

Abstract Submitted  
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**Effect of Stereochemistry and Polydispersity on Diffusion in Polypropylene**<sup>1</sup> ERNST VON MEERWALL, NUMAN WAHEED, WAYNE MATTICE, Univ. Akron — We have performed dynamic Monte-Carlo (MC) simulations and pulsed-gradient diffusion (D) experiments to study the effect of stereochemical composition in linear polypropylene (PP) melts. 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 of differing molecular weight  $M$  and dispersity, with the probability of a meso diad  $P_m = 0.02$  (syndiotactic), 0.23 (atactic), and 0.89 (nearly isotactic). The experiment supplied the fixed conversion between MC steps and real time; no dependence on  $P_m$  is expected. Both simulation and  $M$ -scaled experiment found  $D$  at high  $P_m$  several times faster than at low  $P_m$ . The constant- $M$  simulation also showed a maximum near  $P_m = 0.8$  due to quenched randomness. To find the source of the remaining disagreement with experiment, new simulations tracked the samples'  $P_m$ , mean  $M$ , and polydispersity, producing modest improvement. We suspect that the GPC determination of  $M$  and its distribution, based on linear polyethylene calibration, is somewhat dependent on PP stereochemistry (via  $D$ ), generating misleading results.

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