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1 Development of a skeletal mechanism for heavy-duty 2 engines fuelled by diesel and natural gas

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6 Abstract

7 The purpose of this work is to develop a skeletal dual-fuel mechanism for heavy-duty
8 engines fuelled by diesel and natural gas. With diesel fuel modeled as n-heptane, and
9 natural gas modeled as methane, the skeletal mechanism was constructed by coupling
10 the two skeletal mechanisms reduced detailed mechanisms: n-heptane and methane
11 mechanisms. Directed relation graph error propagation and sensitivity analysis,
12 computational singular perturbation and reaction rate adjustment methods were
13 employed for mechanism reduction. The final skeletal dual-fuel mechanism is
14 composed of 61 species and 199 reactions. So as to validate the fidelity of the novel
15 skeletal dual-fuel mechanism, zero-dimension ignition delay testing against shock
16 tube experimental results and 3-dimensional engine validation about in-cylinder
17 pressures, heat release rates and NO_x and CO emissions against engine testing results
18 were performed under various operating conditions. The validation results indicate
19 that the dual-fuel mechanism can accurately reproduce the ignition behaviors,
20 combustion characteristics and emission trends in heavy-duty diesel/NG dual-fuel
21 engines. Besides, a parallel computing method based on the round-robin algorithm
22 was developed which can significantly save the time for calculating. Combined with
23 the new developed skeletal dual-fuel mechanism, the 3D CFD simulation for the
24 combustion in heavy-duty engines can be done in a reasonable computational time.

25

26 **Keywords:** Natural gas; Pilot diesel; Dual-fuel skeletal mechanism; heavy-duty
27 engines

28

29 1. Introduction

30 Diesel engines are widely used in numerous applications throughout the world. With
31 rapid depleting of fossil fuels and increasingly strict emission regulations, alternative
32 fuels for diesel engines have attracted more and more attention [1-4]. Due to its
33 abundant reserves, high fuel economy and relatively low emissions, natural gas (NG)
34 has been emerging as a promising alternative fuel in recent years, especially in ship
35 propulsion [5-7]. The diesel/NG dual-fuel engines adopt natural gas as primary fuel,
36 while using a small amount of diesel as pilot fuel to ignite NG and air mixture [8-9].
37 Conventional diesel engines can be retrofitted to diesel/NG dual-fuel engines with
38 some modifications, which make it possible for the dual-fuel engines to utilize the
39 high compression ratios of original diesel engines, thus achieving high thermal
40 efficiency as well as relatively lower nitrogen oxides (NO_x) and particulate matter

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