Development and validation of a reduced combined biodiesel–diesel reaction mechanism -
DTU Orbit (14/12/2018)

In this study, a compact combined biodiesel–diesel (CBD) reaction mechanism for diesel engine simulations is proposed through the combination of three component mechanisms using a chemical class-based approach. The proposed mechanism comprises the reaction mechanisms of methyl crotonate (MC), methyl butanoate (MB) and n-heptane which are the surrogate fuel models of unsaturated fatty acid methyl ester, saturated fatty acid methyl ester and straight chain hydrocarbon (HC), respectively. The MC and MB mechanisms are adopted to represent biodiesel fuels, while n-heptane is utilised to characterise the combustion of fossil diesel. Here, the MC and MB mechanisms are reduced before integrating with a compact n-heptane mechanism. CHEMKIN-PRO is used as the solver for the zero-dimensional, closed homogenous reactor with a constant volume in this study. In the first phase, the mechanisms of MC and MB are methodologically reduced. The MC mechanism by Gail et al. with 301 species and 1516 reactions is reduced to 47 species and 210 reactions, while the MB mechanism by Brakora et al. with 41 species and 150 reactions is reduced to 33 species and 105 reactions. The mechanisms are reduced from a combination of methods, including peak molar concentration analysis, reaction flux analysis and the removal of individual species. In the second phase, the reduced MC and MB mechanisms are combined with the n-heptane mechanism by Pang et al. with 46 species and 112 reactions. Upon the combination of the component mechanisms, parametric adjustments to the Arrhenius rate constants of pertinent chemical reactions are performed for better ignition delay (ID) prediction. The final mechanism developed comprises 80 species and 299 reactions. The compact-sized CBD mechanism is validated against 234 test conditions ranging from initial temperatures of 750–1350 K, pressures of 40–60 bar and equivalence ratios of 0.4–1.5. The mechanism is generally found to accurately predict the timing and duration of ID for the combustion of each surrogate fuel. This model is also shown to be feasible for use with multidimensional computational fluid dynamics studies involving a light-duty diesel engine fuelled with biodiesel of different feedstock types, diesel as well as their blends.

General information
State: Published
Organisations: Department of Mechanical Engineering, Thermal Energy, University of Nottingham Malaysia Campus
Contributors: Ng, H. K., Gan, S., Ng, J., Pang, K. M.
Pages: 620-634
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Fuel
Volume: 104
ISSN (Print): 0016-2361
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5.4 SJR 1.891 SNIP 2.127
Web of Science (2017): Impact factor 4.908
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.9 SJR 1.736 SNIP 2.207
Web of Science (2016): Impact factor 4.601
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.46 SJR 1.781 SNIP 2.123
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.14 SJR 1.634 SNIP 2.294
Web of Science (2014): Impact factor 3.52
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.31 SJR 1.762 SNIP 2.544
ISI indexed (2013): ISI indexed yes
Original language: English
Keywords: Biodiesel, Chemical kinetics, Diesel engines, Methyl butanoate, Methyl crotonate
DOIs: 10.1016/j.fuel.2012.07.033
Source: dtu
Source-ID: u:5893
Research output: Research - peer-review › Journal article – Annual report year: 2013