Abstract Submitted for the MAR09 Meeting of The American Physical Society

Effect of Stereochemistry and Polydispersity on Diffusion in Polypropylene¹ ERNST VON MEERWALL, NUMAN WAHEED, WAYNE MAT-TICE, 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 Pm = 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 Pm is expected. Both simulation and M-scaled experiment found D at high Pm several times faster than at low Pm. The constant-M simulation also showed a maximum near Pm = 0.8 due to quenched randomness. To find the source of the remaining disagreement with experiment, new simulations tracked the samples' Pm, 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.

¹Supported in part by NSF (DMR 04-55117)

Ernst von Meerwall University of Akron

Date submitted: 17 Nov 2008

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