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# A Molecular Dynamic Simulation Study to Explore Role of Chain Length in Predicting Useful Characteristic Properties of Commodity and Engineering Polymers

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**Abstract :** This work attempts to use molecular simulations to create equilibrated structures of a range of commercially used polymers. Generated equilibrated structures for polyvinyl acetate (isotactic), polyvinyl alcohol (atactic), polystyrene, polyethylene, polyamide 66, poly dimethyl siloxane, poly carbonate, poly ethylene oxide, poly amide 12, natural rubber, poly urethane, and polycarbonate (bisphenol-A) and poly ethylene terephthalate are employed to estimate the correct chain length that will correctly predict the chain parameters and properties. Further, the equilibrated structures are used to predict some properties like density, solubility parameter, cohesive energy density, surface energy, and Flory-Huggins interaction parameter. The simulated densities for polyvinyl acetate, polyvinyl alcohol, polystyrene, polypropylene, and polycarbonate are 1.15 g/cm3, 1.125 g/cm3, 1.02 g/cm3, 0.84 g/cm3 and 1.223 g/cm3 respectively are found to be in good agreement with the available literature estimates. However, the critical repeating units or the degree of polymerization after which the solubility parameter showed saturation were 15, 20, 25, 10 and 20 respectively. This also indicates that such properties that dictate the miscibility of two or more polymers in their blends are strongly dependent on the chosen polymer or its characteristic properties. An attempt has been made to correlate such properties with polymer properties like Kuhn length, free volume and the energy term which plays a vital role in predicting the mentioned properties. These results help us to screen and propose a useful library which may be used by the research groups in estimating the polymer properties using the molecular simulations of chains with the predicted critical lengths. The library shall help to obviate the need for researchers to spend efforts in finding the critical chain length needed for simulating the mentioned polymer properties.

**Keywords :** Kuhn length, Flory Huggins interaction parameter, cohesive energy density, free volume
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