Sorption in polyolefins: equilibria, diffusion and morphology

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Polyolefins are commercially important due to their massive production and variety of applications. The two most common polyolefins, polyethylene and polypropylene, account for almost 50% of the annual worldwide plastics production. Sorption equilibria and transport of penetrants in polymers significantly influence polymerization processes and subsequent product treatment such as degassing. Sorption also enhances unwanted agglomeration of polymer particles in the reactors, which can lead to the shut-down of the whole production line.

This contribution presents two experimental techniques for the measurement of sorption and diffusion in polyolefin powder: a gravimetric apparatus and a pressure-decay apparatus. Both the sorption of pure compounds and co-sorption are addressed. The measured equilibrium data are correlated with PC-SAFT simulations, while several models are used for diffusion, namely (i) simple Ficks law, (ii) multigrain or bi-disperse model, and (iii) complex model of transport in reconstructed 3D porous particles.

In the case of polyolefins, the sorption processes depend on their morphology. The characterization of semi-crystalline polyolefin morphology is thus essential for the analysis of sorption and diffusion in polyolefins, as it provides input data for mathematical models and as the comparison of experimentally measured sorption data with the morphology enables to study the structure-property relationships. This contribution thus presents several advanced experimental techniques for the characterization of polyolefin morphology, namely: (i) X-ray micro-tomography (μCT), (ii) time-domain NMR (TD-NMR) and (iii) confocal Raman microscopy.

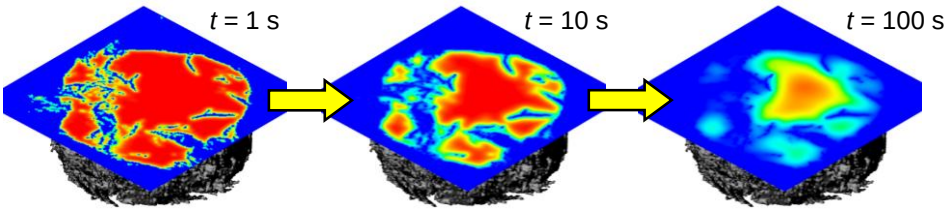


Figure. Simulation of propylene degassing from a porous polypropylene particle. The simulation considers a real 3D morphology based on micro-tomography data.