MOLECULAR MIGRATION IN POLY(VINYL ALCOHOL) MIXTURES

Katarzyna Majerczak and Zhenyu Jason Zhang
School of Chemical Engineering, University of Birmingham, Edgbaston, B15 2TT, Birmingham, United Kingdom
Contact Email: kxm654@bham.ac.uk

Introducing additives such as plasticisers into polymer materials is a common way to enhance their mechanical properties while retaining the inherent advantages of these materials. Although characteristics are improved upon modification with additives, unintended changes in materials' structure (e.g. blooming or segregation) due to guest molecule migration may occur. As a result, these systems can exhibit long term non-equilibrium characteristics, potentially affecting their operational life cycle. Current scientific theories cannot fully explain these phenomena. Therefore, developing a molecular understanding within these systems may result in enhanced, environmentally friendly products with improved performance and shelf life.

This work aims to understand the migration characteristics of small molecules one such complex polymer mixture - poly(vinyl alcohol) (PVA) packaging materials that are in contact with concentrated detergent. Thin PVA films containing glycerol, surfactants of various headgroup chemistry, and Rhodamine B (RhB) as a fluorescent tracer were examined using Fluorescence Recovery After Photobleaching (FRAP) and Fluorescence Correlation Spectroscopy (FCS). It was found that the migration is determined by both molecular arrangement within the film and the magnitude of inter-species molecular interactions. Glycerol initially improved the flexibility of PVA but imposed steric inhibition once the concentration exceeded 44 wt% (Fig. 1a-c). Furthermore, surfactants reduced the diffusivity of RhB in PVA matrix in both thin films and bulk solutions. Steric inhibition effects explain this phenomenon in compositions doped with non-ionic surfactant (Fig. 1d), however, for films containing cationic or anionic surfactant, molecular interactions and consequent change in diffusivity of RhB are the likely explanation (Fig. 1e).

Using thin polymer films as a proxy for industrial formulations, we revealed fundamental migration mechanisms within these materials. Both molecular arrangement and molecular interactions control the migration at the macroscopic scale, therefore, this simplified system can be used to create a set of design rules for commercial polymer film products.

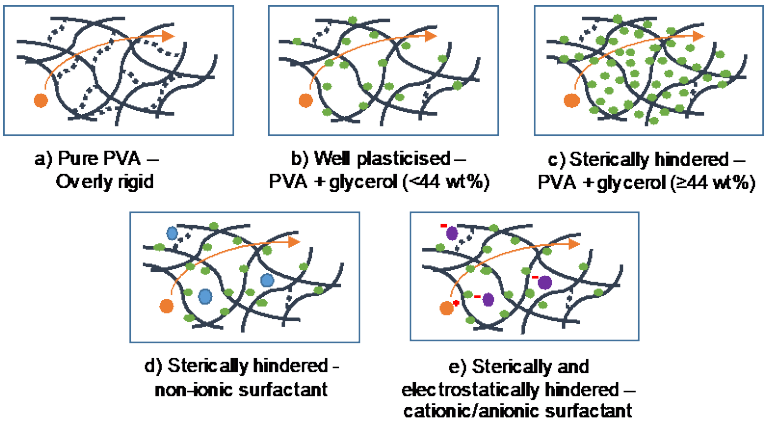

Fig. 1. Scheme of factors controlling RhB (orange sphere) diffusion through a polymer matrix (lines). Dashed lines – PVA-PVA hydrogen bonding, green spheres – glycerol, blue spheres – nonionic surfactant, purple spheres – anionic surfactant.

Back to Programme