

Abstract Submitted  
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**Molecular modeling simulations in phase stability of polyethylene solutions at elevated pressures** MOEED SHAHAMAT, McGill University, ALEJANDRO D. REY, Professor-McGill University — Molecular dynamics (MD) simulations using the OPLS-AA force field are conducted to compute pressure, molecular weight dependence of Hildebrand's solubility parameters (SP) and density of hexane and high-density polyethylene (HDPE) at high pressures from 100 to 3000 bar. The electrostatic energy contribution to the cohesive energy and density leads to increases in the SP with pressure for molecular mechanical models (MMM) with and without electrostatic terms. The Flory-Huggins interaction parameter (IP) predicted from the pressure dependence of SPs and molar volumes decreases upon increasing pressure, indicating that miscibility improves by raising pressure. This is consistent with the solution polymerization process for producing PE, where pressure-induced phase separation (PIPS) is used to separate the polymer from solution. Exclusion of electrostatic potentials in the MMM results in larger IPs while the decreasing trend remains intact with and without electrostatic forces. There is a pressure limit beyond which the IP has less sensitivity to pressure indicating that PE miscibility is not further affected. It is shown that pressure increases the chemical potential factor of the phase stability condition, stabilizing the solution. These results contribute to the fundamental understanding of PIPS, an important demixing process poorly understood when compared to thermally-induced phase separation.

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None

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