

POLYETHYLENE CHANGES DURING LIQUID SORPTION OBSERVED BY LOW FIELD NMR

Patrik Schneider^a, Tomáš Chaloupka^a, Václav Pelc^b, Juraj Kosek^{a,b}

^aUniversity of Chemistry and Technology Prague, Department of Chemical Engineering, Technická 5, 166 28, Prague 6, Czech Republic

^bResearch Centre New Technologies, University of West Bohemia Univerzitní 8, 306 14 Pilsen, Czech Republic

The observation and evaluation of liquid sorption in polyolefins is important for the control and operation of liquid-dispersion (slurry) production processes. However, measuring the sorption equilibria of liquids in polymers and the dynamics of their sorption proves to be a challenging task, so that new approaches tackling these issues are still in the continuous development. We employ a low field NMR, a very robust spectroscopic method. Nowadays, NMR popularity increases due to its wide applicability (e.g., water content in oil), low cost, reasonably fast and non-destructive measurements.

We performed sorption experiments of hexane, which is commonly used as organic solvent/diluent and which shall be thermodynamically similar to 1-hexene, a commonly employed comonomer in the production of ethylene copolymers of various densities. To achieve a major progress in the observation of the sorption process in real time, we modified the Magic sandwich echo and the Goldman-Shen pulse sequence for the sorption experiment. Thus we can now measure the sorption process from the beginning up to the equilibrium. Moreover, we can distinguish individual polymer phases and evaluate their weight content, which can be validated by an independent gravimetric analysis. Thus, we can evaluate the amount of hexane in polyethylene during its continuing sorption.

Data obtained by this work can also be used for the interpretation of the semi-crystalline polymer morphology changes during the sorption process and even for the better understanding of the sorption process itself. Moreover, by using of TD-NMR we can determine diffusion coefficients and to characterize the thickness of swollen amorphous domains. Low field NMR studies are complemented with PC-SAFT simulations of liquid sorption in amorphous PE.