

Experimental Study of the Influence of Molecular Architecture and Morphology on the Gas Solubility in Polyethylene Grades

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The gas solubility of semi-crystalline polymers plays an essential role in various industrial applications, including recycling techniques such as supercritical fluid extraction[1] or CO₂ capture applications utilizing membranes[2]. The prediction of gas solubility in different polymer grades is crucial for developing durable and sustainable products and applications. It is well-understood that gas solubility predominantly occurs in the amorphous areas of the polymer, resulting in heterogeneous solubility distributions in different morphological regions. Moreover, it has been shown that the presence of crystalline domains inhibits the amorphous domains from dissolving gas[3]. To understand and describe these complex interrelations, comprehensive gas solubility measurements linked with molecular architecture and morphological characteristics are important. This information is required to further validate sophisticated modeling approaches, which have been successfully developed, such as Monte Carlo simulations with an *ad hoc* constraint in the osmotic ensemble[4], the incorporation of a constraint pressure in the thermodynamic modeling[5] and multi-scale thermo-mechanical modeling with consideration of eigen pressure [6,7]. In this work, a comprehensive experimentally obtained relationship between CO₂ solubility in different polyethylene grades and polymer's bivariate molecular architecture distribution, i.e. molecular weight distribution and comonomer distribution, as well as morphology, is established. Additionally, the mechanical, thermophysical properties and morphological characteristics of the pure polymer are linked, such that structure-property relationships are fully elucidated which provide a solid base for future thermodynamic model development and validation.

References

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