Estimation of Kinetic Parameters in an Automotive SCR Catalyst Model

A challenge during the development of models for simulation of the automotive Selective Catalytic Reduction catalyst is the parameter estimation of the kinetic parameters, which can be time consuming and problematic. The parameter estimation is often carried out on small-scale reactor tests, or powder samples of the catalyst, which leads to problems when upscaling is done to the full-scale application. This contribution presents a methodology to sequentially estimate the kinetic parameters in 2 steps using steady-state limited small-scale reactor data, with the goal that the parameters should be used directly for accurate full-scale transient simulations. The model was validated against full-scale data with an engine following the European Transient Cycle. The validation showed that the predictive capability for nitrogen oxides (NOx) was satisfactory. After re-estimation of the adsorption and desorption parameters with full-scale transient data, the fit for both NOx and NH3-slip was satisfactory.

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