Analytical rheology of metallocene-catalyzed polyethylenes

SACHIN SHANBHAG, ARSIA TAKEH, Florida State University — A computational algorithm that seeks to invert the linear viscoelastic spectrum of single-site metallocene-catalyzed polyethylenes is presented. The algorithm uses a general linear rheological model of branched polymers as its underlying engine, and is based on a Bayesian formulation that transforms the inverse problem into a sampling problem. Given experimental rheological data on unknown single-site metallocene-catalyzed polyethylenes, it is able to quantitatively describe the range of values of weight-averaged molecular weight, $M_W$, and average branching density, $b_m$, consistent with the data. The algorithm uses a Markov-chain Monte Carlo method to simulate the sampling problem. If, and when information about the molecular weight is available through supplementary experiments, such as chromatography or light scattering, it can easily be incorporated into the algorithm, as demonstrated.

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