114a High-Throughput Experimentation and Statistical Design of Experiments

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Design of experiments in combination with high-throughput experimentation can be a powerful toolbox to systematically study vast parameter spaces encountered in the design and optimization of heterogeneous catalysts. We will present the general approach and, as an example, the study of NOx storage and reduction (NSR) catalysts as a function of cyclic operating conditions and metal/storage material type and loadings using response surface analysis. Empirical models were developed to predict the catalyst performance as a function of cycle time, lean fraction of cycle time, and catalyst composition. Using these empirical models, new catalyst formulations that maximize NOx conversion and selectivity to N2 were found.