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Development and Validation of an N-Dodecane Skeletal Mechanism Using a Hybrid Reduction Method in a Jet Stirred Reactor

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Extended Abstract

Diesel and Kerosene fuels are widely used in transportation, including aviation. However, their complex chemistry and high carbon numbers provide many challenges in simulating real-world conditions. Therefore, researchers are considering surrogates that can help to understand the combustion behaviour of different hydrocarbon fuels. *n*-dodecane is one of the important surrogates for kerosene and diesel due to its same physical properties. The fact that the chemical kinetic in flames is not well noticed.

This study proposes a skeletal mechanism for n-dodecane, further used to investigate the ten species (O_2, CO, CO_2, H_2, H_2O, CH_4, C_2H_2, C_2H_4, C_6H_6, n-$C_{12}H_{26}$) in the jet-stirred reactor. For the first time, the n-dodecane mechanism is reduced using the hybrid reduction method (path flux analysis + artificial neural network). The detailed mechanism [1] of n-dodecane is reduced to 94 species, and 516 reactions from 255 species and 1521 reactions [1] by using hybrid reduction method. The newly reduced mechanism maintained the accuracy of the detailed mechanism in the different reactors (ignition delay time, flame speed, and jet stirred reactor). In the future, the reduced mechanism will incorporate into a 2-D co-flow reactor to analyze the insight information of PAH and soot formation in n-dodecane flames.

References

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