Neural Networks for Modeling of Chemical Reaction Data: a Step by Step Methodology, Support for Reactor Design and Simulation

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A general framework for implementing neural networks for estimation of chemical kinetic reaction data has been investigated. The neural network has been applied to the estimation of the rate equation of Fe-catalyzed gas-solid Fischer-Tropsch synthesis (FTS) for reactor design, scale-up and simulation purposes as a case study. A novel, step-by-step methodology for determination of the optimum network topology and learning criteria, choosing the input-output signals and the number and quality of input data has been presented and common rising problems for optimum designing of neural networks are investigated and discussed. the resulting neural network was used to compare different Langmuir-Hinshelwood-Hougen-Watson type rate equations for FTS over a precipitated iron catalyst and accompanied mechanisms formerly reported in literature. Based on this method detailed statistical analysis of the resulting neural estimators have been performed.