APPLICATION OF DATA-DRIVEN COMPUTATIONAL METHODS TO LLDPE FLUIDIZED-BED REACTORS FOR PREDICTION OF END-USE POLYMER PROPERTIES IN TERMS OF PROCESS CONDITIONS AND MACROMOLECULAR ARCHITECTURE

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ABSTRACT

The linear-low density polyethylene (LLDPE) production is expected to grow significantly owing to its unique end-use properties such as high tensile strength, high impact resistance, and flexibility. The properties of LLDPE makes it suitable for applications in packaging, agriculture, building-construction, and healthcare. By 2025, the LLDPE production is expected to rise to more than 56 million tons. LLDPE is produced via the copolymerization of ethylene with butene, hexene and octene, in the presence of Ziegler-Natta catalysts. Several companies have developed and are licensing gas-phase technologies for production of LLDPE including the Univation's Unipol process, the Innovene G (Ineos), the LyondellBasell's Spheriline, and the Borstar process of Borealis. All of them are based on the same principle of using a fluidized-bed gas-phase reactor, although the operating mode and conditions differ among the different licensors.

The end-use properties of LLDPE (e.g., tensile strength, tear strength, impact strength, puncture, environmental stress crack resistance, etc.) do depend on the reactor operating mode and conditions in the FBR, the resin macromolecular architecture, and post-reactor processing conditions. The effects of all these process conditions and polymer chain architecture on the end-use polymer properties can be quantified via the application of polymer reaction engineering, polymer science, and polymer processing fundamentals. However, gaps in these fundamental theories limit their application, particularly in developing new LLDPE grades with a desired set of end-use properties. On the other hand, machine learning methods including regression techniques (e.g., multivariate statistics, Projection to Latent Structures (PLS), etc.) and Neural Networks can address the present limitations of fundamental modeling methods and identify the underlying relationships between process conditions-macromolecular architecture–end-use polymer properties. In this study, data-driven multivariable statistical regression methods and neural networks are applied to an industrial LLDPE process to establish the underlying relationships between process operating conditions in a gas-phase FBR – macromolecular architecture (i.e., molecular weight distribution from GPC curves; copolymer composition via TREF, etc.) – post-reactor processing conditions (i.e., compounding, extrusion, etc.) – end-use properties of commercial LLDPE grades.

KEYWORDS: LLDPE Manufacturing, Fluidized-bed Reactors, Machine Learning, Mulitvariate Statistical Analysis, PCA, PLS, Neural-Networks

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