501e Online Estimation of Ato Catalyst Reaction Rate Parameter for Fuel Cell System

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An ASPEN Adiabatic PFR model is used to simulate the ATO reactor. Rate information of H2 and CO oxidation reaction from literature in plugged into the above PDF model to generate simulation results for parameter estimation. A nonlinear least square optimization method is applied to the set of partial differential equations to obtain the information of reaction rate parameters from the simulation data. Estimation and Literature results are compared and the deviation is within 10%.