Three-Dimensional Finite Element Simulation of Polymer Melting in a Single-Screw Extruder

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Abstract

Screw freezing experiments in a single-screw extruder were conducted for an ABS resin. The melting of ABS was also simulated by a full three-dimensional simulation of the two-phase flow in the compression section of the extruder. Numerical simulations as well as experiments exhibit the Maddock melting mechanism.

Introduction

Even though Tadmor-type melting models [1], which are based on Maddock melting mechanism [2], have been very helpful in elucidating the qualitative trends in melting of polymers in single-screw extruders, the melting process is too complex for a single melting mechanism to be valid for the complete melting section of all extruders for all polymers. Instead of a priori assuming the existence of a melting mechanism, the objective of the present work is to perform a three-dimensional simulation of the two-phase flow in the melting (compression) region of a single-screw extruder. Extrusion experiments were also conducted to validate the numerical simulation.

Resin

The resin used for the experiments was an acrylonitrile butadiene styrene (ABS) resin that was manufactured by The Dow Chemical Company. The resin was an extrusion grade material with a melt flow rate (MFR) of 2.5 dg/min (230°C, 3.8 kg). The shear viscosity data for this resin and the Cross-WLF viscosity [3] fit are shown in Fig. 1. The values of Cross-WLF viscosity model parameters are $n = 0.35$, $\tau^* = 2.70\times10^4$ Pa, $D_1 = 6.487\times10^{11}$ Pa.s, $T^* = 100$ °C, $A_1 = 27.66$, $A_2 = 89.37$ K. The melt density, heat capacity and thermal conductivity were assumed to be constant at 0.88 g/cm^3, 2345 J/kg.K and 0.18 W/m.K, respectively.

Experimental Data

The extrusion experiments were performed using a highly-instrumented, 63.5 mm diameter, single-screw extruder with a length-to-diameter (L/D) ratio of 21. The extruder was operated at barrel temperatures of 200°C for the feed zone, 230°C for the middle zone, and 250°C for the metering zone and a screw speed of 60 rpm. Experimental melting profiles in the extruder were obtained by performing Maddock solidification experiment. The cross-sectional views of the plastication process from this experiment are shown in Fig. 2.

Numerical Simulations

In the present work, numerical simulations of polymer melting was performed in a coordinate frame fixed on the screw and the barrel was rotated in the opposite direction. To further simplify the simulation, the helical screw channel was unwound into a straight channel, and the barrel was modeled as a plate moving on top of the straight channel at an angle equal to the helix angle of the screw. For numerical simulations, the barrel and screw temperatures were specified to be 230 °C and the compacted solid polymer entered the channel at 30 °C. For the screw rotating at 60 rpm, the equivalent velocity of the top plate (barrel) used in the simulation is $V_x = 0.060$ m/s and $V_z = -0.190$ m/s. Figs. 3 and 4 show the temperature and cross-channel velocity distributions predicted by PELDOM™ software [4]. The two-phase flow was simulated for only the compression section of the extruder. Since the feed section of the screw used was six diameters long and the compression section had an axial length of eight screw diameters, the simulation starts at the location of the cross-section labeled 6 in Fig. 2 and ends at cross-section 14. The glass transition temperature of the ABS is 100 ˚C and almost no flow occurs below 150 ˚C. Therefore, the region below 420 K, shown with blue color in Fig. 3, is solid polymer, whereas other colors show the temperature of polymer melt. The melting pattern in the photographs in Fig. 2 as well as that in simulation results in Figs. 3 and 4 follow the Maddock mechanism. However, the solid bed width in numerical simulation decreases at a higher rate than that in the experimental data in Fig. 2. This faster rate in the simulation might have been caused by the assumption of constant heat capacity and that of a steady state flow.

References

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4. PELDOM software, Plastic Flow, LLC, Houghton, MI 49931 (www.plasticflow.com)

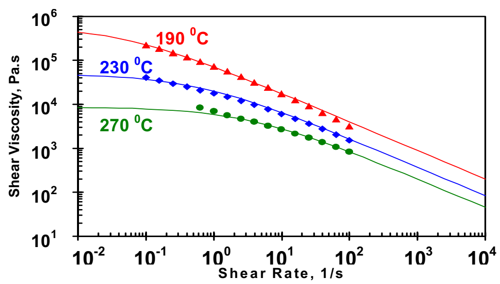

Figure 1: Shear viscosity data (symbols) and Cross-WLF model fit (curves) to the viscosity data for the ABS resin.

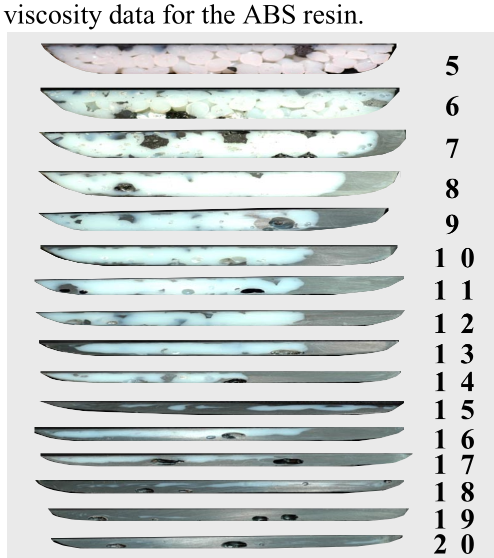

Figure 2: Cross-sections of the solidified polymer obtained from the solidification experiments. The numbers along the cross-sections show the axial location of the cross-section as a multiple of the screw diameter.

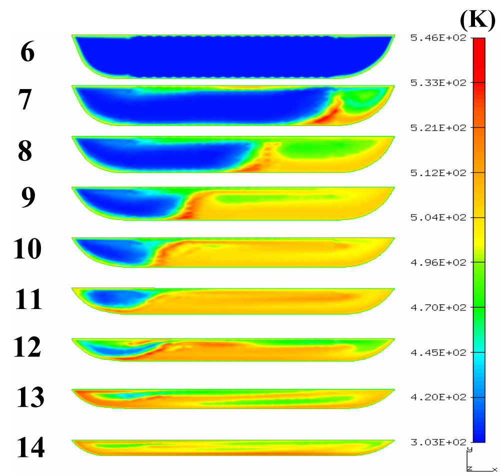

Figure 3: Predicted temperature distribution in the melting section of the extruder.

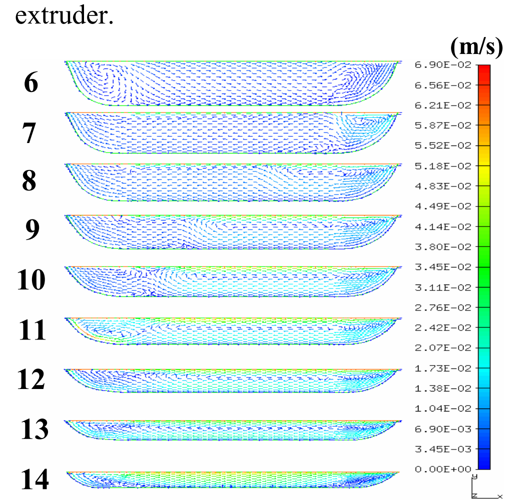

Figure 4: Predicted cross-channel velocity distribution in the melting section.