Investigation of Solids Transport in a Single-Screw Extruder Using a 3-D Discrete Particle Simulation

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A non-isothermal, 3-D discrete particle simulation based on the discrete element method (DEM) was developed to simulate the solids-conveying zone and feed hopper of a single-screw extruder. The method considers each particle in a granular assembly as a separate entity that can interact with other particles or boundaries through collisions or lasting contacts. By using DEM to model the extrusion environment, *a priori* knowledge of the solids flow was not required in order to simulate the motion of a granular assembly with reasonable accuracy, allowing studies to be conducted in the absence of the solid plug assumption typical of classical solids-conveying models. In this paper, predicted results were limited to low levels of compaction in the solids assembly (i.e., no particle deformation), in order to understand the behavior of the polymer pellets in their most dynamic state. The results of the DEM model showed reasonably good agreement with experimental data, providing comparable bulk values like output rate, yet also demonstrating its ability to capture the dynamics of solids particle conveying. The model captured the inherent variability of extrusion such as the low-amplitude, high-frequency fluctuations referred to as "solids pulsing" and the recirculation of pellets in the feed throat. Polym. Eng. Sci. 44:2203–2215, 2004. © 2004 Society of Plastics Engineers.

INTRODUCTION

The granular mechanics of plastics within a single-screw extruder has, for the past five decades, remained a difficult phenomenon to model. It is generally understood that the solids are transported forward by the action of the extruder screw, assisted by the difference in frictional forces between the screw and barrel surfaces (1), and retarded by the throughput capacity of the subsequent downstream mechanisms of melting and pumping (2). Compaction of the polymer solids progresses down the length of the solids-conveying zone, dependent on pressure, temperature, and material type (3, 4). Not so well understood is the exact nature by which pressure develops in this early zone of the extruder or the influence of screw geometry on throughput rate. To simplify the solids-transport phenomenon and allow for an analytical solution, the granular bed has been likened to an elastic plug (1, 5−8), or an elastic fluid (9). However, the isotropic stress distribution inherent to an elastic plug or fluid bears little resemblance to the anisotropic behavior of granules often observed in an extruder (1, 10). Modified variants of the classic model (1) have relied on the use of a "lateral stress ratio" constant (11) to approximate the behavior of solids while maintaining the mathematical simplicity of an isotropic plug, with a modest improvement in predicted pressure and output rate values. The shortcomings of the classic model that the modified models have sought to overcome include: i) no consideration for velocity variation within the solids bed as observed experimentally (10, 12); ii) the need for a non-zero initial pressure at the start of the solids-conveying zone; iii) no allowance for flow to occur in the case where the screw friction coefficient was larger than the barrel; and iv) the lack of consideration for wall slip during solids motion (12). To consider the local influences within the screw channel that give rise to the anisotropic stress distribution, the modeling approach must take a non-plug approach; the non-plug approach attempts to take a discrete view of the solids motion. Multidimensional velocity and pressure distributions are then available from a solids-conveying model through the inclusion of internal frictional forces

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