

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Interaction of Surface Modified Carbon Nanotubes with Supercritical Carbon Dioxide¹ NIHAT BAYSAL, BANU UNSAL, Department of Chemical Engineering, Yeditepe University, Istanbul 34755, Turkey, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180, USA — The properties of carbon nanotube (CNT)-polymer nanocomposites are far below than those calculated, mainly due to poor dispersion or interface quality. This is particularly difficult for single walled carbon nanotubes (SWNTs) as they tend to form bundles or ropes that are difficult to exfoliate. Supercritical fluid (SCF) assisted processing is one of the methods that can be used to exfoliate/disperse CNTs along with modifying the interface of the CNTs. Molecular dynamics simulations were performed to understand how the surface modifiers behave near SWNT surface with and without the presence of SCF molecules. It is also important to understand the diffusivity of SCF molecules between SWNT bundles and the effect of surface modifiers on diffusion. Octane and *n*-perflourooctane molecules were used as surface modifiers with varying tethering density and carbon dioxide (CO₂) was chosen as the SCF. Results showed that the system with highest number of *n*-perfluorooctanes presented the highest degree of success in separating the SWNTs in the presence of CO₂.

¹This material is based upon work supported by the National Science Foundation under Grant 0500324.

Rahmi Ozisik
Rensselaer Polytechnic Institute

Date submitted: 29 Nov 2005

Electronic form version 1.4