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Determining the collision properties of semi-crystalline and amorphous thermoplastics for DEM simulations of solids transport in an extruder

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Abstract

To improve application of the distinct element method (DEM) to polymer processing applications it was necessary to evaluate the contact mechanics of a selection of commonly used polymers. The contact behaviors of high-density polyethylene (HDPE), polystyrene (PS) and polycarbonate (PC) were revealed in this paper from a series of impact studies where spherical polymeric particles struck a steel anvil at various angles of incidence and impact velocity. The coefficients of restitution and friction were calculated from high-speed video analysis of individual impacts. The collected data was used to evaluate the relevance of several popular normal contact force–displacement models to determine their suitability for the tested semi-crystalline and glassy polymers. The models considered were those proposed by Walton and Braun [1986. Viscosity, granular-temperature, and stress calculations for shearing assemblies of inelastic, frictional disks. Journal of Rheology 30, 949–980], with constant (WBCE) and variable (WBVE) normal restitution coefficient, and Thornton [1997. Coefficient of restitution for collinear collisions of elastic-perfectly plastic spheres. Journal of Applied Mechanics 64, 383–386], based on elastic–plastic collisions. Comparison of the impact data with DEM simulations using the various contact force–displacement models revealed that the WBVE model provides the best overall agreement with the viscoelastic-fully plastic behavior of HDPE, while the almost purely elastic nature of PC and PS agreed well with all three models studied in this paper. The influence of the normal force–displacement models on the solids transport zone of an extruder was subsequently discussed based on the findings from the impact study.
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Keywords: Contact mechanics; Granular materials; Polymers; Polymer processing; DEM; Extrusion

1. Introduction

Within the field of polymer processing, the influence of granular mechanics on the process is most often overlooked in favor of the transport of melt. Most currently employed models for solids conveying in a plasticating single-screw extruder (which is the dominant machine in practice) consider the granular assembly as either an elastic plug (Darnell and Mol, 1956; Tadmor and Broyer, 1972; Tadmor and Klein, 1978; Hyun and Spalding, 1997, Derenzinski, 2003) or an elastic fluid (Campbell and Dontula, 1995), which are conceptualizations that do not convey the dynamic, anisotropic behavior of the solids. In view of engineering topics such as process troubleshooting and system design, neglect for the nature of plastics in their granular state can lead to considerable economic loss within an industrial production facility. Recently, a relatively new modeling approach has been demonstrated for the solids-inflow and solids-conveying zone based on tracking the motion of each discrete particle (Potente and Pohl, 2001; Yung et al., 2002, Moysey and Thompson, 2004, 2005). The distinct element method (DEM) builds a macroscopic understanding of the granular flow from the microscopic behavior of the particles as they move and collide with each other and with local surfaces. Through use of DEM to simulate the dynamic motion of the dense granular assembly of polymer solids within a single-screw extruder, reasonably good agreement was found with experimental data. From the DEM simulations, several new aspects of the nature of solids in the extruder were revealed (Moysey and Thompson, 2004) including: (i) the source of the pulsating nature of

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