SKELETAL REDUCTION OF DETAILED MECHANISMS FOR BIOFUELS: ETHANOL AND BIODIESEL SURROGATES

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Abstract: The reduction of two detailed kinetic mechanisms will be performed, one for ethanol and one for biodiesel subrogates. That is, detailed kinetic mechanisms available for biofuels will be reduced to generate reduced skeletal mechanisms that can be used in the analysis of fueled engines with biofuels in CRFD of simple geometries. And also, to serve as a basis for further reductions from optimization methods for more complex CRFD applications. This, due to the great boom in biofuels and the environmental need to reduce the use of fossil fuels. For ethanol, the detailed CRECK mechanism was selected. For biodiesel, the detailed CRECK mechanism for Methyl-Esters was chosen, and a combination of 25% Methyl Decanoate (MD), 25% Methyl 9-decenoate (MD9D), and 50% n-heptane was established as a surrogate for Biodiesel to represent rapeseed oil methyl ester (RME). The objective of this study is to reduce detailed biofuel mechanisms to skeletal level using a combination of different skeletal reduction methods, such as Directed Relation Graph (DRG), Directed Relation Graph with Error Propagation (DRGEP), Directed Relation Graph with Sensitivity Analysis (DRGASA), Directed Relation Graph with Error Propagation with Sensitivity Analysis (DRGEPSA), Path Flux Analysis (PFA), Connectivity Method (CM), and Reaction Flow Analysis (RFA), seeking to have the lowest percentage relative error in relation to the detailed mechanism. Simulations will be performed using Python and for thermodynamic and kinetic calculations Cantera will be used. Both softwares is freely available. The reductions will consider combustion parameters such as ignition delay time, laminar flame speed, and species concentration in a Jet Stirred Reactor (JSR). A wide range of relevant conditions for internal combustion engine applications will be taken into account, including low and high temperatures, while considering conditions with available experimental data in the literature. Finally, graphs comparing the results of ignition delay time (IDT), laminar flame speed (LFS), and species concentration in the JSR will be presented for each evaluated mechanism, including both the detailed and reduced mechanisms. Additionally, the numerical results obtained will be compared with experimental data available in the literature for the same conditions.

Keywords: Detailed chemical kinetics, Mechanism reduction, Internal combustion Engines.