Abstract Submitted
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Dynamic Monte-Carlo Simulations of Diffusion in Polypropylenes: Possible Artifacts of Stereochemistry[1] ERNST VON MEERWALL, NUMAN WAHEED, WAYNE MATTICE, Univ. Akron — We previously reported coarse-grained lattice-based dynamic Monte-Carlo (MC) simulations in polypropylenes (PP), as well as pulsed-gradient diffusion (D) experiments at 180 deg. C., to study the effects of stereochemistry. We had obtained three PP specimens, with probabilities of a meso dyad Pm = 0.02 (syndiotactic, "sPP", Mn = 12,300), 0.23 (atactic, "aPP", Mn = 5,300), and 0.89 (isotactic, "sPP", Mn = 9,900). New simulations copied the samples' Mn and Pm, and for iPP the polydispersity Mw/Mn = 1.24. The conversion factor K between MC steps and real time must be derived from experiment. It was found that K = 3300 MCS/ps for both sPP and aPP, but falls to 1600 for monodisperse iPP, falling further to 800 if polidispersity is coarsely included. As the lack of any M-dependence of K had been verified in our earlier work with n-alkanes and polyethylenes (PE), its Pm-dependence must either originate in a systematic error of the PE-calibrated GPC M values, or else be an intrinsic feature of our MC method. New dilute D measurements, consistent with the Flory $M^{-0.5}$ –dependence, point to the second possibility.

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