

Improvement of Product Prediction in Polymer Flow Synthesis with Computational Fluid Dynamics

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In this study, We aimed to enable the prediction of extrapolated data by using computational fluid dynamics (CFD). We applied CFD to an experimental data, and obtained a new explanatory variable. This is not a simple calculated value, but a chemically based value that combines some CFD calculated values. Simply put, We got a lot of temperature data from each computational cell, and calculated a new explanatory variable from them. The unit for this value is pseudo-length, so I called it “Effective Length”. As a result, the coefficient of determination, one measure of the model’s predictive accuracy, improved by up to about 0.1 compared to before the new explanatory variable was used. The reason why the new variable contributed to the improvement in prediction accuracy is that CFD can represent the internal state of the reactor, which cannot be represented by external information such as the set values of conventional explanatory variables. We also believe that the ability to use temperature, which is an important factor in such reactions, in the derivation of the new explanatory variable has greatly contributed to the improvement of the coefficient of determination.