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Detailed chemical kinetic models for large n-alkanes and iso-alkanes found in conventional and F-T diesel fuels

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Detailed chemical kinetic models are needed to simulate the combustion of current and future transportation fuels. These models should represent the various chemical classes in these fuels. Conventional diesel fuels are composed of n-alkanes, iso-alkanes, cyclo-alkanes and aromatics (Farrell et al. 2007). For future fuels, there is a renewed interest in Fischer-Tropsch (F-T) processes which can be used to synthesize diesel and other transportation fuels from biomass, coal and natural gas. F-T diesel fuels are expected to be similar to F-T jet fuels which are commonly comprised of iso-alkanes with some n-alkanes (Smith and Bruno, 2008). Thus, n-alkanes and iso-alkanes are common chemical classes in these conventional and future fuels. This paper reports on the development of chemical kinetic models of large n-alkanes and iso-alkanes to represent these chemical classes in conventional and future fuels. Two large iso-alkanes are 2,2,4,4,6,8,8-heptamethylnonane, which is a primary reference fuel for diesel, and iso-octane, a primary reference fuel for gasoline. Other iso-alkanes are branched alkanes with a single methyl side chain, typical of most F-T fuels. The chemical kinetic models are then used to predict the effect of these fuel components on ignition characteristics under conditions found in internal combustion engines.

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