

Development of a reduced biodiesel surrogate model for compression ignition engine modeling

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Abstract

Methylbutanoate (MB), a C4 methyl ester, represents the simplest surrogate that captures the chemical effects of the ester moiety in biodiesel and biodiesel surrogates. An updated chemical kinetic model has been developed to characterize the ignition and flame characteristics of MB. The mechanistic elements within this model that relate to the MB and smaller ester/oxygenate sub-mechanisms are drawn from the prototypical Fisher et al. model and from more recent theory and modeling efforts. The MB model development which is based on an iterative procedure involving global sensitivity analyses to identify elementary reactions that govern ignition and subsequent high level ab initio based theoretical updates to these reaction rates are presented. The MB model makes reasonable predictions of ignition delays and laminar flame speeds. The C5–C7 submechanisms from the LLNL n-heptane (NH) model were merged with the present MB model to obtain a detailed chemical kinetics model for a surrogate blend representing biodiesel. The detailed MB-NH model (661 species) was reduced using graph based techniques. The robust reduction techniques employed result in a reduced model (145 species) that is in good agreement with the detailed model over a wide range of conditions. 3-D compression ignition (CI) engine simulations utilizing this reduced chemistry model for MB-NH blends as a surrogate for biodiesel show good agreement with the experimental data suggesting the utility of this model for predictions of combustion and emission characteristics of biodiesel in realistic CI engine simulations. Copyright 2012. The Combustion Institute. Published by Elsevier Inc. All rights reserved.