A Method for Predicting Sensitive Rate Coefficients with High Accuracy Tested for the $H_2/CO/O_2$-System

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Triggered by concerns about global climate change in conjunction with an increase of energy demands while fossil resources decrease, many efforts are ongoing, with a wide range of fuels, including renewable ones, to be exploited. To address fuel flexibility, natural gas like fuels, hydrogen rich fuels, syngases, as well as low-caloric fuels such as vent gases and biogenic gas mixtures are discussed. However, their major combustion properties must be known, to ensure a safe and efficient energy production, with almost no pollutants released [1-5].

Chemical-kinetic reaction mechanisms offer an excellent method to study the combustion of a particular fuel or fuel mixture by running numerical calculations when integrated into appropriate simulation software such as Chemical workbench [6]. Today, it is recognized that detailed mechanisms are inevitably needed to predict fuel oxidation, pyrolysis, and the formation of pollutants associated with it. This is especially true for gas turbine combustion where a wide range of temperature, pressure, and fuel-air-ratio needs to be covered by the reaction model [7].

However, when using chemical kinetic reaction mechanisms erected from different groups a significant spread in predictions of the data of interest (target) is often found, depending on temperature, pressure, fuel-air ration, and type of fuel. Within this context, an optimization tool is desirable that results in a better prediction of the target values by a fast analysis of the model parameters, such as rate coefficients.

In the current work, a newly developed optimization tool will be presented [8]. An evolutionary strategy and a gradient-based solver are presented [8], for the optimisation of chemical kinetic reaction models. The novel approach with the linear transformation model is based on new variation methods of rate coefficients and new evaluation methods of the distance between target values (experimental) and simulation values.

Both solvers are tested on OH*-and CH* chemiluminescence data of 120 shock tube experiments. For validation, the target data is simulated and random errors are added. Both solvers fit the simulation and experimental data with high precision. Furthermore, the gradient based solver is capable of predicting sensitive rate coefficients with outstanding accuracy compared to present confidence intervals.

Results will be shown for a biogenic gas mixture, of a typical composition, using ignition delay time data as input for the optimization

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