Title: Tailor-making Chain Microstructures of Ethylene/1-Butene Copolymers using Machine Learning

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Abstract:

Note: maximum length of 400 words.

Ethylene/1-butene copolymers with desired microstructures can be produced with specific polymerization conditions. Important question is how to find these conditions effectively for the system of interests. Copolymerization kinetic model can be used to predict chain microstructures for a given set of polymerization conditions, but it cannot be inversely solved to estimate polymerization conditions from desired chain microstructures. The denoising autoencoder (DAE) model, a specific machine learning technique based on artificial neural network (ANN) concept, may be the solution for this important question.

In this work, DAE model was developed to help estimate polymerization conditions (i.e., monomer and comonomer concentration, hydrogen concentration, cocatalyst concentration, and temperature) for producing polymers with desired microstructures (i.e., molecular weight distribution (MWD), chemical composition distribution (CCD), number and weight average molecular weights). To illustrate the potential of this approach, the system with two catalytic site types, which can produce either unimodal or bimodal microstructural distributions, was used as an example.

There were two models tested in this work: model A with microstructural distributions (MWD and CCD) and model B with additional information on average microstructures and polymer yield. The results showed that both proposed DAE models can adequately estimate polymerization conditions from desired microstructures with acceptable mean square error (MSE). As expected, more microstructural information (model B) lead to better estimation of polymerization conditions with lower MSE. Robustness of both models were also considered by testing with ±5% and ±10% uniform random noises in average properties and yield of input data, which represent common experimental errors during GPC analysis and weight measurement. Although the results showed that estimated polymerization conditions may be significantly deviated from the diagonal line, the average properties recalculated from estimated polymerization conditions were mostly well within the range ±5% and ±10% errors. Therefore, these results provide the great proof of concept for the future applications in the complex industrial system.