

Abstract Submitted
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Diffusion in Polypropylene Melts: Role of Stereochemistry.¹

ERNST VON MEERWALL, NUMAN WAHEED, WAYNE MATTICE, University of Akron — We have performed numerical simulations and experiments at 180°C to study the effect of stereochemical composition on the diffusion (D) of linear polypropylene melts of moderate polydispersity. The coarse-grained Monte-Carlo (MC) simulations were based on the rotational isomeric state model and repulsive Lennard-Jones potentials. For the pulsed-gradient ¹H NMR diffusion measurements the three specimens used had probabilities of meso diad $P_m = 0.02, 0.23, \text{ and } 0.89$. The conversion factor between MC steps and real time was obtained by comparison with the measured D; no dependence on stereochemistry was evident. Using a molecular-weight (M)-scaling known from earlier work on n-alkanes, results were normalized to a common M after accounting for differences in experimental polydispersity. Results agreed closely with the monodisperse simulations. D at high P_m was found to be several times faster than at low P_m , but the simulation also showed a maximum in D at P_m near 0.75, an effect attributed to quenched randomness. Likely for similar reasons the experimental D-distribution for the $P_m = 0.89$ sample greatly exceeded that expected from the known polydispersity.

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Ernst von Meerwall
University of Akron

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