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An optimized kinetic model for H_2-O_2 combustion in jet-stirred reactor at atmospheric pressure

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ABSTRACT:

An optimized kinetic model for hydrogen combustion in a jet-stirred reactor was proposed based on a validated mechanism. The rate constants were optimized using a genetic algorithm to minimize the prediction error of the outlet species' concentrations. The reference experimental data of jet-stirred reactor were selected from the literature. Optimization was established with and without constraints. Then, the kinetic models were evaluated using the relative errors in predicting the concentrations of major species at the outlet (H_2, O_2 and H_2O) and their accuracy in the calculation of ignition delay times. The comparison of experimental and calculated ignition delay time using unconstrainedly optimized model, rejected the optimization of kinetic model without any constraints. The optimized kinetic model showed a relatively better performance than the original model, especially under atmospheric conditions. At higher pressures and very rich conditions, the deviations from experimental data became greater than the original model.

Keywords:
Hydrogen combustion, genetic algorithm, jet-stirred reactor.