Dynamical modelling of morphology development in multiphase latex particles

Executive summary

In this project a dynamic model was designed to predict the development of the morphology of multiphase waterborne systems, such as polymer-polymer and polymer-polymer-inorganic hybrids.

Challenge overview

Waterborne polymers are used in a wide range of applications including synthetic rubber, paints, adhesives, additives in paper and textiles, leather treatment, impact modifiers for plastic matrices, additives for constructing materials, cosmetics, flocculants, diagnostic tests and drug delivery. Although homogeneous particles meet the requirements of many of the applications, multiphase waterborne polymer particles provide advantages in more demanding applications. Thus, 2-phase soft-hard particles have been used for coatings, which combine a low minimum film forming temperature and a high blocking resistance. Rubber thermoplastic core-shell particles are useful to impart toughness to thermoplastics resins. Waterborne polymer-polymer hybrids (e.g. alkyd-acrylic, polyurethane-acrylic and epoxy-acrylic) have been developed in an attempt to combine the useful properties of both polymers, avoiding their drawbacks. Waterborne polymer-inorganic (e.g., silica and clay) hybrids led to improvements in mechanical and thermal resistances.
Performance of multiphase waterborne polymer particles depends on particle morphology. The synthesis of new morphologies is time and resources consuming as it largely relies on heuristic knowledge. Therefore, there is a need for developing models describing the kinetics of phase morphology development of multiphase systems, which could be used to guide the design and synthesis of high performance waterborne polymers.

Implementation of the initiative

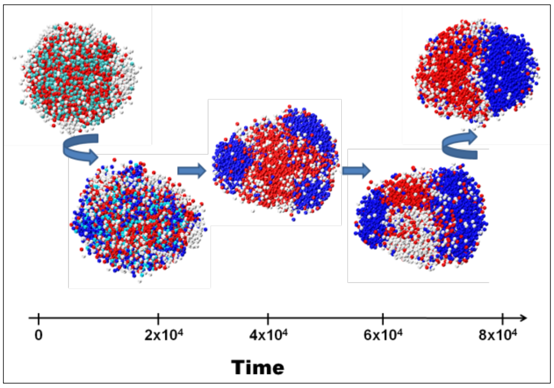
The Institute for Polymer Materials of the University of the Basque Country (POLYMAT) and the Basque Center for Applied Mathematics (BCAM) joined efforts to develop such a model. Both institutions have complementary expertise: POLYMAT is proficient in waterborne dispersed polymers and polymerization in dispersed media. It works in close collaboration with industrial companies such as Akzo Nobel, Arkema, BASF, Comex, Cytec, Nuplex Resins, Solvay, Stahl and Wacker Chemie. BCAM has a rich experience in mathematical simulation. The project was funded using POLYMAT / BCAM own resources with additional financial support from Ikerbasque, Basque Foundation for Science.

The problem

The morphology of the particles is the result of the interplay between kinetics and thermodynamics during the polymerization of a monomer in the presence of preformed polymers and/or inorganic materials in particles dispersed in water. Therefore, the model should account for the simultaneous polymerization and phase migration. The dynamics of the particle morphology development was simulated by means of the velocity Langevin dynamics performed in the NVT ensemble.

Results and achievements

For the first time, a model able to describe the dynamics of the development of the morphologies for multicomponent waterborne particles is available. The model accounts for the formation of graft copolymer, which can be used to control the particle morphology. This opens the possibility of a knowledge-based design and synthesis of materials for a wide range of applications.



Evolution of 3-phase particle morphology predicted by computer simulation

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