CORRELATING THE DEPENDABILITY OF NANOPARTICLE DISPERSION WITH THE PRESENCE OF MATRIX POLYMER IN NANOPARTICLE COMPOSITES

Abayomi Adeleke and Venkat Padmanabhan
Department of Chemical Engineering and Center for Energy System Research

Abstract

The systems investigated are polymeric systems identical shown in LAMMPS simulations. Three solvent systems, 0.1 and 0.5, were used to model the nanoparticles, grafted polymer and matrix polymer. Finite extensible nonlinear elastic potential was used to model all the polymers chains in the system. Degree of polymerization

System parameters

- Matrix polymer = 40
- Grafted polymer = 10
- All monomers are chemically identical
- mass \( m \) = 1
- intermolecular distance \( \sigma_p \) = 1
- All nano-particles are chemically identical
- mass \( m \) = 1
- intermolecular distance \( \sigma_p \) = 5

Polymer grafting

- \( N_k \) chains were grafted on the surface of nanoparticle such that the grafting density:
  - \( \Sigma_g = 0.4 \) (chains/ \( \sigma_p \))
  - Soft potential was used to ensure good distribution of the grafted chains on the nanoparticles to avoid depletion effects.
  - Parking fractions were calculated using:
    - \( \eta_T = \frac{1}{2} (\sigma_g^3 \rho_p + \sigma_g^3 \rho_n + \sigma_g^3 \rho_B) \)
    - Volume fractions were calculated using:
      - \( \phi_T = \frac{1}{3} \rho_p + \frac{2}{3} \rho_n + \frac{1}{3} \rho_B \)

Furthermore, the radial distribution function (RDF) will be used to investigate the structural properties of the systems.

Results:

Presented below are the results of calculations of RDF and MSD from the three systems that were simulated.

Fig 1: MSD of nanoparticles before evaporation. The figure shows that we have the highest displacement in system with matrix polymers. This can be attributed to improved steric effect on the nanoparticles.

Fig 2: RDF of nanoparticles before solvent evaporation. Wide peak in system 1 agrees with results from Fig 1 as we have good dispersion in system 1.

Fig 3: MSD of nanoparticles after evaporation. Improved dispersion of nanoparticles seen in system 3 can be attributed to the more effective steric effect due to longer polymer chains.

Fig 4: RDF of nanoparticles after solvent evaporation. Reduction in first peak in systems 2 and 2 suggest there is better dispersion in the absence of solvents.

Methodology

Coarse-grained molecular dynamics simulations using LAMMPS parallel MD packages is used in simulating a system which includes solvents, matrix homopolymer chains and nanoparticles grafted with linear polymer chains (PGNPs). Three systems were developed with different but related compositions namely:

- Solvent, matrix polymers and polymer grafted nanoparticles
- Solvent and polymers and polymer grafted nanoparticles
- Solvent and PGNPs with extended polymer grafted nanoparticles

The mean squared displacement (MSD) of the nanoparticles in the systems will be calculated to understand the diffusivity of the nanoparticles. This will be done to shed light on some dynamic properties of the nano-particles in the system.

Acknowledgments:

Tennessee Tech University, Department of Chemical Engineering Center of Energy systems research

Table 1: Some parameters of the systems simulated

<table>
<thead>
<tr>
<th>S/N</th>
<th>System type</th>
<th>( \phi_{nano} ) (with solvent)</th>
<th>( \phi_{nano} ) (No solvent)</th>
<th>( \Phi - sol )</th>
<th>NPs</th>
<th>Matrix Poly</th>
<th>Graft-len</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sol+mat+pgnp (RED)</td>
<td>0.05</td>
<td>0.1</td>
<td>0.5</td>
<td>40</td>
<td>815</td>
<td>10</td>
</tr>
<tr>
<td>2</td>
<td>Sol+pgnp (BLUE)</td>
<td>0.05</td>
<td>0.3</td>
<td>0.83</td>
<td>40</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>3</td>
<td>Sol+extpgnp (BLACK)</td>
<td>0.05</td>
<td>0.1</td>
<td>0.5</td>
<td>40</td>
<td>0</td>
<td>36</td>
</tr>
</tbody>
</table>