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Multiscale Modeling of Poly(lactic acid) Production: From Reaction Conditions to Rheology of Polymer Melt

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Abstract. Poly(L-lactic acid) (PLLA) is a fully biodegradable bioplastic with promising market potential. The paper deals with systematic development and analysis of the modeling framework allowing direct mapping between PLLA production process conditions and rheological properties of the polymer melt. To achieve this, the framework builds upon three distinct elements that approach the production process from different scales: (i) macroscopic deterministic model of L,L-lactide ring opening polymerization taken from the literature, (ii) microscopic stochastic simulation of the polymerization process based on hybrid Monte Carlo approach, and (iii) mesoscopic public domain model of polymer chain reptation dynamics. Based on the input reaction conditions, the macro-scale model predicts L,L-lactide conversion and averaged molar mass of PLLA, while the micro-scale and meso-scale simulations allow prediction of full molar mass distribution and melt viscosity of the product. The developed predictive tool is validated by literature data, i.e. experimentally measured rheological characteristics of three commercial PLLA samples with different molecular architecture. Moreover, comprehensive global sensitivity analysis has been carried out to support exploration of the process conditions space in relation to target polymer melt properties. Computational efficiency of the developed model achieved so far foreshadows its potential use as soft sensor for molar mass distribution and melt viscosity in the optimization and control of PLLA production.

Keywords: Poly(lactic) acid; Mathematical modeling; Monte Carlo simulation; Polymer melt rheology; Global sensitivity analysis; Identifiability analysis.

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