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Performance Comparison of Different Regression Methods for a Polymerization Process with Adaptive Sampling

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Abstract : Developing complete mechanistic models for polymerization reactors is not easy, because complex reactions occur simultaneously; there is a large number of kinetic parameters involved and sometimes the chemical and physical phenomena for mixtures involving polymers are poorly understood. To overcome these difficulties, empirical models based on sampled data can be used instead, namely regression methods typical of machine learning field. They have the ability to learn the trends of a process without any knowledge about its particular physical and chemical laws. Therefore, they are useful for modeling complex processes, such as the free radical polymerization of methyl methacrylate achieved in a batch bulk process. The goal is to generate accurate predictions of monomer conversion, numerical average molecular weight and gravimetrical average molecular weight. This process is associated with non-linear gel and glass effects. For this purpose, an adaptive sampling technique is presented, which can select more samples around the regions where the values have a higher variation. Several machine learning methods are used for the modeling and their performance is compared: support vector machines, k-nearest neighbor, k-nearest neighbor and random forest, as well as an original algorithm, large margin nearest neighbor regression. The suggested method provides very good results compared to the other well-known regression algorithms.

Keywords : batch bulk methyl methacrylate polymerization, adaptive sampling, machine learning, large margin nearest neighbor regression
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