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DETERMINATION OF THE RATE PARAMETERS OF N/H/O ELEMENTARY REACTIONS BASED ON H₂/O₂/NO_x COMBUSTION EXPERIMENTS

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Environmental regulations of industrial processes require accurate reaction mechanisms for the simulation of nitrogen oxides in combustion systems. A mechanism for the description of hydrogen–oxygen combustion systems doped with NO, NO₂ or N₂O was optimized using the method that had been developed in our laboratory [1]. Literature experimental data (ignition delay times and concentration profiles measured in flow reactors) were collected. In total, 2116 experimental data points in 93 data sets from 13 publications were used. These indirect experimental data were reproduced using ten recent NO_x mechanisms. The performance of the Glarborg-2017 [2], Curran-2017 [3] and POLIMI-2017 [4] mechanisms were the best. Ten elementary reactions were selected from the Glarborg-2017 mechanism based on sensitivity analysis and their Arrhenius parameters (A, n, E) were fitted not only to the indirect experimental data, but also direct experimental and theoretical determinations of the rate coefficients. This way more accurate rate parameters of these reactions could be obtained and the temperature dependent uncertainty of the rate coefficients was calculated. The Glarborg-2017 mechanism modified with the optimized rate parameters described the experimental data better than any other investigated reaction mechanism.

References:

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