Title: Application of Machine Learning on Estimation of Propylene Polymerization Conditions in a Two-Reactors System

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Reference 5:
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Reference 9:
Reference 10:
Reference 11:
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Abstract:

Polymerization via the two-reactor system is widely used in industry to produce polymers with desired microstructures and properties. The system allows control of polymerization conditions in each reactor; therefore, it can be used to produce polymers with a wide range of structures and applications. However, the system is complicated as the polymerization conditions in both reactors may contribute differently to final product microstructures. Therefore, finding “the right” polymerization conditions for this system to produce the desired product can be a challenging problem. The purpose of this study was to explore the concept of using artificial neural network (ANN) model, one of the machine learning techniques, for describing the relationships between polymerization conditions and polymer microstructures though model learning dataset. This will show the potential application of machine learning concept to model forward-inverse polymerization processes, which typically are complex and non-linear problems.

In this work, the ANN model was developed to describe the relationships between the polymerization conditions (i.e., hydrogen amount, residence time) and the microstructures (i.e., molecular weight distribution, MWD) of polypropylene produced with Ziegler–Natta catalysts in the two-reactor system. The forward model was developed to predict the microstructures from a given set of polymerization conditions, while the inverse model was developed to estimate the polymerization conditions for desired microstructures. The results showed that the forward model can impressively predict the yield and microstructures. The inverse model can also adequately estimate the polymerization conditions. This provide the evident that our approach can be an effective solution for product development in a complex polymerization system.