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Research Article

A Simple-to-Implement Simulator for the Reactive Extrusion of Poly(Lactic Acid) in a Corotating Uniform Twin-Screw Extruder

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The present paper deals with the poly(lactic acid) (PLA) reactive processing simulation in a uniform corotating twin-screw extruder that can be readily turned into practical applications in pilot and industrial equipment. The simulator provides a cause-effect guide that can be useful for starting an experimental setup in a reactive screw extruder for a biopolymer in a growing industry. The proposed model considers a free radical ring-opening mechanism involving the main characteristic flows inside the extruder and the non-Newtonian behavior of PLA. The characteristic behavior relating reaction rate, average molecular weights, and polydispersity against chamber number are described by S-shaped and monotonically decreasing curves, for the equipment. Numerical predictions show that this simple and easy to implement model accurately reproduces previously reported data and that the impurity concentration exhibits a marked effect over all the variables, except conversion.

1. Introduction

Poly(lactic acid) (PLA) belongs to the family of aliphatic polyesters, commonly made from α-hydroxy acids, which include polyglycolic or polymandelic acids, and is considered biodegradable and compostable [1]. PLA is a thermoplastic, high-strength, high-modulus polymer that can be made from renewable resources yielding articles for use in either the industrial packaging field or the biocompatible/bioabsorbable medical device market [2]. For further applications, the property profile and price of PLA can be changed by combining PLA with other biocompatible or bioacceptable polymers, fillers, or reinforcements [3, 4]. Alternatively, PLA can be modified by adding plasticisers to obtain more flexible materials [5, 6].

To process PLA on large-scale production lines in applications such as injection molding, blow molding, thermoforming, and extrusion, the polymer must possess adequate thermal stability to prevent degradation and maintain its molecular weight and properties [7]. PLA can be prepared in two ways: either by a polycondensation or by free radical polymerization [7, 8]. The free radicals pathway offers high molecular weight polymers with nearly no remaining monomer. The catalyst currently used industrially is stannous octoate [8], which leads to the ring-opening polymerization of L-lactide and obtains a linear high molecular weight polymer [9]. The choice of initiator system, coinitiator as chain control agent, catalyst concentration, monomer-to-initiator ratio, and polymerization temperature and time, significantly affects the polymer properties, such as the molecular weight, degree of crystallinity, and residual monomer content, which in turn affect the physical-mechanical properties and range of temperature use of the polylactide and its copolymers [10, 11]. Mehta et al. [8] provided a selective summary of the literature on PLA synthesis. The determination of individual rate constants requires the propagation rate constant k_p knowledge, a difficult task that has not been performed properly for this polymer [8]. Evaluation of the rate constants by modeling and simulation in conjunction with the experimental results offers several advantages: initiation, propagation, and