

Meso-scale description of polyolefin powders: electrostatic charging, agglomeration and sorption processes

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Mathematical models of various levels of fidelity are basic tools of process and reaction engineering. These tools can describe almost all essential phenomena in the catalytic polymerization of olefins or the combination of these phenomena: reaction kinetics, mass, heat and momentum transport, thermodynamics, reactors, process flowsheets, residence time distribution, catalyst/polymer particle morphology evolution, melt rheology and evolution of hetero phase polymers (such as high-impact polypropylene). These tools can serve multiple purposes: better understanding (research), computer-aided tailoring of products with desired properties, off-line optimization of grade transitions and even on-line control and optimization of processes. In this contribution we focus on the experimental research and modeling of insufficiently understood phenomena of particle agglomeration and thermodynamics of (co-)sorption in relation to meso-scale, i.e., particle and/or semi-crystalline morphology.

Particle agglomeration is affected by electrostatics (i.e., generation, transfer and neutralization of charge formed on the particle surface), adhesion dynamics (i.e., evolution of particle-particle or particle-wall bonding forces) and softening (caused by temperature and swelling). We are going to present experimental results systematically characterizing all three above described contributions to particle agglomeration (i.e., electrostatics, adhesion dynamics and softening). We shall concentrate especially on the poorly understood problem of electrostatic charging of particles. The developed model coupling DEM (discrete element method) for the description of particle dynamics and TEA (trapped electron approach) for the description of charging dynamics will be presented and demonstrated to provide good prediction of charging in dependence on temperature and particle size distribution.

The thermodynamic description of (co-)sorption and diffusion of penetrants in polyolefins and the swelling of polyolefins at conditions relevant to catalytic polymerization of olefins is still not at the predictive level required by process models of various fidelity. We shall explain underlying reasons for this state of current knowledge. We will present excerpts from the probably largest database of sorption and swelling data measured in our laboratories for PE densities from 0.90 to 0.96 g/cm³ covering practically all relevant grades and reactor conditions including sorption of both gaseous and liquid penetrants. We will demonstrate how to interpret the sorption data in the context of our recently proposed semi-crystalline structure of PE based on SAXS, TD-NMR and AFM measurements, i.e., measurements independent of sorption isotherms. Moreover, we will demonstrate the modeling of diffusion in the reconstructed semi-crystalline spherulites and compare the results to experiments.

Chmelař J., Matuska P., Gregor T., Bobak M., Fantinel F., Kosek J.: *Chemical Engineering Journal* 228, 907-916 (2013).

Chmelař J., Pokorný R., Schneider P., Smolná K., Belsky P., Kosek J.: *Polymer* 58,189-198 (2015).

Chmelař J., Smolná K., Haškovcová K., Podivinská M., Marsalek J., Kosek J.: *Polymer* 59, 270-277 (2015).