Kinetic modeling of Diesel autothermal reforming in tubular micro-reactor

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A kinetic model of the autothermal reforming of Diesel to syngas is proposed for the 1kW class reformer modeling, simulation and optimization. Among the possible reaction sets and reaction rate equations in literatures, the best set and equation type are chosen by comparing the accuracy of data fitting for different combinations. Parameters in the equations are estimated by using least squares estimation which minimizes the summation of squared error between experimental data and calculated values. GC is used for obtaining the experimental data which is the molar flow rate of reformates at the exit of the reactor. And the plug flow reactor model describing the tubular micro-reactor used in the experiment is solved to obtain the calculated exit molar flow rate of reformates. As a result, the reaction rate equations with power law type for the total oxidation, steam reforming and water gas shift reactions show the best accuracy of data fitting.