

Abstract Submitted
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Stereochemical Effects on Diffusion in Polypropylenes: Simulation and Experiment¹ ERNST VON MEERWALL, NUMAN WAHEED, WAYNE MATTICE, Univ. Akron — In support of our dynamic Monte-Carlo (MC) simulations we performed pulsed-gradient NMR diffusion (D) measurements at 180°C on moderately disperse polypropylene (PP) melts to study the effects of stereochemical composition. The coarse-grained simulations were based on the rotational isomeric state model and Lennard-Jones potentials. For the proton NMR diffusion measurements we obtained three PP specimens, with probabilities of a meso dyad $P_m = 0.02$ (syndiotactic), 0.23 (atactic), and 0.89 (nearly isotactic). After accounting for differences in polydispersity, results were normalized to a common molecular weight M , using a scaling law taken from our earlier work with n-alkanes. Conversion between MC steps and real time was derived from experiment; no dependence on P_m was expected. Both experiment and simulation found D at high P_m several times faster than at low P_m , but the simulation also showed a maximum in D near $P_m = 0.8$. The latter effect is attributed to quenched randomness; no specimen was available for experimental verification. For reasons not well understood, the experimental D -distribution on the $P_m = 0.89$ sample exceeded that expected from the known M -distribution.

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