

### Modules Used

MAPS  
LAMMPS  
Amorphous Builder  
SciDPD

The phase behavior and morphology of two additives, Glycoltristearate and Glycoltrinonane in a PET polymer matrix has been studied using classical molecular dynamics and Dissipative Particle Dynamics within the MAPS framework.

In order to identify the miscibility and distribution of the two additives in the matrix, Dissipative Particle Dynamics calculations have been performed using the SciDPD plug-in. To generate the appropriate parameters for the simulations, solubility parameters for the fragments needed to be obtained.

The solubility parameter for PET is reported as  $20.9 \text{ Mpa}^{0.5}$ , for the hydrophobic tail beads of the glycoltriolefins the solubility parameter for polyethylene ( $15.8 \text{ Mpa}^{0.5}$ ) has been used [1].

In order to determine the repulsive parameter for the glycol section atomistic simulations using the LAMMPS plug-in and the Dreiding force field with Buckingham potentials [2] have been performed on bulk structures of glycoltrimethane. The starting structures were generated using the Amorphous Builder followed by a series of molecular dynamics simulations. The solubility parameter was determined as a result of these calculations with  $23.5 \text{ Mpa}^{0.5}$ .

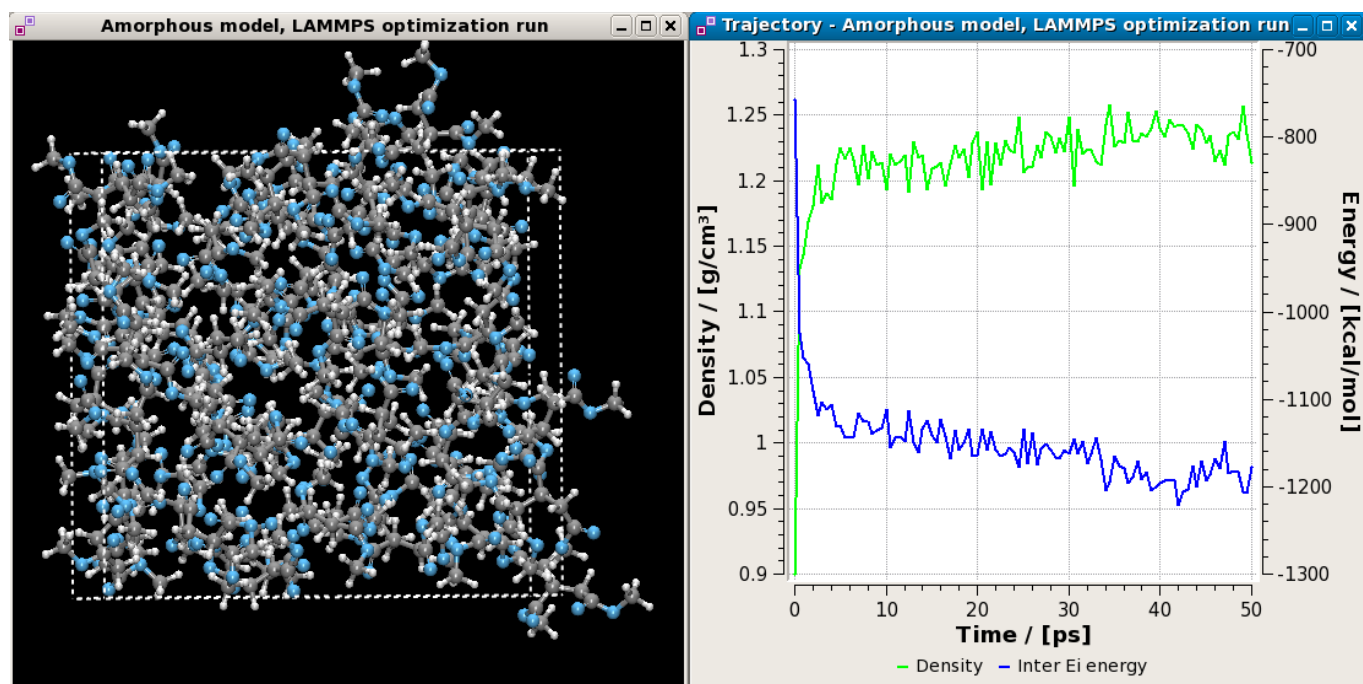


Figure 1: Structure and time evolution of density and cohesive energy for glycoltrimethane

## Dispersion of additives in a PET polymer matrix

## Application Note

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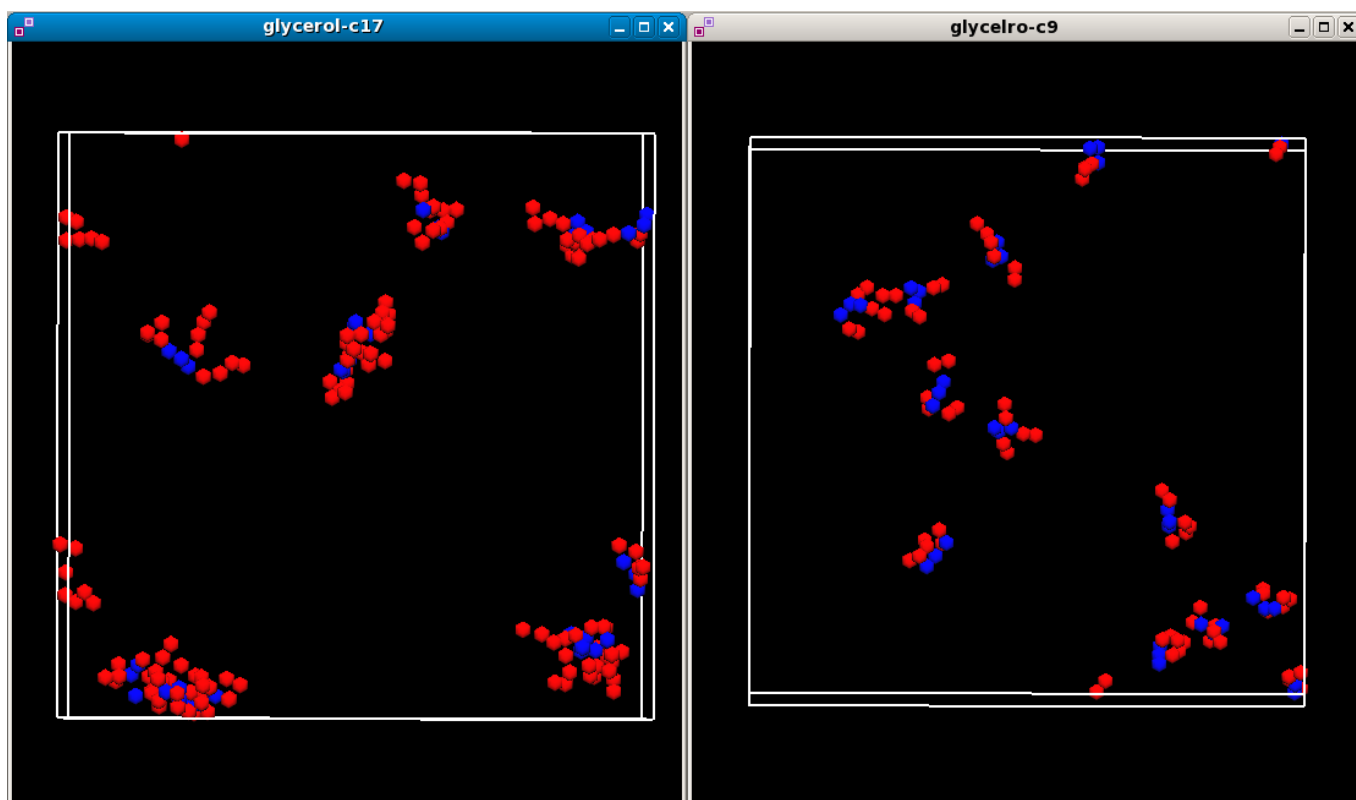


Figure 2: Glycoltristearate (left) and Glycoltrironane(right) in a PET matrix, polymer is not displayed

Figure 1 shows the end structure of the simulation as well as the evolution of the density and cohesive energy of the model system.

The picture in page 4, figure 1 shows the end structure of the simulation as well as the evolution of the density and cohesive energy of the model system.

These solubility parameters have been translated into repulsive parameters for the DPD coarse grained simulation. Here one Ethyleneterephthalate monomer was represented by two beads, resulting in a bead volume of  $155 \text{ \AA}^3$ .

The repulsive parameters were:

All self 25

Tail/ head 32

Tail/PET 30



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Head/PET 26

A higher number stands for a higher repulsion, units are reduced units. The PET chain was considered semi rigid with a bending force constant of 30 reduced units/rad.

100mers of PET were simulated with 5 % additive respectively. A simulation box of 20 reduced units was simulated for 20000 time steps. This represents a box length of about 16 nm in each direction.

The results of the runs can be seen in figure 2.

An agglomeration of the additive (two and three molecules) in the polymer matrix can clearly be observed in the stearate case, the short tail additive disperses evenly through the matrix.

The relative diffusion coefficient of the short tail additive is about 40 % higher than the diffusion coefficient of the long tail additive.

In order to quantify the results, longer runs on larger systems will be necessary. In this case also reliable diffusion coefficients for the additive could be determined.

### References:

1. *Properties of polymers*, T. W. van Krevelen, Elsevier, London, 1990
2. S.L. Mayo, B.D. Olafson and W.A. Goddard, *J. Phys. Chem.*, 94, 8897, 1990