Abstract Submitted
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Diffusion in Polypropylenes: Effects of Stereochemistry and Polydispersity[1] ERNST VON MEERWALL, NUMAN WAHEED, WAYNE MATTICE, University of Akron — We have performed pulsed-gradient diffusion (D) experiments at 180 deg. C and dynamic Monte-Carlo (MC) simulations to study the effect of stereochemical composition of linear propylene (PP) melts. The coarse-grained simulations were based on the rotational isomeric state model and Lennard-Jones potentials. For the proton NMR difusion measurements we obtained three PP specimens of differing molecular weight M and dispersity, with the probability of a meso diad Pm = 0.02 (syndiotactic), 0.23 (atactic), and 0.89 (nearly isotactic). Conversion between MC steps and real time was derived from experiment; no dependence on Pm is expected. Both simulation and M-scaled experiment found D at high Pm several times faster than at low Pm, but the constant-M simulations showed a maximum in D near Pm = 0.8 due to quenched randomness. To find the source of the remaining disagreement with experiment, new simulations tracked the samples' mean M and polydispersity, but the disagrement actually increased. We suspect that the GPC determination of M and its distribution, based on linear polyethylene scaling, is strongly dependent on PP stereochemistry, producing the misleading result.

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