عنوان مقاله:

A new method for Monte Carlo simulation of chain molecules with soft potentials

محل انتشار:

پنجمین کنگره بین المللی مهندسی شیمی (سال: 1386)

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خلاصه مقاله:

A new Monte Carlo simulation for chain molecules with the soft potential, Lennard-Jones, with novel boundary conditions is presented. The new method is more accurate in prediction PVT behavior of chain molecules in comparison with other simulations and analytical Equation of states. The accuracy of obtained data is also examined with experimental data of chain molecules with similar molecular parameters. A Configurational Biased Monte Carlo algorithm (CBMC) is developed in a new manner for hydrocarbons from C1 up toC7 and for C7 to C10 the recoil growth (RG) method is also applied to increase simulation speed.

کلمات کلیدی:

Configurational Biased Monte Carlo; Computer Simulation; Hexagonal Cells; Linear Chain Molecules; PVT Data