation are used to define flow using velocity vector and thermodynamic data (pressure, temperature, specific volume). [2] With assumption of incompressibility of the melt (constant density), thus the above formula can be simplified to

\[ \nabla \cdot \mathbf{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0 \]

(1.1)

2.2 Restrictive assumptions and boundary conditions
In analysing melt flow, solving the above systems of conservation equations is not straightforward calculation. Some important assumptions to simplify the derivations are needed. However, care must be given to the resemblance of the assumption and the reality to solve these problems accurately. Most important assumptions for extrusion die design are given below [2];

- Steady state flow-no back ward flow
• Slow moving flow-inertia of the melt is neglected
• Isothermal flow-the whole melt have the same temperature
• Incompressible flow-the density is constant
• No external force including effect of gravity
• No wall slip in other words wall adhesion under reasonable shear stress range.
• Constant pressure difference in the channel.
• Convection in the flow direction is more dominant than conductive heat transfer.
• Heat transfer perpendicular to the flow direction occurs due to conduction. The temperature of the melt at the wall is equal to the wall temperature.

When a uniform velocity is considered as in the assumption, the above equation will be reduced to \( \sum F = 0 \). Hence it is simplified to obtain the pressure drop and shear forces on the system from the reduced conservation equation, boundary conditions and the material law (i.e. \( f = f(\dot{\gamma}) \)). By integrating the introduced boundary conditions to equation (2.18) the velocity functions, flow rate, forces occurring at channel walls and pressure drop \( \Delta p \) can be obtained. [1]

3. Theory;
Drag flow: is flow between two surfaces caused by the movement of one relative to the other. Assuming none slipping of melts, the fluid is literally dragged by the moving walls of the screw and the barrel. [3]

Drag flow \( (Q_d) = \frac{1}{2} \pi^2 \dot{\gamma} N \sin \theta \cos \theta \)  
(3.1)

Pressure flow: is the kind of flow only noticed when the die or the head is present. It is a flow caused by a pressure difference. This flow occurs in the metering zone of the screw is characterized by the back ward flow of materials down the screw channel. This scenario is symbolized as \( Q_p \).

\[ Q_p = \Delta p \frac{k}{\mu} \]  
(3.2)

Where \( k \) is a function of the geometry for a given die (e.g. capillary, annulus, or slit).

![Figure 1. Operational point in Extrusion](image)

4. Methods;
In this study a 3-dimensional flow analysis for an existing die was successfully investigated using COMSOL Multiphysics software. The operational point of a die was obtained and the results were compared to both theoretical and experimental values of the operating point values of the die. This enhances the current operation point calculation by including the most realistic temperature dependent varying viscosity values instead of just using a constant viscosity. The non-Newtonian module of the software was used to study the flow of an exemplary material LDPE at 220 Degree Celsius. The model used was an exact replica of the 2 holes capillary die in Arcada University of Applied Science. The material data for LDPE was obtained from the manufacturer to plot the logarithmic viscosity-shear rate graph. After retrieving the necessary rheological information of the polymer melt, it was fitted to the Carreau-Yasuda viscosity model. Using the extruder maximum output value as an input value for the initial sub-boundary condition the pressure was solved using the parametric solver. The results were compared to the continuity equation and the pressure which fulfils the condition was identified.

5. Numerical Model;
After having the necessary information about the rheology of the polymer at hand, the next step was to study the 3-D model analysis of the flow geometry for an exemplary actual die in the
Arcada workshop. The purpose of this model was to visualize the viscosity and pressure distribution of the flow domain. And most importantly to compare the result of the simulation to the real value of the operating point.

The 3-D FEM analysis for the flow of LDPE was done using the COMSOL Multiphysics, non-Newtonian (Chemical Engineering Module). After re-modelling the existing die in the Solid edge 3D software, the Boolean feature was used to obtain the flow domain of the melt. Then the resulting model was imported to COMSOL software work station. In order to do this the solid edge file had to be saved as .stl file format.

5.1 Parametric
This is the most important part of the modelling where the parameters for solving any complicated function are defined. In this case, the aim of this model is to solve for the pressure drop in the die. Since the pressure at the outlet is zero, finding the operating pressure, $p_{in}$, at the inlet of the die is sufficient.

To help the convergence of the solution and reduce solution time and error of the iteration, a range of arbitrary but reasonable $p_{in}$ parametric values were inserted. An approximated range for $p_{in}$ values of 400 kPa to 2.8 MPa with a sweep of 400 kPa was chosen as a range since that is extruder common operating range.

5.2 Subdomain setting
Another important input in the subdomain setting of the model is the initial domain value. At this stage of the model, the only known flow value is the maximum output of the extruder without any resistance of the die (i.e. $Q_{max}$ for an open discharge). Thus, it is easier to visualize this scenario assuming the die as a closed boundary where the initial flow $Q_{max}$ entered and the effect of resistance of the die and the pressure flow will be calculated by the software and the resulting fully developed flow $Q$ is obtained as the operating flow throughout the domain.

The value of initial velocity in the $x$ direction (in the direction of flow) was calculated from a quantity of melt discharged due to the drag flow of a screw rotating at $N=15$ rpm, barrel diameter $D=0.0175$ m and channel depth $H=0.004$ m. Using equation [30] the value of $Q_{max}$ was obtained by substituting this values in equation (3.1).

6. Result and Discussion

6.1 Post processing
The parametric solver solves the different inputs values of pressure in an ascending order. And hence, the value of $p_{in}$ solved last (the highest value) will be displayed as a contour plot by default as the software converges.

![Figure 2](image)

**Figure 2.** Pressure distribution in the die

The above figure shows a condition when $p_{in}$ value is equal to 28 MPa. This figure does not necessarily imply that this value of 28 MPa is the value of operating pressure. For a pressure to be an operating point pressure it should deliver a uniform quantity of melt complying with the assumption of fully developed and uncompressible flow. In other words, when the operating pressure is applied the flow should obey the continuity equation given in equation (1.1). Thus, for a uniform flow, the ratios of the inlet velocity to the outlet velocity should be
equal to the ratio of the outlet area to the inlet area in the direction of flow. The area ratio of the die was measured to be of a value 8.3. Thus, the operating pressure velocities will have ratio of \( \frac{V_{in}}{V_{out}} = 0.3 \)

And similar procedure is made for the other \( p_{in} \) values and the velocities were compared.

\[ \text{Figure 3. Velocity distribution at 20 MPa} \]

Figure 3 shows a velocity distribution with a quite close velocity ratio of 8.2. Thus implies the flow at this pressure is stabilized and continues. Thus, it can be used as the operation pressure for this condition.

The next step after finding the operating pressure is to calculate the corresponding operating point output.

The operating flow \( Q \) velocity at the exit*outlet area =
\[
(8.2 \times 10^{-2} \text{ m/s}) \times (1.59 \times 10^{-5} \text{ m}^2) \\
= 1.3 \times 10^{-5} \text{ m}^3/\text{s}
\]

As in the continuity assumption, \( Q = \) velocity at the inlet*inlet area
\[
(1 \times 10^{-2} \text{ m/s}) \times (1.33 \times 10^{-4} \text{ m}^2) \\
= 1.33 \times 10^{-6} \text{ m}^3/\text{s}
\]

As can be seen from the above calculation the value of \( Q \) is less than the \( Q_{max} \) value \( 2.3 \times 10^{-6} \text{ m}^3/\text{s} \) which was entered as an initial condition in the sub boundary settings.

This result shows that the percentage of the actual flow to the drag flow through flow domain is:

\[ (1.33/2.3) \times 100\% = 57.78\% \]

This result implies the rest 42.22\% is a pressure flow.

\[ \text{Figure 4. Pressure drop across symmetry line of the die} \]

Figure 4 shows a particle tracing pressure curve plotted for a particle of melt flowing through the central part of the die where the pressure drops from an initial value of 20 MPa which rapidly continues to decrease until it reaches the wall that divides the flow to the cylindrical outlets. Then a small amount of rise in pressure occurs due to build up pressure flow of the melt.

\[ \text{Figure 5. The operating pressure distribution} \]

Other interesting results that can be observed from this model are the dynamic viscosity and shear rate values throughout the flow range.
Figure 6. Dynamic viscosity curve

Figure 7. Shear rate distribution curve

Figure 6 and 7 shows the inverse proportionality of shear rate and viscosity. The dynamic viscosity drops from a value of around 1400Pa.s to a 6.2 times lower value of 225Pa.s while the shear rate rises from around 10/s to 650/s as the flow enters the cylindrical channels.

8. Result Comparison

The experimental output value when extruding at 220 Degree Celsius and 30\(\pi\) was found to be \(9.4 \times 10^{-7}\) m\(^3\)/s.

Comparing the result of the operating output computed in this study, \(1.3 \times 10^{-6}\) m\(^3\)/s, to the experimental result;

\[\frac{13}{9.4} = 1.38\]

This indicates that the computed value is 1.38 times higher than the experimental result.

The experimental value is 30% lower than the simulated result of the model. The experimental value suggests that the die was able to extrude at the rate of \(9.4 \times 10^{-7}\) m\(^3\)/s from quantity of \(2.3 \times 10^{-6}\) m\(^3\)/s melt supplied by the extruder screw. That is,

\[
\frac{(23-9.4)}{23} = 59.1\%
\]

This indicates that the die has extremely high resistance. This could be a result of impurities or temperature difference of the die and the metering zone of the screw. The fact that the operating pressure of extruder could not be measured makes this result comparison less realistic.

Another comparison was made with a theoretical calculation of the operational points for the same.

Figure (8) shows an operating pressure and output value of 11 MPa and 1.75 \(\times 10^{-6}\) m\(^3\)/s respectively. These values were obtained using the power law model assuming the viscosity to be constant.

Thus, comparing to the result obtained from this study,

- Operating pressure of 20 MPa and corresponding operating output value of \(1.33 \times 10^{-6}\) m\(^3\)/s

which was evidently close result.
4. **Conclusion**

In this study a 3-dimensional flow analysis for an existing die was successfully investigated using COMSOL Multiphysics software. The operational point of a die was obtained and the results were compared to both theoretical and experimental values of the operating point values of the die.

This enhances the current operation point calculation by including the most realistic temperature dependent varying viscosity values instead of just using a constant viscosity.

The non-Newtonian module of COMSOL Multiphysics software was used to study the flow of an exemplary material LDPE at 220 Degree Celsius.

8. **References**