Modeling syngas, formaldehyde and methanol combustion: An updated comprehensive kinetic model

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Continuing interest in syngas (CO/H_2) as a next-generation fuel has motivated recent studies on its combustion, including several kinetic models. However, several of the new experimental results, such as ignition delays, laminar burning velocities and species concentration profiles, from various experimental set-ups can not be simulated with satisfactory agreement using these existing combustion kinetic models. The goal of this work is to address these issues by updating and improving the model of Li et al. [1] for syngas and as well formaldehyde and methanol combustion (C_1 combustion).

Burke et al. [2] recently published an updated, detailed hydrogen/oxygen model, incorporating new evaluations for the thermodynamic and kinetic data and successfully tested against a wide range of validation targets. This forms a first set of updates to the C_1 model of Li et al. [1]. Secondly, more recent experimental and theoretical studies are considered for C_1 combustion such as for the sensitive reactions $OH+CO \rightarrow$ products, $CO+HO_2 \rightarrow CO_2+OH$ and $CH_3OH+HO_2 \rightarrow$ products. Simulations with the new mechanism are tested against both the original validation targets of Li et al. [1] and new validation data over a wide temperature range at higher pressures and mixtures with high amounts of H_2O or CO_2 present.

The present hierarchically-constructed, comprehensively validated C_1 model can serve both as a powerful C_1 mechanism and as a core around which to construct kinetic models for larger hydrocarbons and oxygenates.

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References
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