142l Simulation of Contraction Flow of a Polystyrene – Carbon Dioxide Solution through an Axisymmetric Extrusion Foaming Die

Shunahshep Shukla and Kurt W. Koelling

We have attempted to simulate the contraction flow of a polystyrene-carbon dioxide solution in an extrusion die under adiabatic conditions using the computational fluid dynamics package FLUENT. The simulated pressure drops across the die length were compared with experimental data obtained previously in our laboratory.

Detailed rheological characterization is required for accurate simulation of the flow dynamics of a gas charged polymer solution through an extrusion foaming die. Small amplitude oscillatory shear measurements of complex viscosity of pure polystyrene melt were made on a parallel plate rheometer in our laboratory for a temperature range of 140°C to 240°C. The depression in the glass transition temperature of polystyrene melt on addition of various amounts of carbon dioxide to it was estimated using the Chow model. Classical linear viscoelastic scaling techniques were then used to carry out a concentration shift of the complex viscosity data for different concentrations of carbon dioxide in polystyrene melt. Time temperature superposition was carried out on the concentration-shifted data to estimate the WLF constants for the polystyrene – carbon dioxide system. The shear-rate dependence of viscosity of the polymer – gas system could be adequately represented using the three-parameter Cross model and reasonable predictions of the viscosities at the higher shear-rates characteristic of extrusion flows could be made by extending the model to the shear rates of interest. The pressure and temperature corrections of the viscosity were incorporated into the simulation in a dynamic way by writing appropriate user defined functions and linking them to the FLUENT solver.

Values of pressure drops across the die obtained through the simulations show good qualitative agreement with experimental pressure drop measurements on the foaming extrusion die. Non-isothermal effects were localized but significant – the bulk temperature of the fluid did not increase significantly but the simulations predicted a temperature rise of up to 30°C in the polymer – gas solution exiting the capillary in the region near the wall at higher shear rates. The field values of temperature and pressure were extracted from FLUENT and fed to a separate program, which computed the surface of incipient nucleation in the die using the Sanchez-Lacombe Equation of State. The pressure drop rates and temperature rise rates were then estimated at the surface of incipient nucleation – quantities which have been reported previously to have significant impact on the number of bubbles nucleated in a supersaturated polymer – gas mixture. Since the mean residence time of the fluid in our die is small enough so as not to allow significant bubble growth in the die, and since little is known regarding the time lag in nucleation that occurs in a die for the polystyrene – carbon dioxide system, we believe that the assumption of approximating the flow as a single phase flow in our simulations is not very unreasonable and can give useful insights into the dynamics of flow in a non-isothermal foaming die.

We also carried out simulations for the case of an isothermal die wall and comparisons are made with the adiabatic die wall case for different temperatures and flow rates.

Finally, in order to assess the convergence properties of the solution, selective grid adaption in domains of high cell property gradients was carried out and the solutions on the refined meshes were compared with results on the coarse mesh. Grid refinement does not appear to have an appreciable effect on the solution properties for lower shear rates or at higher temperatures. But at the lowest temperatures and for the highest flow rates investigated, grid adaption can have an important effect on the final converged solution.