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Revision of experimental data collection for the evaluation of recent hydrogen combustion mechanisms

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To facilitate the use of alternative fuels with zero or low-carbon content, including pure hydrogen and its blends with ammonia or other fuels, it is vitally important to develop a reliable hydrogen combustion mechanism with good performance under various conditions, including those relevant to practical applications. However, while the detailed combustion chemistry of H_2 has been studied for a long time, the continued publication of new experimental data indicates that most available mechanisms are accurate only under specific conditions. Additionally, several recent updates to the hydrogen combustion scheme have been proposed and tested in sample simulations; however, they have not been tested against experimental data under a wide range of conditions.

A quantitative evaluation of existing hydrogen combustion mechanisms using a large collection of experimental data allows identifying which of these recent modifications to the hydrogen combustion scheme are viable and which combustion mechanism is better suited for further improvement and optimization. A collection of 30 detailed combustion mechanisms developed for H_2 or syngas fuels and published over the last decade, including mechanisms optimized by different methods, was selected and tested alongside several other widely used mechanisms, using the method proposed by Turányi et al. [1].

We have utilized the data collection used at the ELTE Chemical Kinetics Laboratory for the validation [2] and optimization [3] of hydrogen combustion mechanisms. Additionally, the new experimental results on the combustion of neat hydrogen flames were gathered from more than 70 recent research articles, encoded in the RKD format, and added to the ReSpecTh database [4]. This included concentration measurements in jet-stirred reactors, flow reactors, and burner-stabilized flames; ignition delay measurements in shock tubes and rapid compression machines; laminar burning velocity measurements; and extinction strain rate measurements. While this study aims to utilize as much experimental data as possible, sometimes different experimental data from the same or similar conditions contradict each other. To address this, an additional procedure was developed and implemented to exclude inconsistent datasets from the analysis.

While evaluation has shown the advantages and deficiencies of different mechanisms, it has also been noted that combustion mechanisms developed for syngas or hydrocarbon fuels are considerably better under experimental conditions where CO_2 is used as a diluent gas.

References

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