

Brownian dynamics studies to portray DNA conformation in roll coating process

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Recent developments in direct visualization methods, coupled with Brownian dynamics simulations, have allowed the dynamics of a single large molecule in homogeneous and non-homogeneous flows to be investigated. In this study, we have numerically estimated DNA dynamics in small-scale coating flow, based on its experimental observations (Duggal and Pasquali, J. Rheol., 2004). In order to depict configuration of DNA molecules in non-homogenous coating flow, we have calculated λ -DNA molecules via Brownian dynamics simulation technique in roll coating flow field solved by Flow-3D. All configurations portrayed by Brownian dynamics simulation quantitatively coincided with the experimental observations. This theoretical investigation will be useful to find optimal processing conditions to improve physical properties of coated film incorporated with the orientation of polymer chains.