Application of Digital Technology in Catalyst Design

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Digital technologies of machine learning and multiobjective optimization were introduced to develop the catalyst for fluid catalytic cracking (FCC). Response surface methodology (RSM) was applied for machine learning with the data set which consists of a variety of catalysts compositions, feedstock properties, pseudo-equilibrium conditions, cracking performance test conditions as input parameters and the cracking test results as outputs. Then the virtual experiments were carried out based on the obtained response surfaces and catalyst design was optimized using multiobjective genetic algorithm (MOGA). In this study, all investigations on the computer were carried out with the commercial software "modeFRONTIER".

At first, 1000 sets of data on many FCC catalysts and each laboratory performance test were prepared before conducting machine learning. Regarding RSM, some methods were examined to build the machine learning model and finally radial basis function (RBF) was found to contribute to the best accuracy in the prediction of cracking performance. Furthermore, additional 15 actual experiments were examined in the laboratory and verified to be good correlation with the prediction by RSM (Fig. 1). This suggested the possibility of the replacement of laboratory experiments by virtual experiments.

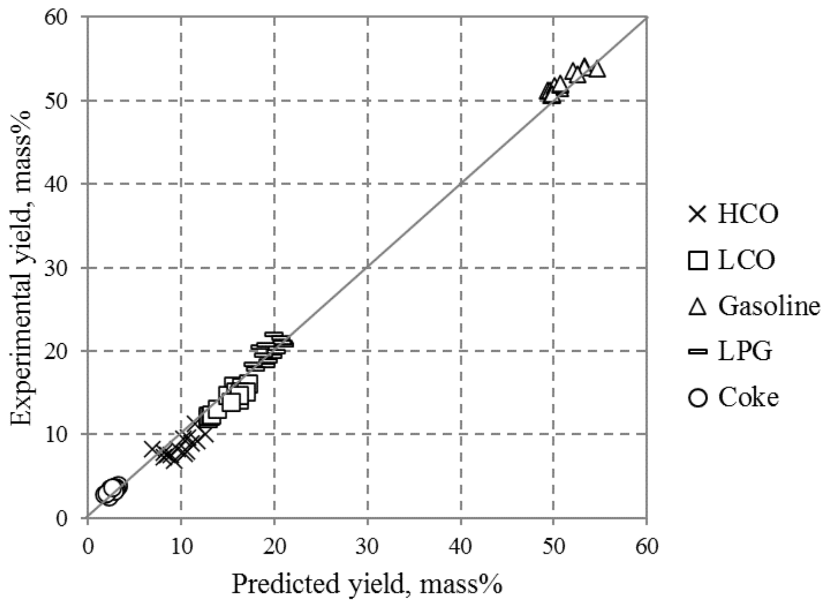

Fig. 1 Validation result of prediction accuracy for product yield

Multiobjective optimization is useful in such case where there are more than two objectives and these relationships are trade-off. For example, as the main role of FCC is to convert heavy oil to lighter valuable products such as propylene and gasoline, it must be difficult to be satisfied with both objectives, bottom product (HCO) to be reduced and gaseous by-products to be reduced, at the same time. In such case, the number of optimal design would not be only one but multiple designs exist on the trade-off line. In multiobjective optimization, the designs on the trade-off line could be found out by the functions of MOGA and many virtual experiments (Fig. 2). In this study, 5000 virtual experiments were examined to achieve four objectives. A design which was mostly expected to match the demand within some constraints was selected among 5000 designs and verified to have better performance than our commercial catalysts in the laboratory experiment.

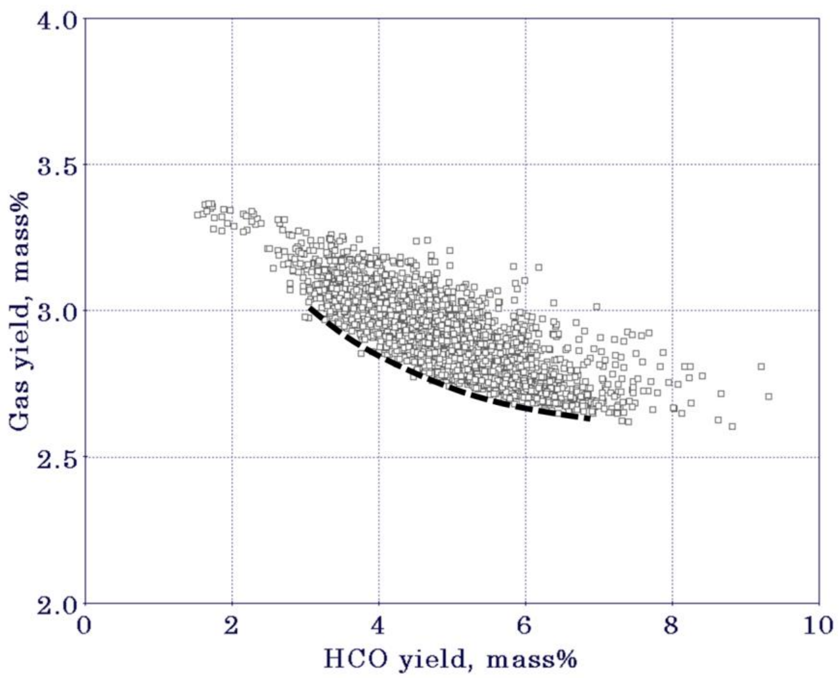

Fig. 2 Virtual experimental results

The digital technologies including machine learning and multiobjective optimization were applied in the field of catalyst design. FCC catalyst design was quickly optimized with the technologies and its performance was in the level to be hard to overcome with the human effort.