

Abstract Submitted  
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**Dynamics of Adsorption-Desorption of Linear Polymer Chains to Spherical Nanoparticles: A Monte Carlo Investigation**<sup>1</sup> PETER J. DIONNE, CATALIN R. PICU, Mechanical, Aerospace and Nuclear Engineering, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — Dynamics of attachment/detachment processes of chains to/from spherical fillers in a polymer nanocomposite is investigated by means of numerical simulations using a chemistry-specific model for the polymer. The effects of chain length, chain-to-filler distance, filler radius, and polymer-particle interaction energy on the attachment/detachment processes are studied. It is found that the time a chain is in contact with a filler scales with the number of attached beads as expected from Rouse behavior. A deviation from Rouse behavior is observed at long attachment times where a plateau value in the number of attached beads is observed. This deviation was found to depend on the relative size of the chain and adsorption volume but was not related to entanglement effects. Changing the polymer-particle interaction energy from repulsive to attractive slows down the detachment process. An average characteristic detachment time was calculated as a function of polymer-particle interaction energy that follows an Arrhenius equation, where the activation energy is proportional to the polymer-particle interaction energy.

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Rahmi Ozisik  
Rensselaer Polytechnic Institute

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