Modeling of reactive extrusion: a new method. Application to PLA

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Modeling a reactive extrusion process presents some difficulties. First, the knowledge of the kinetic scheme and of the different constants is necessary. Second, the characteristics of the flow inside the extruder are needed. In previous publications, we used the axial dispersion model as model. The corresponding data may be deduced from the residence time distribution. These distributions can be determined experimentally, although some uncertainty is due to the important variation of the viscosity along the screw, related to the polymerization. The knowledge of the flow can be reached using a simulation software. This simulation allows a finer knowledge of the flow. It is possible to know the position and length of the filled sections, generally the kneading disks and left handed elements, and the partially filed sections, usually the conveying sections. Since an observation inside of the extruder is impossible, using a simulation software is a solution. We used the LUDOVIC® commercial software, which computes the filling ratios section after section, and the local residence times as well. The filled sections are considered as stirred reactors, while the conveying sections as plug flow reactors. The integration of the balance equations of the reactors, section after section, leads to the conversion of the monomer and to the molecular weight distribution.