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ORIGINAL PAPER

# From molecular weight distribution to linear viscoelastic properties and back again: application to some commercial high-density polyethylenes

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**Abstract** The aim of this study was to predict broad molecular weight distribution (MWD) of commercial high-density polyethylene (HDPE) samples from their linear viscoelastic (LVE) responses using a tube-based model. In the first step, a forward model based on time-dependent reptation mechanism was applied to predict LVE properties from MWD. Material parameters of the considered tube-based model were adjusted by comparing experimental and theoretical dynamic storage and loss moduli values. Adjusted parameters were compared with previously reported values and the effects of important parameters on the LVE properties were studied. It was found that higher polydispersity may lead to more relaxation which will be reflected in model by increase of mixing exponent. In the second step, the adjusted material parameters of one of the samples were used for prediction of MWD of all samples from their dynamic storage and loss moduli values. Two standard distribution functions were used for prediction of MWDs and the results were compared. It was shown that the Gaussian distribution function is suitable for prediction of broad unimodal MWD specimens, as they regularly appear in Ziegler–Natta catalyzed polyolefins, but the GEX function brings about optimal combination of flexibility and generality and is more appropriate for samples with asymmetric MWD curves. Considered combination of modeling elements including a Gaussian distribution function, a time-dependent diffusion relaxation function, a double-reptation mixing rule and the Nelder–Mead simplex optimization algorithm offers a practical tool for prediction of broad MWD of the commercial HDPE samples which can be used for online measurements.

**Keywords** Molecular weight distribution · Computer modeling · Viscoelastic properties · Rheology · Polyethylene

## Introduction

All the aspects of chain microstructure, e.g., molecular weight (MW) and its distribution (MWD), comonomer content and its distribution (CCD), long-chain branching (LCB) and its distribution and short-chain branching (SCB) and its distribution, are important characteristics that intensely affect the mechanical and rheological properties of polymers, in particular. Polymer materials are heterogeneous and compressible at the solid state and therefore the impact of microstructure on mechanical properties is affected by disturbing parameters, i.e., crazes and cracks, while in the molten state homopolymers are incomprehensible and homogeneous and the influence of microstructure on rheological properties is not affected by such distractions. MW and SCB are largely related to the mechanical properties while MWD and LCB are responsible for rheological properties.

One of the main goals of polymer science has been to relate the microstructure of macromolecular chains to their final properties. Such a relationship can inversely be used for characterization of polymer structures based on their properties. Some early attempts have been based on dynamic melt viscosity measurements [1, 2]. Prediction of MWD of entangled linear polymers from their linear

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