

A Multi-Dimensional CFD-Chemical Kinetics Approach in Detection and Reduction of Knocking Combustion in Diesel-Natural Gas Dual-Fuel Engines Using Local Heat Release Analysis

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ABSTRACT

Dual-fuel diesel-natural gas (NG) engine exhibits higher power density and lower specific emissions compared to dedicated diesel engines. However, high intake temperatures, high compression ratios, combined with high engine loads may lead to engine knock. This is potentially a limiting factor on engine downsizing and getting higher power. In the present study, the combustion process under knocking conditions has been investigated in a dual-fuel diesel-NG engine. A comprehensive multi-dimensional simulation framework was generated by integrating the CHEMKIN chemistry solver into the KIVA-3V code. A detailed chemical kinetics mechanism was used for *n*-heptane and methane as diesel and NG surrogates. Combination of detailed chemical kinetics and detailed fluid dynamics calculation enabled the model to take into account the characteristics of most pronounced knock type in dual-fuel engines, so called end-gas knock. Within the CFD computational domain, eight regions that are the representatives of the dual-fuel heat release patterns have been selected to extract local properties. Using local knock identification factors, end-gas knock was observed in abnormal combustion cases. A new Knock Intensity factor (K.I) was introduced based on local heat release rate. Using developed knock prediction method, results showed knock could be mitigated by using EGR. Moreover, effect of premixed methane equivalence ratio on knocking combustion was investigated.

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INTRODUCTION

Dual-fuel diesel-NG engines use NG as the main fuel and benefit from the auto-ignition characteristics of diesel fuels for combustion initiation. With limited changes in the engine fuel delivery system and without any structural modification, a normal diesel engine can be retrofitted to a dual-fuel diesel-NG engine. Dual-fuel diesel-NG engines have comparable performance to that of conventional diesel engines, while most of the energy is obtained from NG as a relatively clean burning fuel [1, 2, 3]. In a dual-fuel diesel-NG engine, NG provides the majority of chemical energy and injection of a small amount of diesel fuel as the pilot-fuel is used to trigger the ignition of premixed NG and air mixture. The small quantity of the liquid fuel and clean burning nature of the gaseous fuel provide the potential of producing relatively lower NO_x and lower particulate emissions (PM) comparing to the conventional diesel cycle [4]. Despite the great benefits of the dual-fuel engines in terms of fuel economy, they suffer from low thermal efficiency and high CO and UHC emission levels at light engine loads [4]. At high engine loads, knocking combustion may be resulted due to applying high intake pressure and temperature [5 and 6]. The abnormal combustion process caused by knock leads to high frequency oscillation of the engine structure, high noise level and it can be a limiting factor on engine downsizing and its persistence may damage engine structure and parts.

Under specific operating conditions Dual-fuel engines share one similar aspect with the spark-ignited (SI) engines and that is the end-gas auto-ignition known as SI engine knock. In a dual-fuel engine, diesel pilot-fuel acts as an ignition source and triggers combustion of the premixed NG and air mixture. NG combustion is a premixed flame which propagates through the combustion chamber, leading to compression of the end-gas and possible auto-ignition of the gaseous fuel caused by high pressure and temperature. This abnormal combustion is characterized by extremely rapid temperature rise and energy release and noticeable fluctuations in local pressure [7]. On the other hand, knock tendency depends on the auto-ignition characteristics of the applied fuel. In gaseous fuels, the Methane Number (MN) is used to represent the gas quality or its ability to resist auto-ignition. This is equivalent of Research Octane Number (RON) used for liquid fuels [7]. Although NG has considerably high MN, under high engine loads, compression ratio or boosted intake pressure and temperature could be subjected to the end-gas knock.

Heat release analysis is one of the tools that have been used to identify knocking conditions [7, 8, 9]. It should be noted that knock occurrence mechanism in dual-fuel engines is different compared to SI engines due to persistence of both injected diesel and premixed NG in an engine cycle. Karim and Liu [9] theoretically described that energy release of a dual-fuel diesel-NG engine is made up of three distinguished parts namely pilot-fuel combustion, combustion of gaseous fuel in vicinity of pilot-fuel, and combustion of remained

gaseous fuel as parts I, II, and III, respectively. They explained that combustion is initiated by the energy release of the diesel pilot-fuel, while the maximum heat release occurs in part II and then combustion propagates into the remained NG-air mixture near the cylinder wall boundaries. It is also indicated by them that increasing the concentration of the gaseous fuel in the air, coolant water jacket temperature and pilot-fuel type and injection timing could cause the knock onset in dual-fuel engines. They theoretically claimed that once the dual-fuel engine was incurred knocking combustion, overlap between part II and part III of the heat release pattern would be increased [9].

Comparing to SI engines limited experimental researches have been reported in the literature for dual-fuel engines under knocking conditions. An experimental analysis of knock in dual-fuel engines has been done by Karim et al [6]. It was concluded that initial mixture temperature, pilot-fuel quantity, type of the engine aspiration and equivalence ratio are important factors in knock occurrence. Kubesh and Brehob [7] used Waukesha CFR cetane engine to study knocking combustion in dual-fuel mode. They used in-cylinder pressure gradient and maximum pressure as the knock detection parameters to investigate the diesel and end-gas knock occurrence in a dual-fuel engine and concluded that Fast Fourier Transform (FFT) on cylinder pressure fluctuations was a good indicator of end-gas knock. They also concluded that the different NG compositions used for the premixed fuel fraction did not have a definite effect on the presence or intensity of knock in the engine as methane concentration of the applied gaseous fuel blends was greater than 90 percent.

In the numerical analysis of the knock phenomenon, the onset of knock is defined by steep rise in pressure, HRR and end-gas temperature [5 and 7]. Based on a previous study [8], Karim and Liu developed a quasi two-zone model with detailed chemical kinetics sub-model including 31 species and 105 elementary reactions in order to study knock in the dual-fuel engines [9]. The chemical kinetics mechanism was only used for the predictions of the gaseous fuel auto-ignition process. Pilot-fuel chemistry was neglected and considered as an ignition source to simplify the calculations. They concluded that sudden increase in HRR diagram was the evidence for knock onset. Saidi et al developed a quasi two-zone model [5] and conducted experiments [10] to study the combustion process of a dual-fuel engine operating under normal and knocking conditions. GRI-MECH 3 chemical kinetics mechanism was used in the model. It was concluded that existence of large amounts of free radicals before the flame arrival was the evidence of knock. Saikaly et al [11] developed a two-zone thermodynamic model to study end-gas knock in CFR engine fueled by NG. They used predefined knock factor based on HRR analysis introduced by Karim and Gao [12]. They inferred that the developed model was unable to simulate local temperature and HRR increments and could not predict the knocking conditions correctly.

Overall, paying particular attention to the governing chemistry is the common feature among all numerical simulations discussed above. This is why detailed chemical kinetics mechanisms are used as chemistry directly affects knock occurrence as far as auto-ignition conditions are provided. By referring to extensive researches on modeling of the knock phenomenon in SI engines [13, 14, 15, 16, 17, 18, 19, 20], there are quantitatively limited publications on dual-fuel engines. Furthermore, most of the numerical studies on these engines were performed by the use of thermodynamic models and considering only NG chemistry. In multi-zone models, this was done along with assumption of uniform temperature and composition distribution inside the considered zones [5, 8 and 9]. Therefore, key parameters such as: pilot-fuel chemistry and its distribution, local rate of pressure rise, local temperature and local HRR, and their effects on knocking behavior were neglected. Moreover, use of mean temperature, pressure and HRR values in identification of the knocking combustion is not an appropriate tool and only very strong knock can be captured by using these simplified models. The present work aims to accurately model and demonstrate knocking combustion by developing a coupled 3D CFD/Chemistry model. This has been done by taking into account the effects of fluid flow and chemical kinetics simultaneously not only for in-cylinder mean values of pressure, temperature and HRR, but also for local regions where knock is likely to occur.

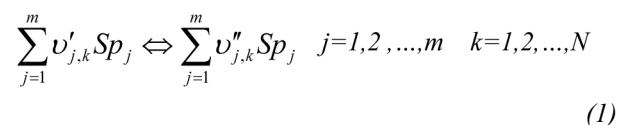
ANALYTICAL MODEL

In reality, not only the combustion process, but also the knock phenomenon is a three-dimensional event which relies on numerous physical and chemical aspects [18]. This requires utilization of a multi-dimensional CFD coupled with chemical kinetics to accurately account for the effects of fluid flow, spray combustion and detailed fuel oxidation chemistry. In this study, fluid flow simulation was carried out using the Los Alamos National Laboratory (LANL) CFD code, KIVA-3V [21], with improved turbulence and spray/wall interaction models. KIVA is a computer code for the numerical calculation of transient, two and three dimensional chemically reactive flows with sprays. It uses a time-marching, finite-volume scheme which solves the conservation equations of mass, momentum, energy and accounts for turbulence using an Arbitrary Lagrangian Eulerian (ALE) method in three solution phases. The combustion calculations in the original KIVA code are based on a global reaction for fuel oxidation chemistry and it involves only 12 active chemical species [21]. The assumption of single-step global reaction ignores essential features of the combustion and auto-ignition of hydrocarbon fuels so called “double-stage ignition” [1]. Fuels with tendency of exhibiting double-stage ignition, are more prone to knock as the first stage ignition happens at relatively low temperature, but provides free radicals and enthalpy for the initiation of the main ignition stage. The phenomenon is

completely ignored by global single step mechanisms. Obviously, combustion model has a key role in reliable and accurate predictions of the global engine performance data such as: in-cylinder pressure, HRR and emissions. Hence, in this work the gas phase kinetics library of CHEMKIN-II [22] was integrated into the KIVA code to generate an advanced computational framework.

KIVA-CHEMKIN INTEGRATION

Accurate simulation of the dual-Fuel combustion under knocking conditions is highly dependent on detailed prediction of pilot-fuel ignition delay as well as methane auto-ignition chemistry. Hence, utilization of detailed chemical kinetics mechanism is essential. Considering a typical chemical kinetics mechanism which consists of N elementary reactions with participation of m chemical species, the general form of the reactions is in the form of [2]:



Molar production rate of the participated chemical species is obtained as the difference of the molar creation and destruction rate:

$$\dot{\omega}_j = N_j \sum_{k=1}^N (v''_{j,k} - v'_{j,k}) [A_{f,k} T^{b_{f,k}} \exp(-\frac{E_{f,k}}{RT}) \prod_{j=1}^m c_j^{v'_{j,k}} - A_{b,k} T^{b_{b,k}} \exp(-\frac{E_{b,k}}{RT}) \prod_{j=1}^m c_j^{v''_{j,k}}] \quad (2)$$

Introducing detailed chemical kinetics into the KIVA code, if the net molar production rate, $\dot{\omega}_j$, is calculated for each time step, different combustion source terms in the conservation equations can be updated. To achieve further details about species molar production/destruction rates, the chemistry routine in KIVA was modified. A considerable amount of FORTRAN programming was needed to enable internal integration of the CHEMKIN-II library within the KIVA code. Detailed and thorough examinations were needed to avoid conflicting parameters or data arrays among both codes. Species concentrations and thermodynamic information of each individual cell at every time step were provided by the KIVA code to pass to the CHEMKIN chemistry solver. N -set of stiff ordinary differential equations was constructed by the CHEMKIN library. Then, the DVODE package [23] was called to compute the species net production rates at the end of each time step. In such a process, gas phase reactions and species thermodynamic data were identified by the CHEMKIN prior to integration with the KIVA code. Using this procedure, the flow and chemistry solutions were fully coupled. Heat transfer routine in the KIVA code was also modified to calculate wall heat flux based on Han and Reitz formulation [24] for better accuracy.

Table 1. OM-355 engine specifications

Engine aspiration	Turbocharged (Garret)
Engine cycle	Diesel – 4 Stroke
Number of cylinders	6 – Inline
Injection pressure [bar]	195
Injector nozzle number	4 - Centric
Nozzle diameter [mm]	0.31
Injection angle [deg]	76
Bore * stroke [mm]	128 * 150
Displacement volume [lit]	11.58
Compression ratio	16.1 : 1
Max. output power [hp]	240 @ 2200 [rpm]
Max. output torque [N.m]	824 @ 1400 [rpm]

Moreover, the RNG k- ϵ model was used as the turbulence model. This model was demonstrated in the literature to obtain better results than previous versions under wide range of engine operating conditions [1].

Chemical Kinetics Mechanism

NG used in the experiments was consisted of more than 98% methane by volume [10] and hence, pure methane/air mixture was assumed at IVC. Moreover, *n*-heptane was considered as a surrogate of the diesel fuel. The *n*-heptane chemical kinetics mechanism of Zheng and Yao [25] was used in this study to model pilot-fuel chemistry in knocking conditions. The mechanism includes 42 chemical species and 58 elementary reactions and was derived from the detailed *n*-heptane mechanism developed by Lawrence Livermore National Laboratory (LLNL) [26]. It was successfully used in simulation of HCCI engines with low D.I ratios [25]. As described earlier, during a knocking cycle methane was experiencing the end-gas knock. Li et al developed a reduced chemical kinetics mechanism of the methane auto-ignition and validated the mechanism by conducting experiments on a dual-fuel engine [27]. In the present study, reduced reaction mechanism developed by Li et al was added to the Zheng and Yao's *n*-heptane mechanism and was used in modeling of dual-fuel combustion under knocking conditions. Since mass ratio of NG/diesel was high in the conducted experiments [10], only characteristic of end-gas knock was considered in this study. Nevertheless, dual-fuel diesel-NG engines can be subjected to both diesel and end-gas knock types as discussed by Kubesh and Berhab [7].

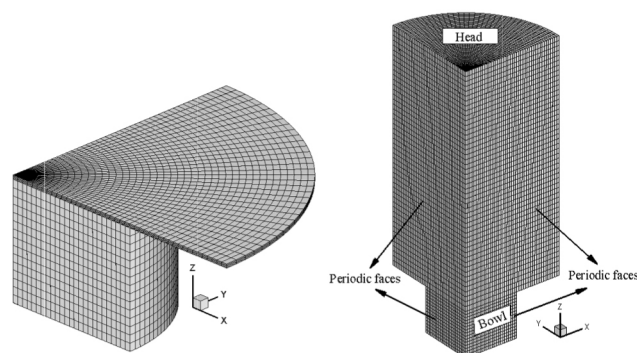
Experimental Setup and Operating Cases

The experiments for the OM-355 dual-fuel engine were conducted by Pirouzpanah et al [10] in the Diesel-Gas research facility [28]. As discussed in introduction part, they have also performed numerical simulations [5] using measured experimental data under knocking conditions. Engine specifications are presented in Table 1. Numerical calculations were performed on four experimental cases. The specifications of the cases are presented in Table 2.

Table 2. Selected experimental cases used for model validation taken from [10] (IVC = -120 CAD ATDC, EVO = 118 CAD ATDC)

Case number	1	2	3	4
IVC Pressure [bar]	1.28	1.75	2.25	2.3
IVC Temperature [K]	320	350	362	350
Engine speed [rpm]	1600	1000	1000	2200
NG EQR	0.54	0.57	0.6	0.58
Diesel/NG [% mass]	9:91	13:87	6:94	7:93
SOI [CAD ATDC]	-17	-16	-15	-22
Knock onset CAD	No-knock	11	7	14
Knock strength	No-knock	Medium	Heavy	Light

Computational Mesh

**Figure 1. Computational mesh for OM-355 engine at BDC (right) and TDC (left)**

A 90 degree computational sector mesh was generated for OM-355 dual-fuel engine, assuming symmetry for a four-hole injector configuration. Periodic boundary conditions were assumed for the side faces of the sector computational mesh which is shown in figure 1. The independency of the results from the mesh size was ensured using various computational mesh sizes. Considering computational time, the mesh depicted in figure 1 was selected including 44*34*65 cells (at