March 6, 2003

Scintillator Extrusion and Die Design Project for NICADD/Fermilab

Progress Report (by M. Kostic)

- **Learning and understanding PolyFLOW software features and numerical simulation:**
  - **With and w/out INERTIA terms simulation**
  - **Quantity and QUALITY of meshing**
  - **Comparing PolyFLOW with FLUENT and/or other Refs.**
- **Learning fundamentals of polymer dynamics and heat transfer**
  - **Understand wall- and average-shear rates in non-uniform velocity field**
  - **Calculate f & Nu values (wall- and bulk-averages) from CFD velocity and temperature fields independently from CFD software (using Excel for example)**
  - **Evaluate CFD simulation against well-established reference data (including Newtonian flow and HT)**
- **Polymer Properties:**
  - **Dow-Chemical Styron: limited shear-rate range viscosity**
  - **AltAir (HyperXtrude) report: inconsistent model and graph data**
  - **No full-range data available for actual Styron used**
  - **Viscoelastic properties?**
- **Die Design and Geometry meshing:**
  - **2-D die-lip with free-surface flow is first approximation**
  - **3-D actual die geometry simulation is a MUST**
  - **Mechanical die design (ProE) and “blueprints”**

A Finite Element Simulation of Flow of Polymer in an Extrusion Die Using PolyFLOW®
A Preliminary Report (March 6, 2002)

Executive Summary

by Prof. M. Kostic's group: Most work done by Srinivasa Vaddiraju with help from Dan Wu.

In this report, we present the results related to the Finite Element Analysis of flow of Carreau model polymer through a profile 3-D extrusion die. The analysis was performed using Fluent's PolyFLOW, a CFD application software. The desired extruded profile is a rectangular cross section with a single circular hole at its center. The analysis performed was based on the available information till date.

A replica of an existing die at Fermi Lab was reproduced using Pro-e. Various flow simulations of extrusion through the die were performed using the dimensions of the existing die in Fermi Lab, the process conditions given by Fermi Lab, and material data provided in Altair Inc. report. The desired output profile of the extrudate in this case is a rectangular cross section with a single circular hole at the center. The profile of the die-land length is an irregular rectangular cross section with an elliptical-like hole at its center so as to give the desired output shape. The polymer flows through the extruder barrel and is pushed out under pressure through a 3-D die with non-uniform (varying) cross sections. Here, the question arises, "How will the final result depend on the upstream flow and heat transfer conditions, and for what die portions the simulation has to be performed?"

The flow through the entire die was divided into two portions, one through converging and diverging portion (section 1) and the other through die transition (sections 2 & 3). The converging and diverging section is not symmetric about both axes, so the complete portion is taken into account for flow simulation. The outlet velocity hence obtained is also not symmetric about both axes. As the polymer enters the die at 466 K and the die walls are maintained at that temperature, no heat transfer takes place during the flow and the temperature is maintained constant. Shear rates of less than 47 sec^{-1} are encountered during the flow.

Next the simulations were performed by taking the whole section of the die transition into account. When the simulation is performed by considering only the die transition region, ignoring the flow occurred in converging and diverging sections, i.e., by taking the inflow condition as fully developed, the velocity profile at the inlet is different from the outlet velocity profile of the converging and diverging section. Various simulations were performed for the above two cases, i.e., one with neglecting the velocity profile from converging and diverging section and other by considering it. The geometries of the extruded profiles for the above two cases were compared, which shows a difference of 1 % in dimensions of final extrudate. Regardless that it is a small difference, it is still critical if the profile accuracy within about 0.1% tolerance is required. This preliminary trial shows that a quarter domain of the model of the die transition, by ignoring the velocity profile obtained from the converging and diverging sections, is sufficient for simulations only if 1% dimension differences could be tolerated. The temperature in the die is almost maintained at a temperature of 466 K and the polymer cools to 463 K in air as it exits the die. Shear rates of less than 230 sec^{-1} are encountered in the die but most of the flow occurs at shear rates of less than 30 sec^{-1}.

Various simulations were performed to show how the final shape of the extrudate depends on the velocity profile in the converging section of the die transition region (section 2). A simulation was also performed by considering the flow only in the die-land length (section 3) and giving the velocity profile at its inlet as fully developed, and then another simulation was performed by considering the flow both in the converging section and the die-land length (sections 2 & 3), so that the inlet velocity profile at the die-land length is not fully developed, but a more realistic one. The final shapes of the extrudate so obtained shows that a greater difference is possible if we neglect the converging section in die transition region.

Various simulations were performed to describe the effect of inertia terms in developing flows using PolyFLOW. The inertia terms can be neglected when the flow is fully developed, as all the terms related to inertia become negligible. But for developing flows, the inertia terms have considerable effect on the velocity profile. Various simulations have been performed for flow of water through square duct (for which a well-established data are available in the references) using PolyFLOW at different Reynolds numbers from 10 to 2000, by neglecting inertia terms and then by considering inertia terms, and the entrance length at which the flow becomes fully developed is observed, which showed that the error in neglecting inertia terms is less than 10 % at Reynolds numbers below 100 but the error increased to almost 100 % at Reynolds numbers above 500. This shows the importance of considering inertia terms in our case, where the flow is not necessarily fully developed.

The plots/values of polymer viscosity as a function of shear rate and temperature from the reports provided by Altair Inc, Dow's Chemical Company and the analytical values from various sources are compared. The Polymer used in Fermi National Accelerator Lab is Styron 663, a non-Newtonian viscoelastic incompressible melt. The best viscosity function for these types of polymers is Carreau model. Altair Inc. has provided some graphs of viscosity as a function of shear rate & temperature and values of parameters of Carreau model according to the properties of Styron 685d, which they claim to have similar properties to Styron 663. When graphs were plotted using their parameters, they are not in agreement with their graphs provided. A comparison was made between the graphs and percentage difference was calculated between the relative values, the maximum being 1170 %.

A set of values of viscosity as a function of shear rate have been supplied by 'The Dow Chemical Company' for Styron 663 at a temperature of 190 ^{0}C (463 K) for shear rates above 35 sec^{-1} . These values and the values of viscosity obtained by equation of Altair were plotted and the percentage difference between them was calculated, which showed a great difference, up to 80 %. From various references, any extrapolation performed using the viscosity values for shear rates above 35 sec^{-1}, to obtain the viscosity at lower shear rates may be extremely erroneous. This can be illustrated by the fact that the viscosity models of different fluids can be characterized by identical constants for values of shear rates above 1, yet they vastly differ at lower shear rates. Zero shear viscosity must be obtained experimentally and using the viscosity values above it, a good curve fit has to be made and the time constant and other parameters are treated as additional adjustable parameters. It is not required to obtain the values of infinite shear viscosity experimentally, as shear rates above 500 sec^{-1} are actually not encountered in flow though extruder die. It would be erroneous to predict the zero shear viscosity by taking the value of time constant. Prof. Maribel Vazquez, in his experiments to curve fit the viscosity model, has explained that the viscosity data obtained experimentally for shear rates of order of 10^{-2} sec^{-1} were good estimates of the zero shear rate viscosity. From the comparison of the values of viscosity as a function of shear rate provided by Altair Inc and Dow's Chemical Company, it is observed that the viscosity values at shear rates less than 35 sec^{-1} has to be measured experimentally to predict the exact values of parameters in Carreau model.

A thorough study of entrance flow and heat transfer of Newtonian fluids through a square duct was made to understand the fundamentals, for which well-established references data are available. The same phenomena were simulated using PolyFLOW and a detailed analysis was made, which helped in evaluation and limitation of the software.

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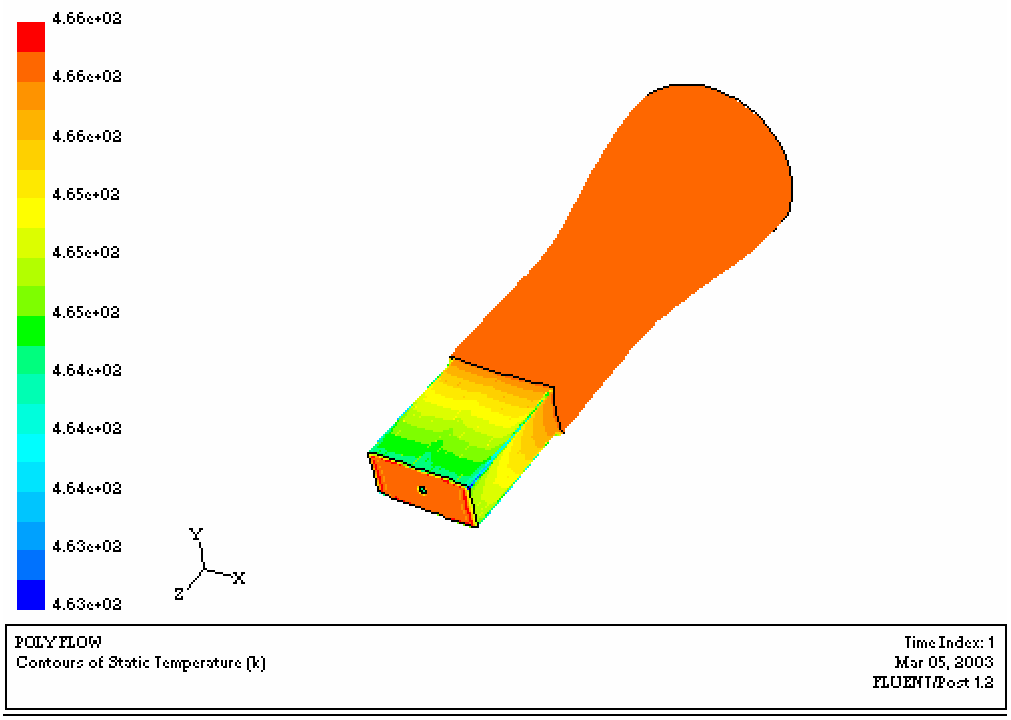

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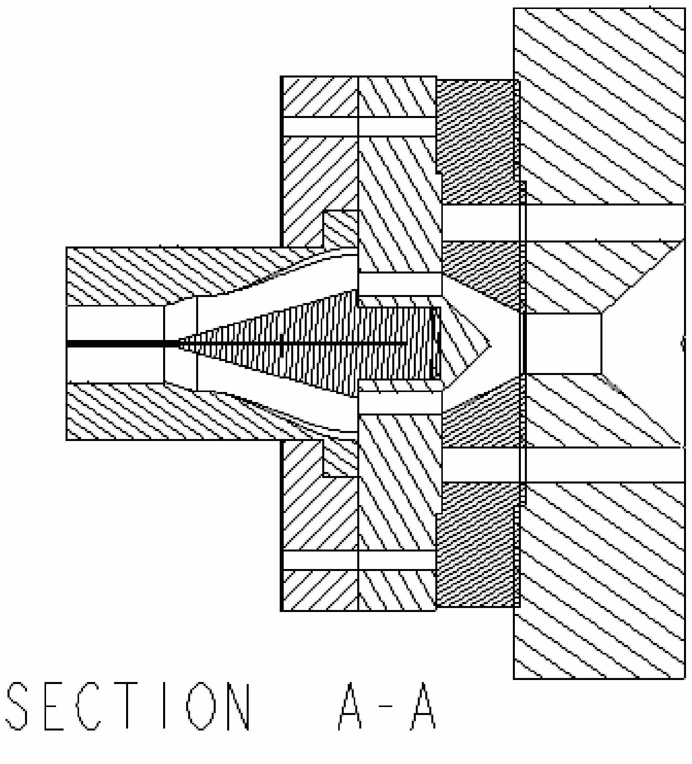
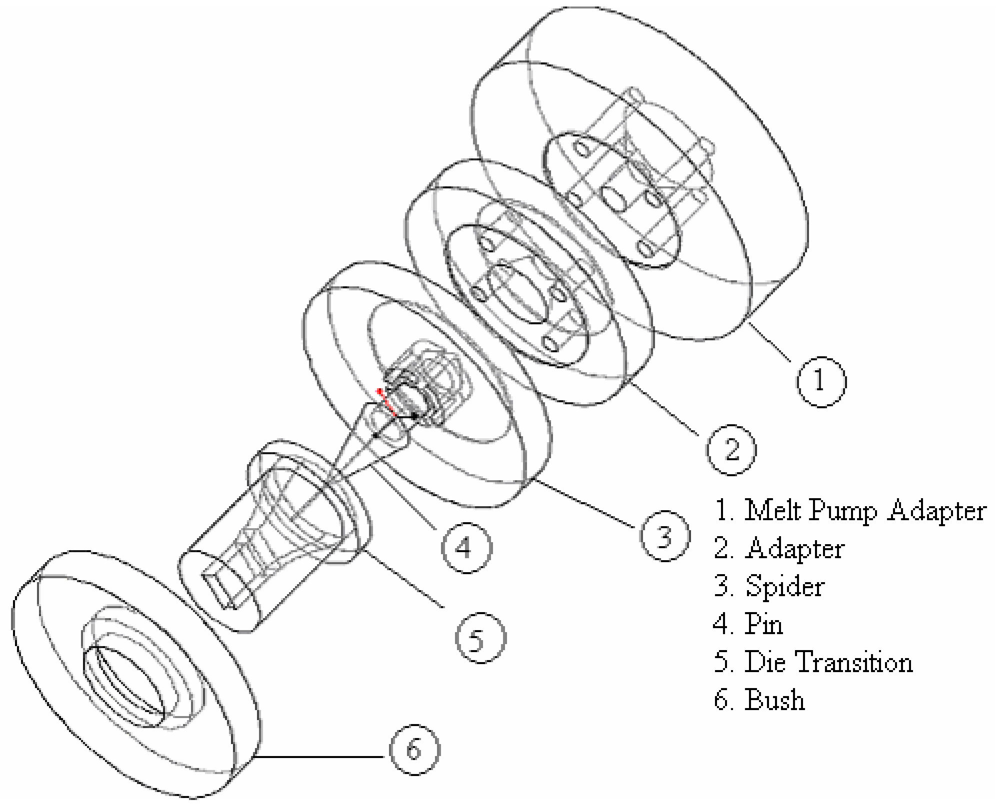
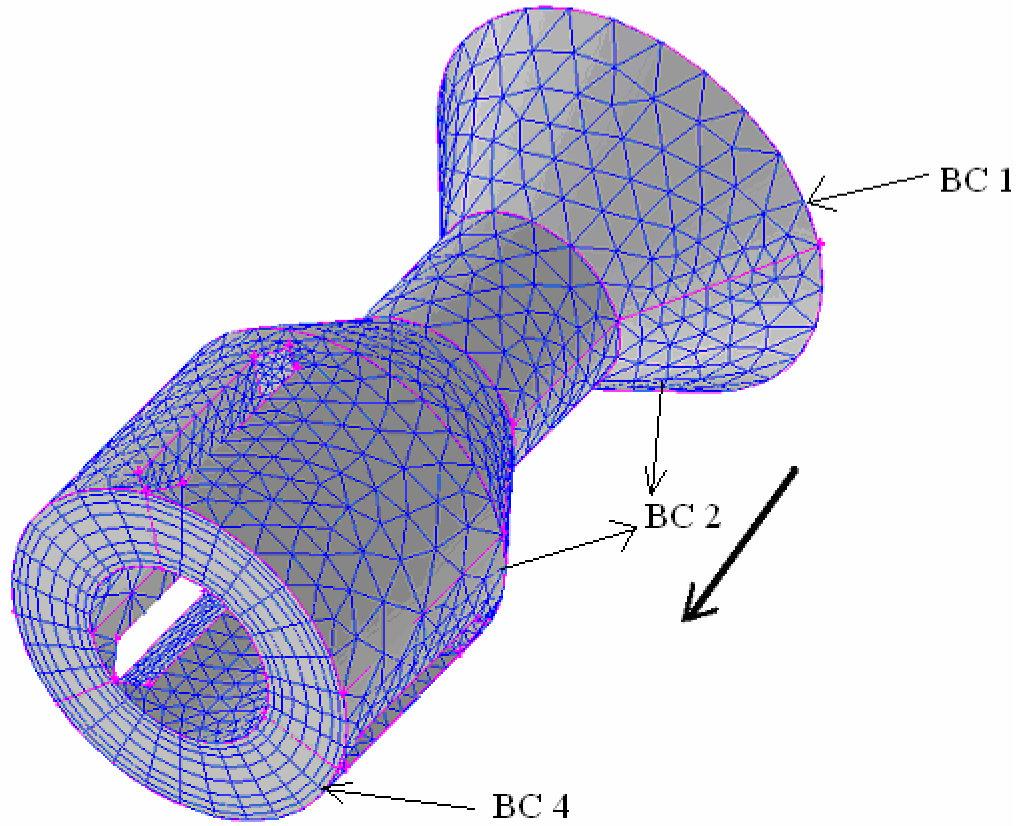


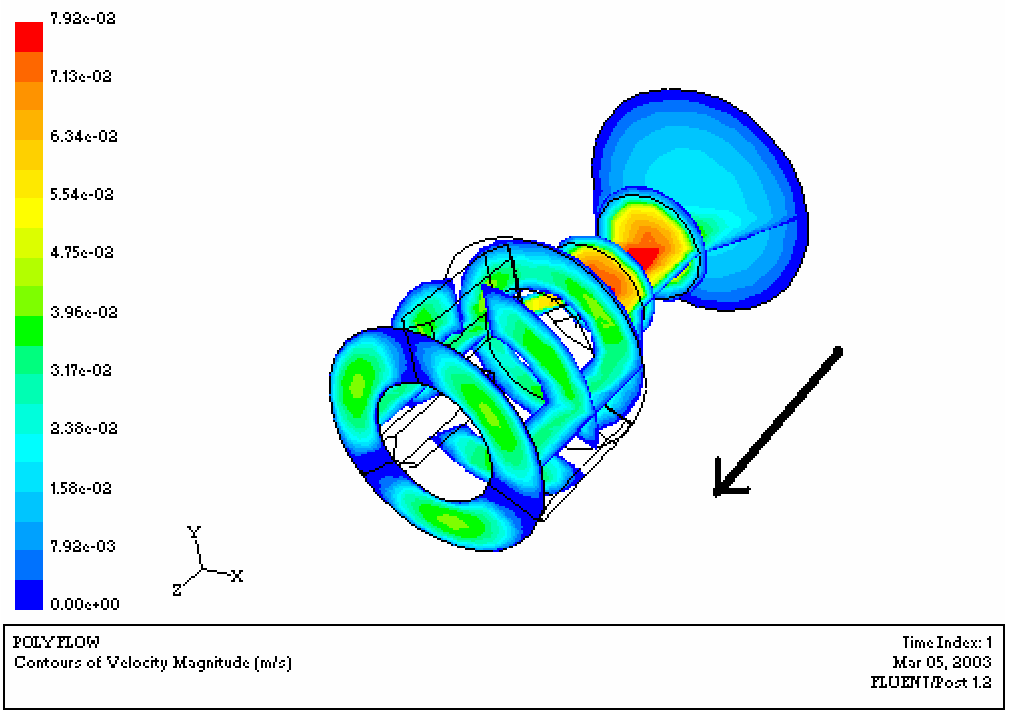
2-D Cross Sectional View of Complete Die



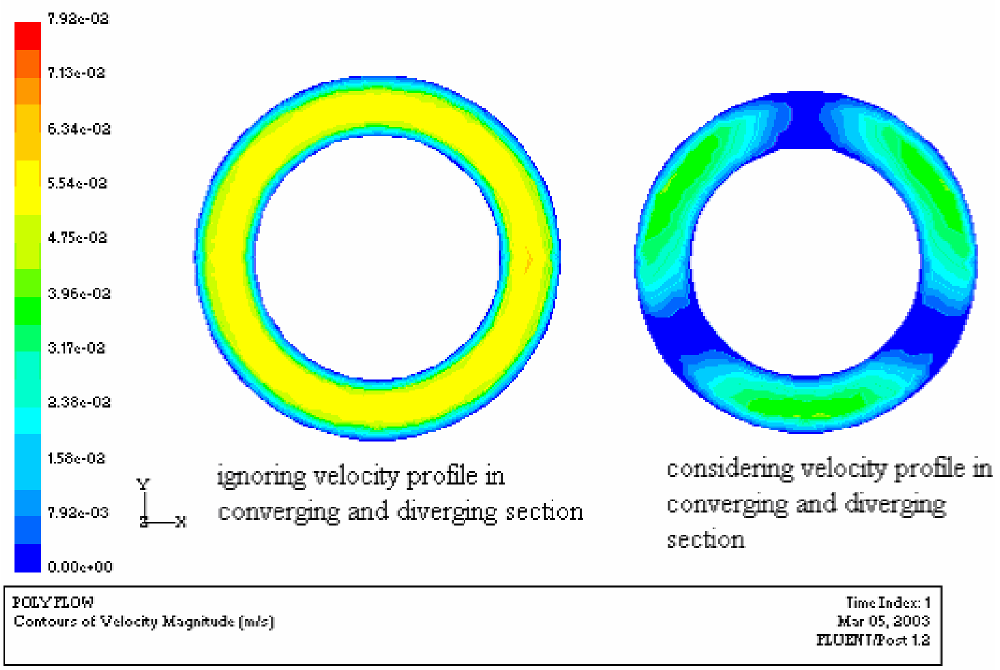
Three Dimensional exploded view of Total Die



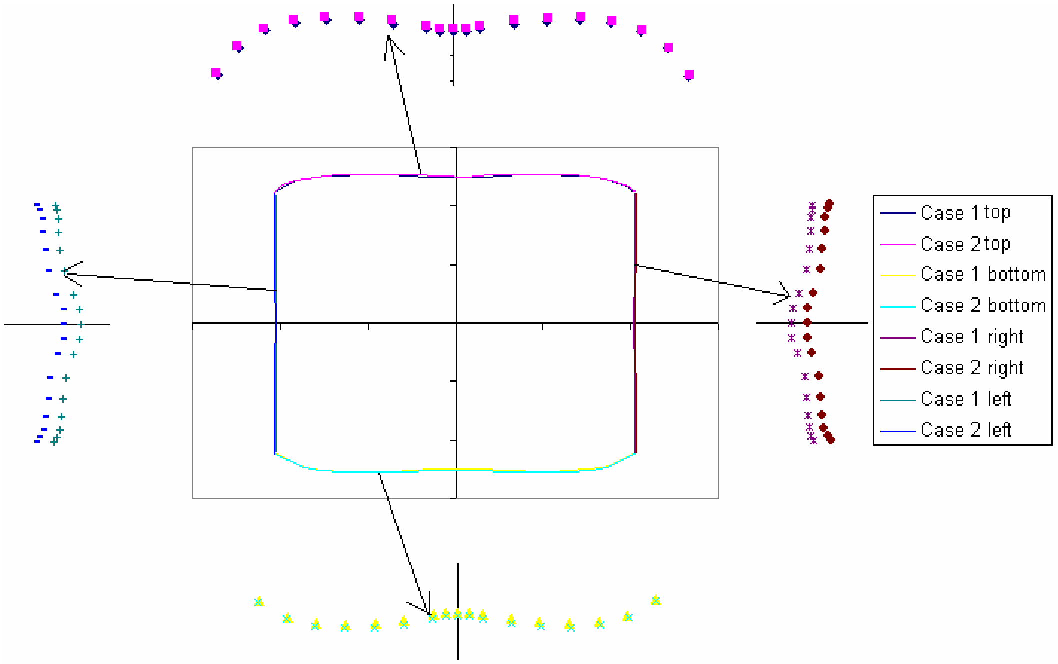
Geometry and Finite Element Mesh of the Model



Contours of Velocity Distribution

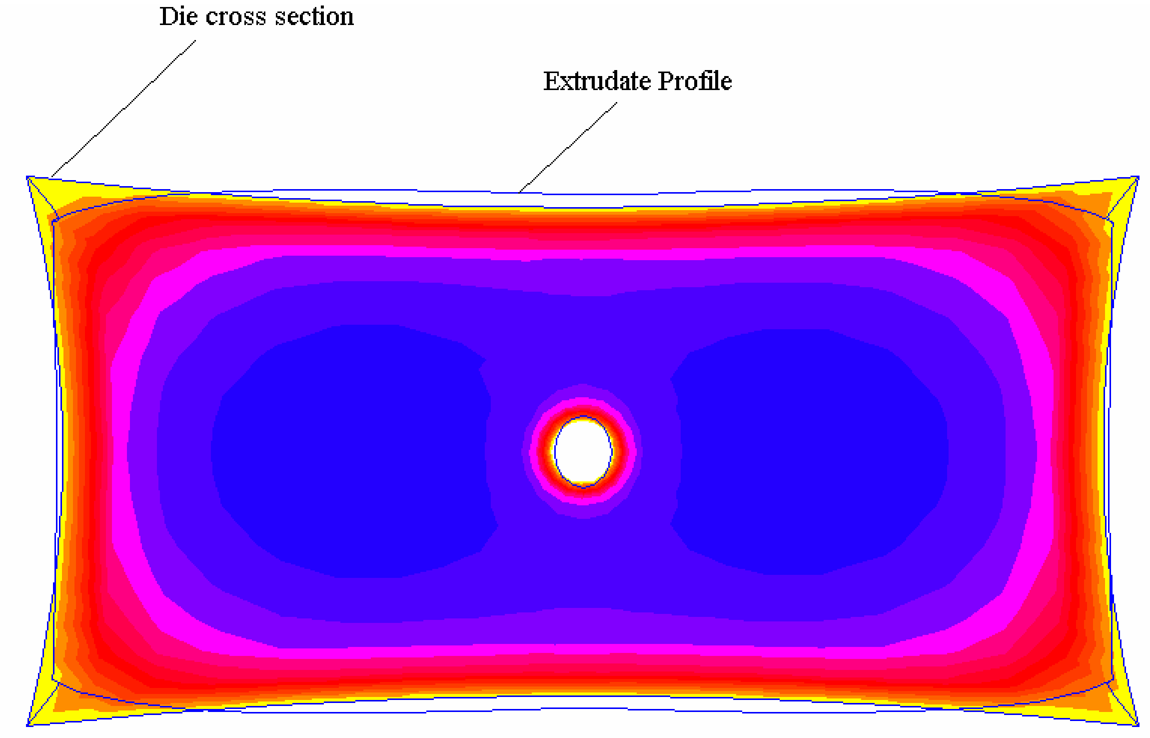


Effect of considering velocity profile in converging and diverging section

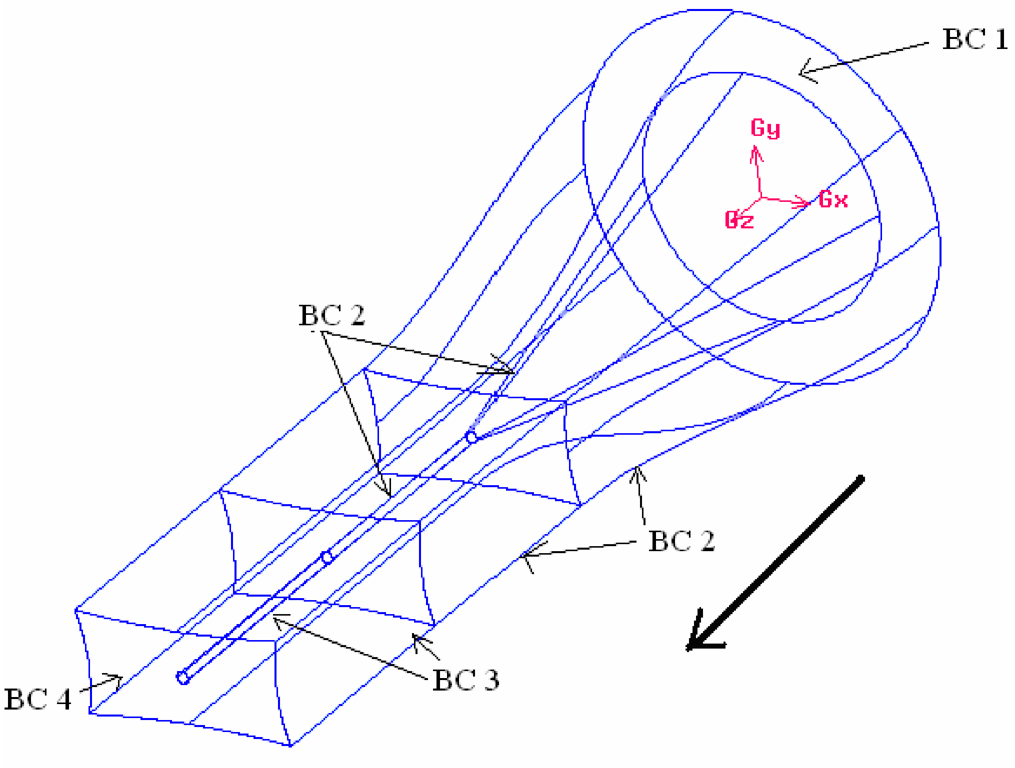


Case 1: Flow simulation neglecting velocity profiles in converging and diverging section
Case 2: Flow simulation considering velocity profiles in converging and diverging section

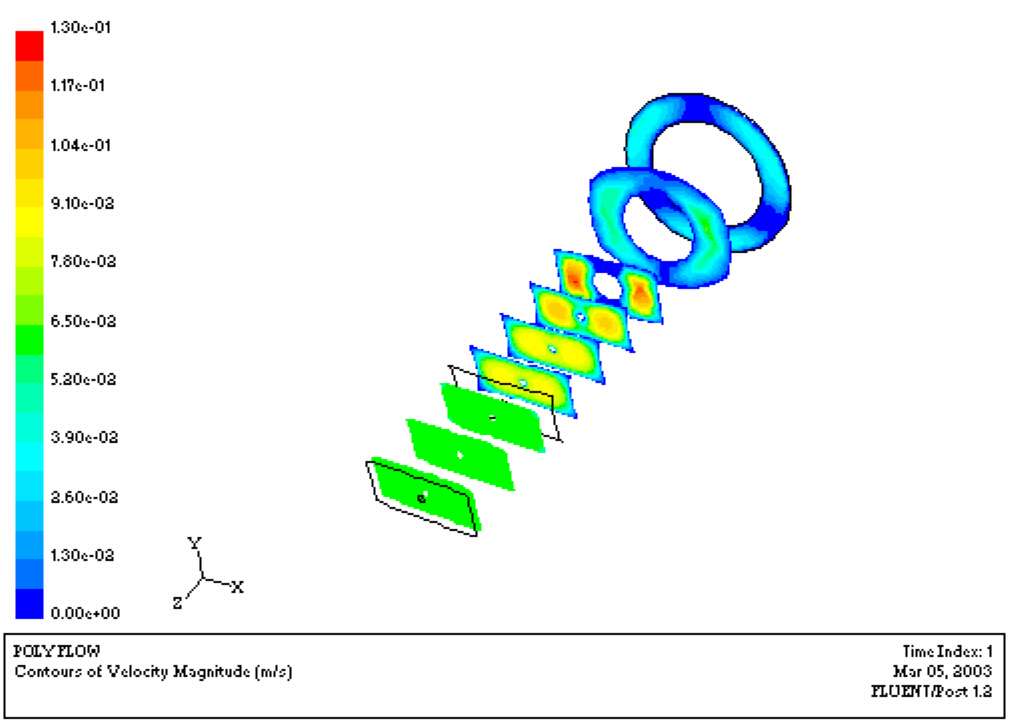
Shapes of extruded profiles when flow in converging and diverging section is considered and neglected



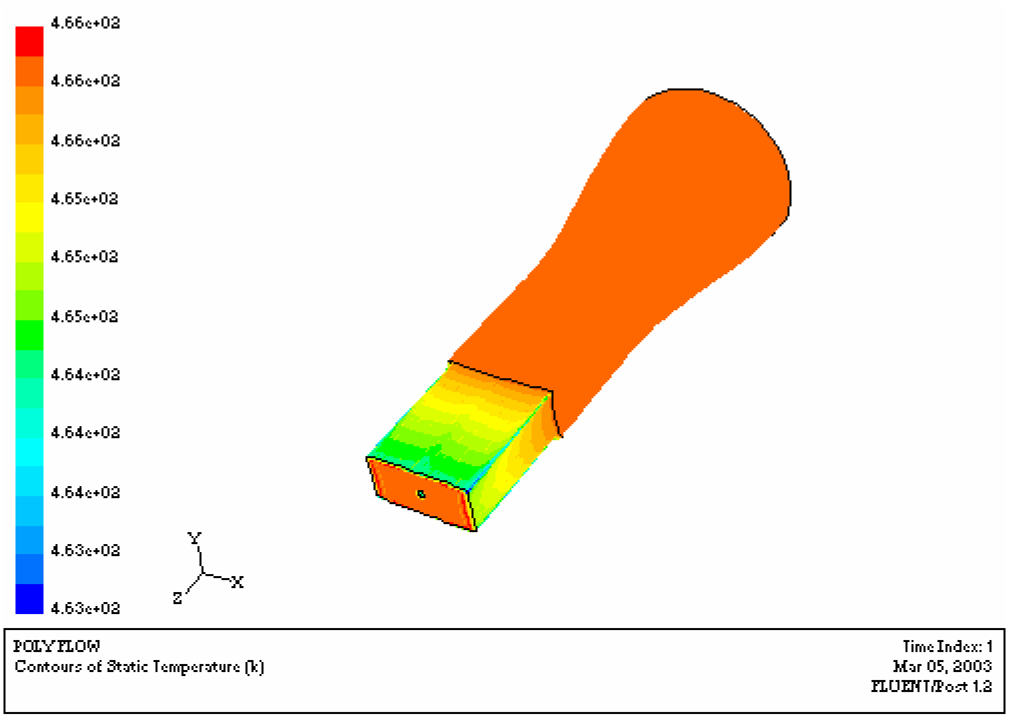
Die cross section and Extrudate Profile



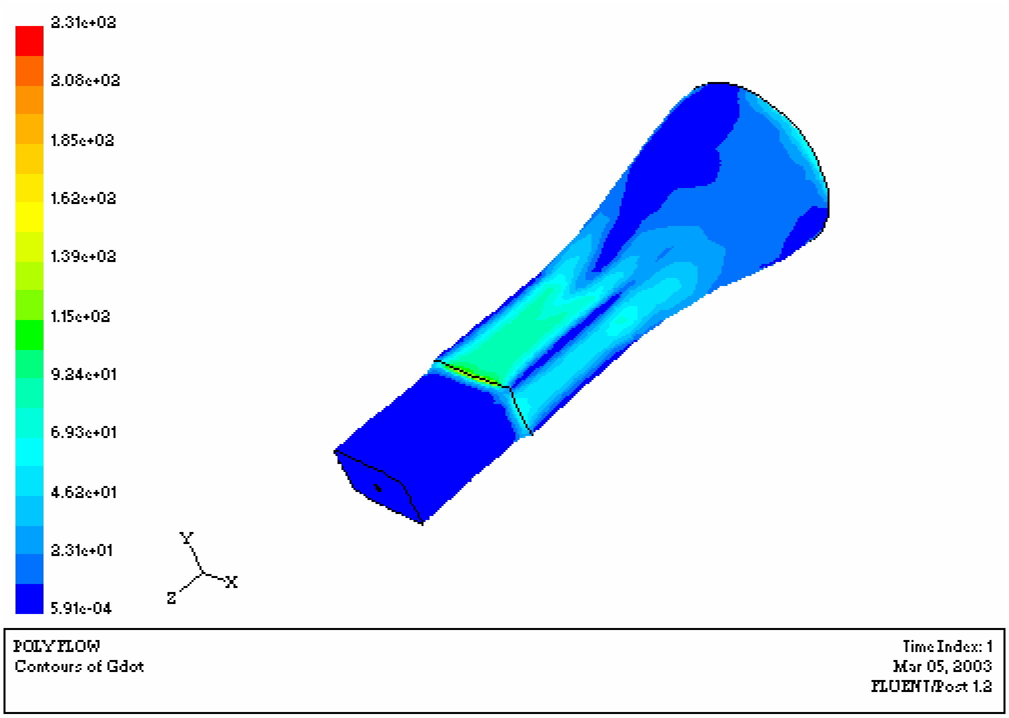
Geometry and Boundary conditions of the model



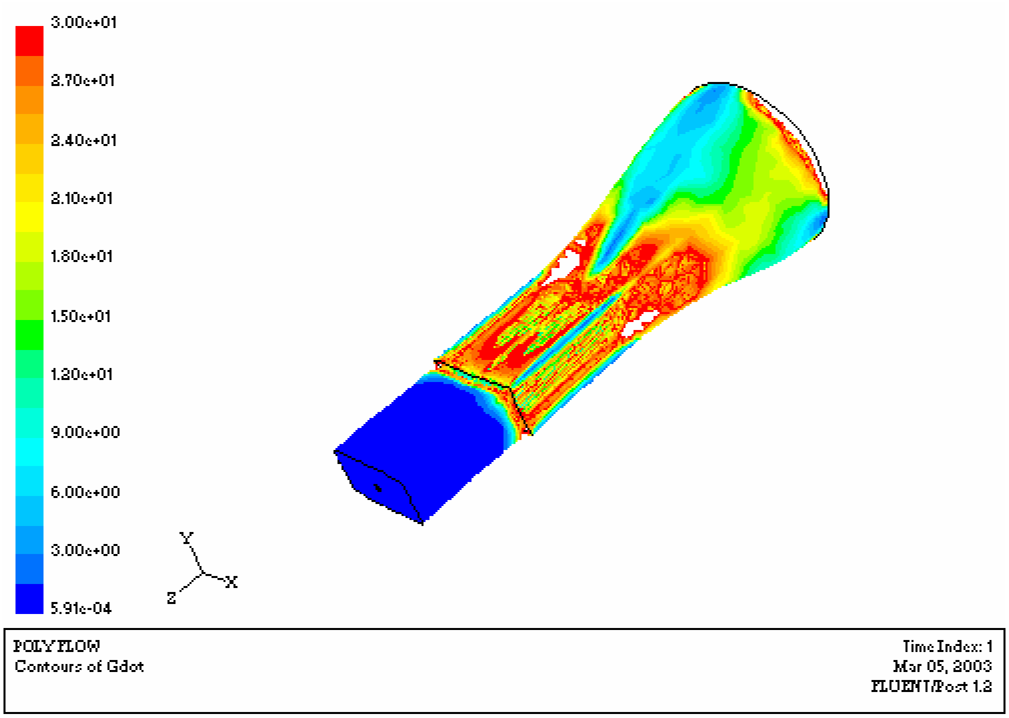
Contours of Velocity Distribution along planes perpendicular to z-axis



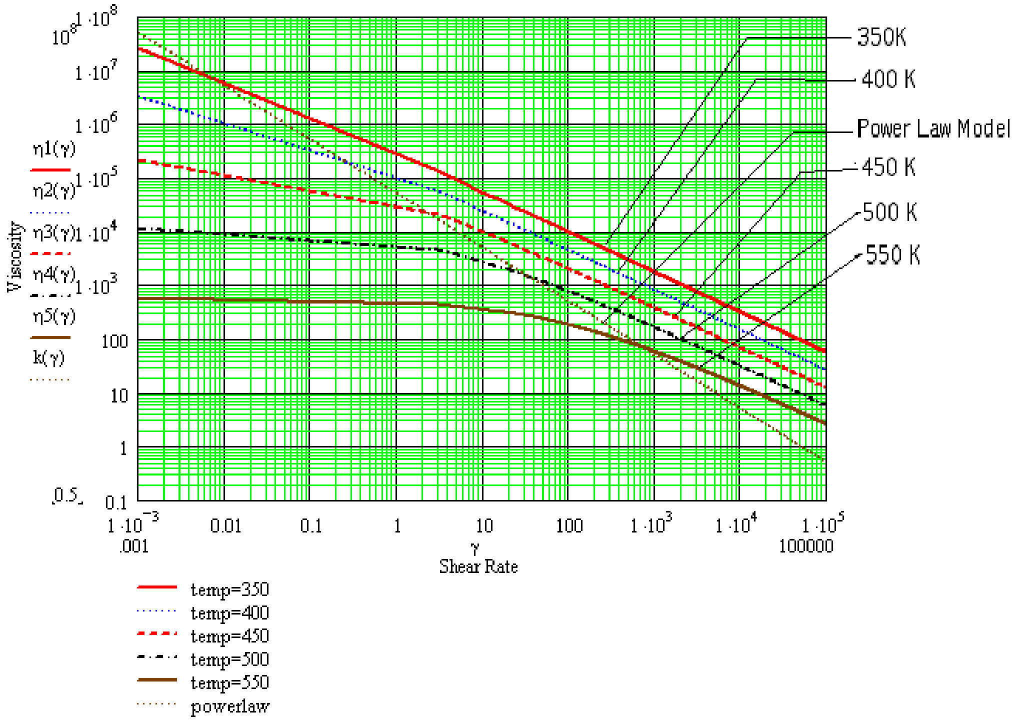
Contours of Temperature Distribution



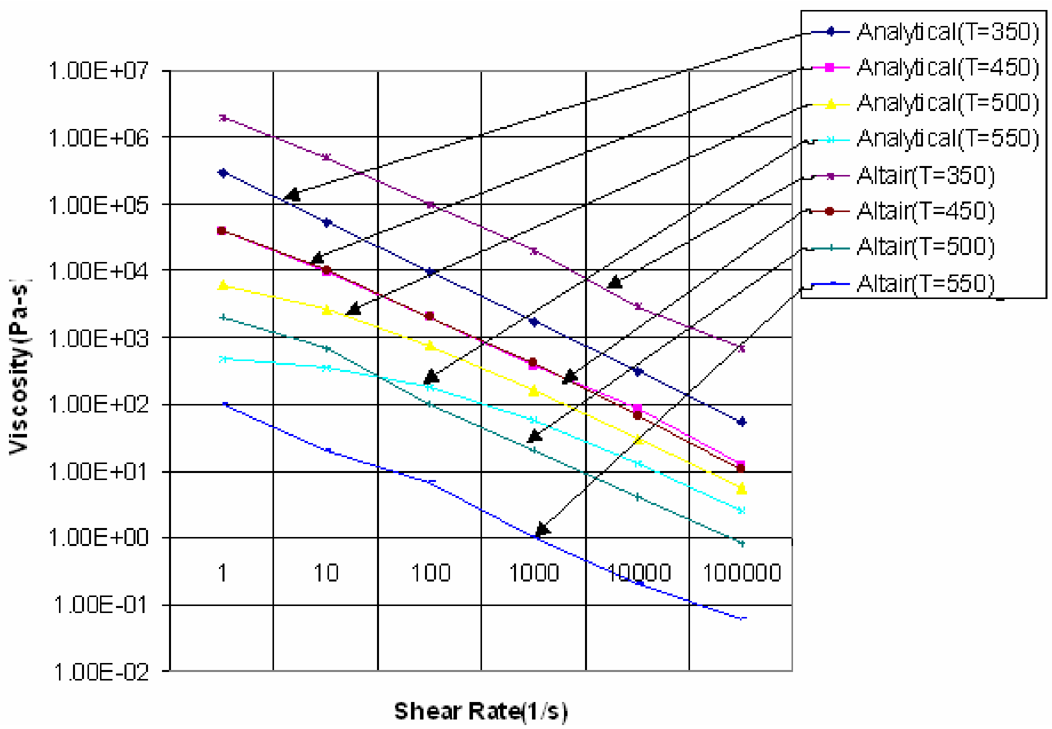
Contours of shear rate



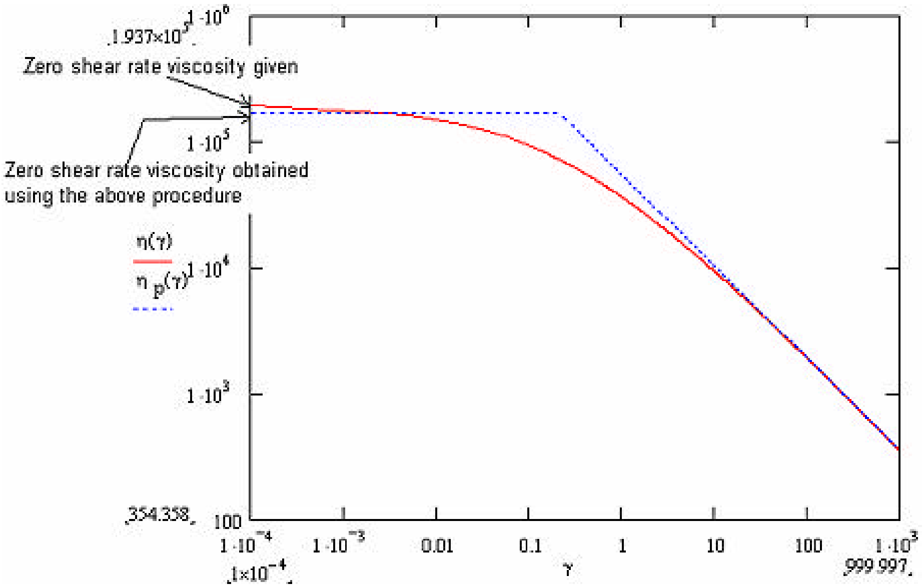
Contours of Shear rate of less than 30



Plot of polymer viscosity (in Pa-s) as a function of shear rate and temperature from analytical values from Eq.(5)



Comparision of plots of Viscosity vs shear rate at different temperatures from Analytical values and values provided by Altair Inc.



Effect of extrapolating the values of Viscosity

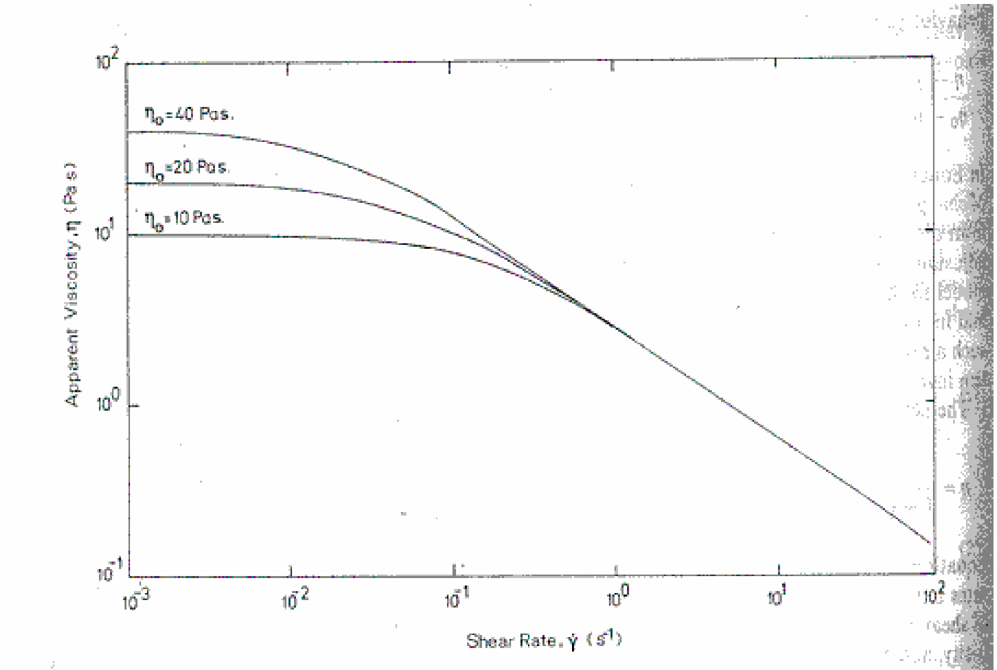
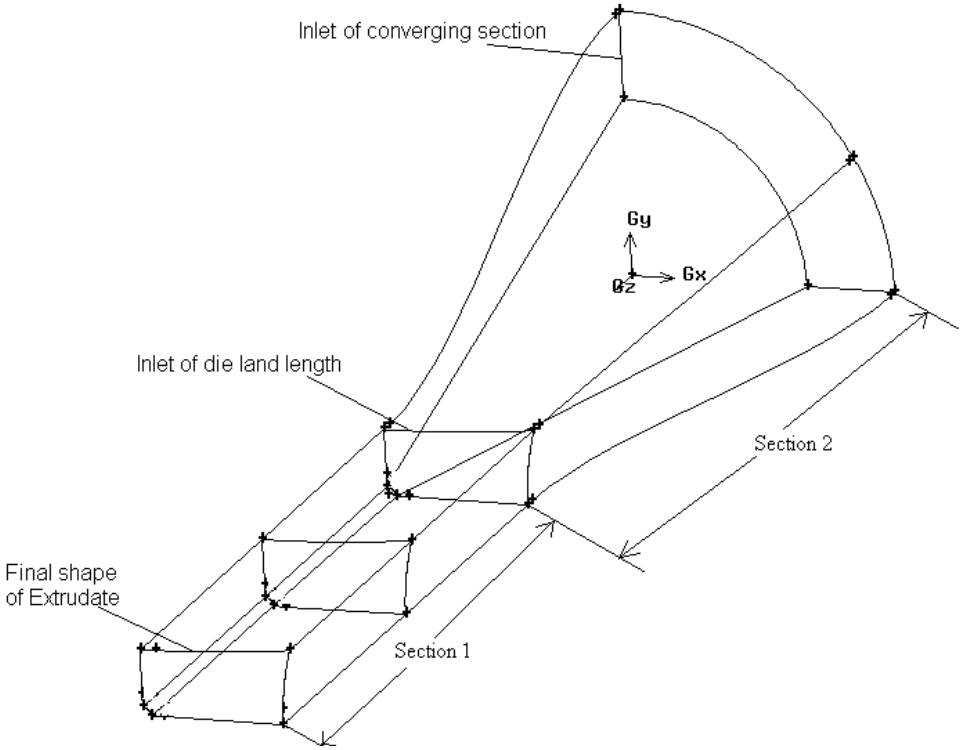
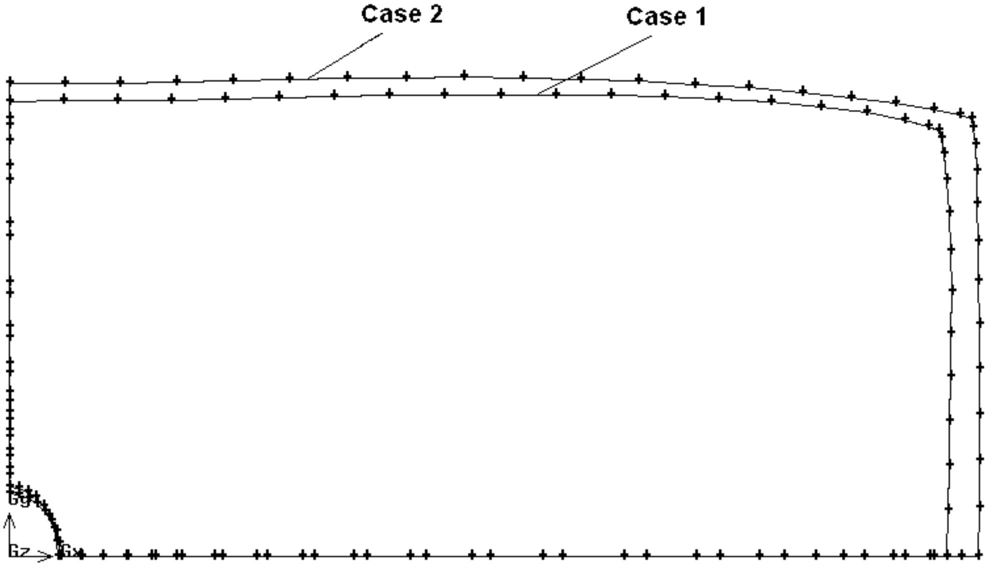


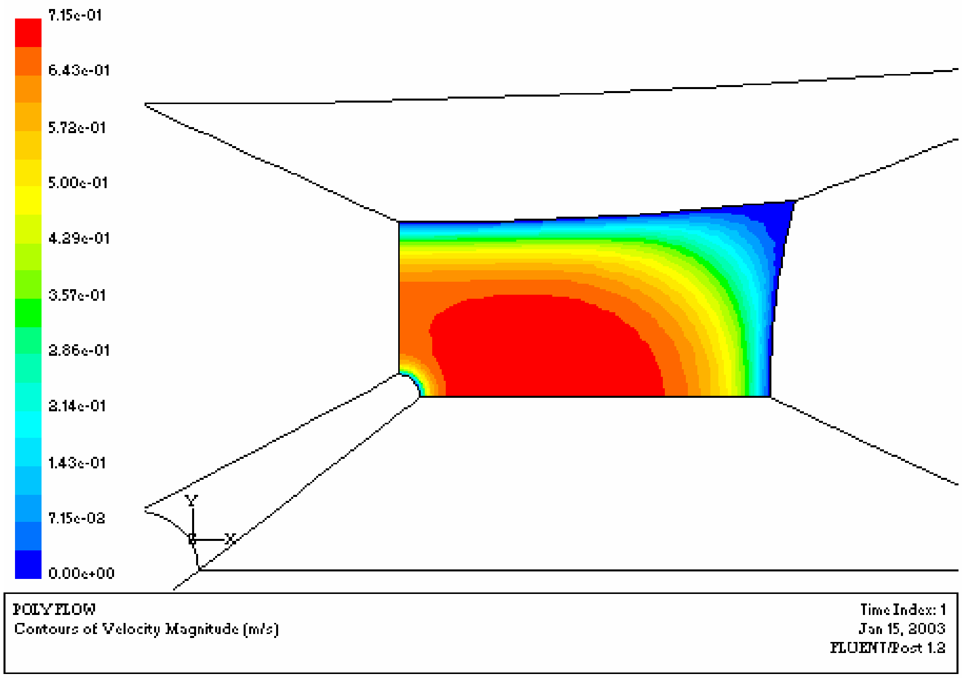
Figure 6. Apparent viscosity as a function of shear rate for three hypothetical fluids that could be characterized by the identical power law constants ($n = 0.4$ and $K = 2.83\ \mathrm{Nm^{-2}\,s^{4}}$), yet are vastly different and accurately characterized by the following sets of values for Ellis model parameters: (a) $\eta_0 = 10$ Pa s, $\alpha = 2.95$ and $\tau_{1/2} = 1.64$ Pa; (b) $\eta_0 = 20$ Pa s, $\alpha = 2.95$ and $\tau_{1/2} =$ 1.18 Pa; (c) $\eta_0 = 40$ Pa s, $\alpha = 2.95$ and $\tau_{1/2} = 0.80$ Pa. (Modified after Boger [25]).



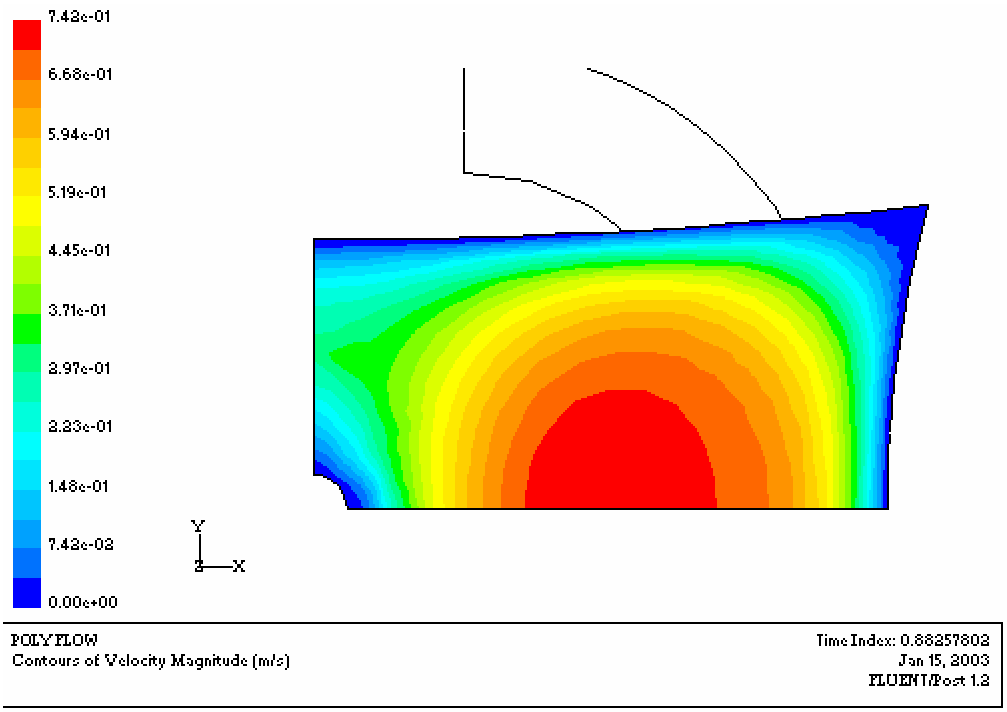
Shape of the die



Comparison of final shapes of the extrudates in both cases



Velocity profile at the inlet of the die land length for case 1



Velocity profile at the inlet of the die land length for case 2

Effect of Inertia Terms in Developing Flows