Influence of chain branching on topological constraint of entangled polyethylene melts

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The topological constraint, entanglement, is closely related to molecular conformation which could be influenced by chain branching effect. In this study, we show the effect of long- and short-chain branching on the structural properties and topological measure on entangled network of polyethylene (PE) melts via Advanced Monte Carlo simulation and Z-code, by comparing with several linear PE melts that has same number of carbon atoms, based on total chain length, longest linear, and backbone of branched chain dimension. From these systems, we quantified some important topological properties: (a) the primitive path contour length, (b) the number of entanglements per chain, (c) the end-to-end length of an entanglement strand, and (d) the number of carbon atoms per entanglement strand. The results show that short-chain branched PE have more compact chain conformations with smaller number of entanglements per chain compared to linear PE, while long-chain branched have more extended chain conformation and relatively larger number of entanglements than linear PE.