

Mathematical Modeling for Continuous Reactive Extrusion of Poly Lactic Acid Formation by Ring Opening Polymerization Considering Metal/Organic Catalyst and Alternative Energies

Authors : Satya P. Dubey, Hrushikesh A Abhyankar, Veronica Marchante, James L. Brighton, Björn Bergmann

Abstract : Aims: To develop a mathematical model that simulates the ROP of PLA taking into account the effect of alternative energy to be implemented in a continuous reactive extrusion production process of PLA. Introduction: The production of large amount of waste is one of the major challenges at the present time, and polymers represent 70% of global waste. PLA has emerged as a promising polymer as it is compostable, biodegradable thermoplastic polymer made from renewable sources. However, the main limitation for the application of PLA is the traces of toxic metal catalyst in the final product. Thus, a safe and efficient production process needs to be developed to avoid the potential hazards and toxicity. It has been found that alternative energy sources (LASER, ultrasounds, microwaves) could be a prominent option to facilitate the ROP of PLA via continuous reactive extrusion. This process may result in complete extraction of the metal catalysts and facilitate less active organic catalysts. Methodology: Initial investigation were performed using the data available in literature for the reaction mechanism of ROP of PLA based on conventional metal catalyst stannous octoate. A mathematical model has been developed by considering significant parameters such as different initial concentration ratio of catalyst, co-catalyst and impurity. Effects of temperature variation and alternative energies have been implemented in the model. Results: The validation of the mathematical model has been made by using data from literature as well as actual experiments. Validation of the model including alternative energies is in progress based on experimental data for partners of the InnoREX project consortium. Conclusion: The model developed reproduces accurately the polymerisation reaction when applying alternative energy. Alternative energies have a great positive effect to increase the conversion and molecular weight of the PLA. This model could be very useful tool to complement Ludovic® software to predict the large scale production process when using reactive extrusion.

Keywords : polymer, poly-lactic acid (PLA), ring opening polymerization (ROP), metal-catalyst, bio-degradable, renewable source, alternative energy (AE)

Conference Title : ICP 2015 : International Conference on Polymer

Conference Location : Paris, France

Conference Dates : February 23-24, 2015