The Study on Dual Fuel Spray and Characteristics of Combustion of Diesel, Natural Gas and Dual Fuel

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Abstract

Combustion of fossil fuels provides around 88% of total energy supply for modern society, and meanwhile causes many environ mental problems and social problems such as air pollution and energy crisis. Therefore，both at home and abroad are focusing on the research and development of natural gas engine recently. However, the mass production and application of this kind of engine are restricted by some unsolved technical difficulties. This paper explored the injection, combustion and emission processes of diesel/ natural gas and dual fuel engine based on Chemkin II, Fire software and Schlieren method. The experimental study on the mixing process of dual fuel jet was carried out by using high-speed Schlieren method in a constant volume bomb. Based on the Fire software, and then applied to Chemkin II software to analyze the effect of the initial temperature and pressure on the net heat production and combustion emissions. The results show that Dual fuel mechanism is capable of producing different heat production behaviors when varying the initial pressure and temperature CO_2 emissions are minimized by changing the initial pressure above or below the atmospheric value. However, CO emissions are peaked when diesel fuel is used. The dual fuel engine minimizes the CO emissions amount caused by diesel fuel. Increasing the initial pressure eliminates dual fuel CO_2 combustion emissions. The research of this paper is important to optimize the in cylinder combustion processes of natural gas engine, and have a certain important meaning to guide the development of diesel ignition dual fuel engine.

Introduction

Although tremendous studies on alternative energy solutions such as combined fuels and hybrid-engines have been under focus for many years, yet there's still a lack of a complete substitution of the conventional internal engines [1-5]. Therefore, conventional engines are employed through a lot of applications to utilize the engine's optimum conditions [6]. Internal combustion engines generally are nominated to reduce the emissions amount below the emissions regulations. Commonly, conventional diesel engines are modified to work as dual fuel engines in which methane fuel provides most of the chemical energy while diesel fuel plays a main role in a pilot ignited one with the methane-air mixture [7-11]. However, adding the natural gas fuel option as a supplement for conventional diesel fuel proved that it's not only a very clean choice but also its more economically viable[12-15]. Combining these two types of fuel will elevate the conventional diesel engine's heating value, lower the fuel cost, and reduce the engine's adiabatic flame temperature [10, 16, 17]. Most of the existed conventional diesel engines can be modified to serve as dual fuel engines maintaining its compression ratio with less emissions of NOx and particles [13, 14]. However, adding methane fuel to the engine makes it more competitive in terms of fuel air mixing and knocking resistance [18].

Recently, the natural gas/diesel combined fuel engine's implementations have been under focus both theoretically and experimentally to specifically understand the reaction nature [15, 19, 20]. The natural gas/diesel fuel ratio, the natural gas initial percentage and the natural gas initial composition with their initial temperatures and pressures conditions were studied and evaluated taking in consideration the intake air temperature [15, 21, 22].The most significant drawback of the dual fuel engines compared with the conventional diesel engine is represented in efficiency redundancy in addition to higher CO emissions in case of low fuel loads [23, 24]. At high and intermediate loads both of the engine's output and CO emissions are better than those in the conventional diesel engines [20, 23, 24]. Changing the engine parameters, increasing the pilot fuel amount and changing the injection time might have a better effect on the engine's output along with CO and HC emissions.

However, it also increases the effect on NO_x emissions [20, 25].

Many efforts have been made toward overcoming these drawbacks and reducing NO_x emissions at the same time. Exhaust gas recirculation (EGR) was suggested [18]. The main objective of this study is to explore the injection, combustion and emission processes of diesel/ natural gas and dual fuel engine based on Chemkin II, Fire software and Schlieren method. The complete measurements options for the initial pressure and temperature were conducted for various engines operating mode; particular analysis were conducted on the combustion process such as the engine's efficiency along with all the associated emissions. For further tests, a high digital CCD in-cylinder camera FASTCAM was used to observe the combustion development. Injection images were post-processed then numerical calculations were obtained using Chemkin II software.

Experimental and Numerical Simulation Study

In this paper, the experimental study on the mixing characteristics of dual fuel injection is carried out by high speed filming combined with constant volume bomb. In order to acquire more accurate and reliable results; three-dimensional numerical simulation of dual fuel iscarried out as shown in Fig .1.The AVL-Fire software used in this article is a CFD software - developed specifically for the engine - is widely used in the engine spray cylinder, combustion and emission simulation studies.

Application of Fire software

Fire software is software developed by AVL in Austria for the study of complex transient flow and combustion problems in the cylinder. The software has a powerful function of solutions and calculations; therefore it has been widely recognized in the field of the engine. Comparing with Fluent, Converge and other similar software, it has the advantages of: (1) The user is simple, clear, easy to operate and efficient; (2) Advanced pre-processing FAME mash generator which can automatically generate hexahedral mesh, and simplify the use of the FAME mash generator;(3) It has provided a technique for solving any shape polyhedron mesh;(4) In addition to the commonly used turbulence model, it can also provide a k-ζ-f compound turbulence model; (5) Its flow model has the highest level in the same software,
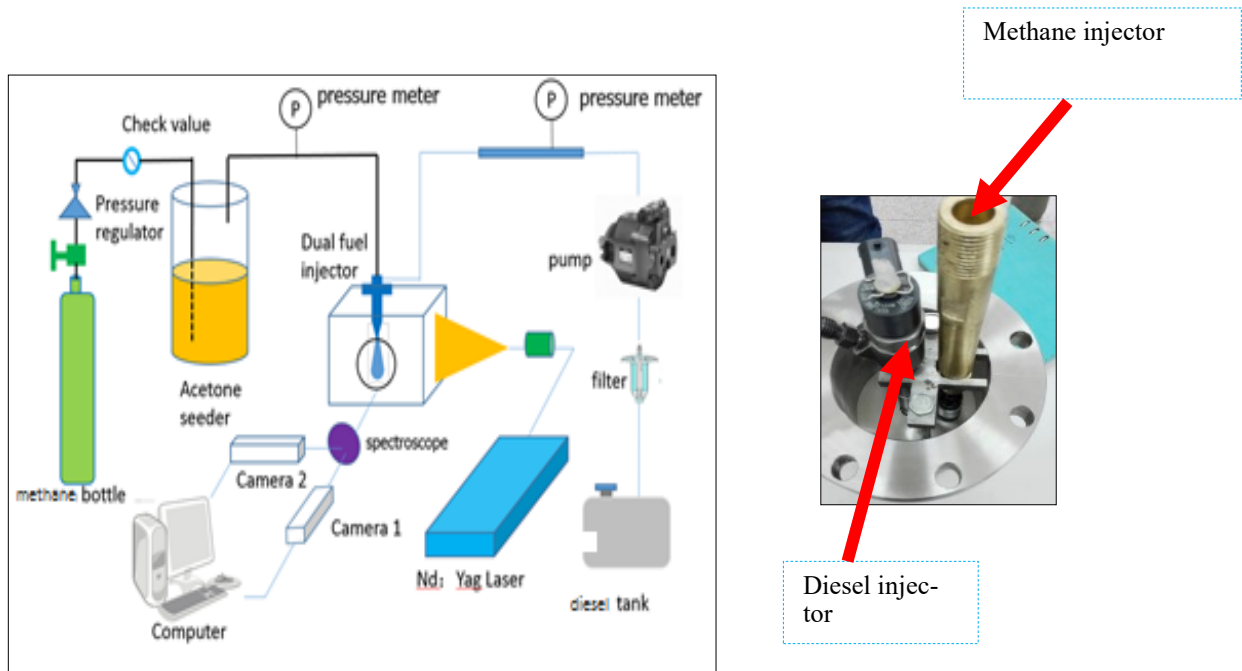
Methane injector

Diesel injector

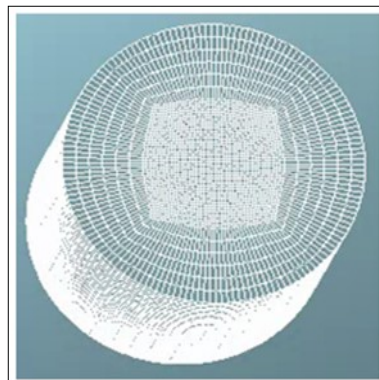Fig 1. View of the experimental layout (left) and the fuel injectors of the engine (right).

Fig 2. the mash of constant volume bomb.

and the interaction between multiple phases can be calculated.

$$\frac{\partial(\rho u)}{\partial t} + div(\rho uu) = div\left(\mu \operatorname{grad} u\right) - \frac{\partial p}{\partial x} + S_u \qquad \text{Eq. (1)}$$

$$\frac{\partial(\rho v)}{\partial t} + div(\rho vu) = div\left(\mu \operatorname{grad} v\right) - \frac{\partial p}{\partial y} + S_v \qquad \text{Eq. (2)}$$

$$\frac{\partial(\rho w)}{\partial t} + div(\rho wu) = div\left(\mu \operatorname{grad} u\right) - \frac{\partial p}{\partial z} + S_w \qquad \text{Eq. (3)}$$

Where ρ denotes the force on the fluid, μ is the dynamic viscosity, Su, Sv and Sw are the source term.

Mass Conservation Equation

The increase of fluid mass is equal to the mass of the inflow into the fluid in unit time：

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho w)}{\partial t} = 0 \qquad \text{Eq. (4)}$$

In which, t is the time, ρ is the density, u, v and w are the velocity vector components of u in the x, y and z directions.

Energy Conservation Equation

The increase of the energy in the fluid is equal to the sum of the net heat flow and the external force on the fluid in unit time. The energy conservation equation is:

$$\frac{\partial(\rho T)}{\partial t} + div(\rho uT) = div\left(\frac{k}{c_p} \operatorname{grad} T\right) - \frac{\partial p}{\partial x} + S_T \qquad \text{Eq. (5)}$$

In which T is the temperature, Cp is the Specific heat capacity, k is Heat transfer coefficient, S_T is the source term.

Physical Model and Research Program

The physical model is a conceptual model modeled by small or large species, which allow visualization, from examining the model, of information about the thing the model represents. The physical model investigates the geometry of the model and the mathematical correlations applied in this model:

Geometric Model of Constant Volume Bomb

A cylindrical constant volume bomb is used in the experiment, the structure is simple, and the location of the nozzles, size, direction and other parameters in the simulation process were directly defined. Therefore, geometric model of constant volume bomb and meshing is directly built in the Fire software, as shown in Fig.2.The volume of the constant volume bomb is larger, The mixing process of diesel spray, natural gas jet and diesel jet mainly occurs in the center area of the constant volume bomb. In order to shorten the calculation time and ensure the accuracy of the calculation results, the center of the constant volume bomb center is refined. The surrounding area grid size is about 3.5 times than the volume of the encrypted location grid, and the total number of meshes is 120393, which belongs to the structured grid.

Mathematical Model and Boundary Condition

For natural gas jets, there will be an incomplete expansion phenomenon under very high ejection pressure conditions; the jet process is very complex therefore; in this paper, the Pure Gas Jet model is selected as the gas jet model and KH-RT is the broken model. Because the injection mixing process of natural gas/diesel dual fuel in the fixed

volume is researched in this section, it does not involve the combustion process. The ambient temperature is represented by the room temperature; the collision model Walljet2 is suitable for the cold wall.

Analysis of Mixing Process of Natural Gas / Diesel Dual Fuel Injection

In order to be able to analyze the mixing process of natural gas/diesel injection the following must be investigated;

Experimental and Numerical simulation conditions

This section mainly studies the effect of the ambient pressure on the mixing characteristics of dual fuel injection, so the numerical simulation and the parameters of the experiment are consistent by varying the ambient pressure. In this paper, four different ambient pressures of 0.1MPa, 0.3MPa, 0.5MPa and 1MPa were selected and analyzed. Table.2. gives several major parameters in the study.

The Influence of Ambient pressure on Natural Gas / Diesel and Dual Fuel Jet Development

The pilot ignited diesel fuel is introduced inside the combustion burning chamber as illustrated in Table.1. High digital CCD in-cylinder camera FASTCAM was established to observe the dual fuel combustion development. Photos were taken under different time zones. The results are compared with the results from fire software simulation.

Table.1 shows the dual fuel jet image with different injection back pressure at 0.3ms, 0.5ms, 1.0ms, 1.5ms, and 2.0ms. As can be seen from Fig.3, the numerical simulation is carried out under different back pressure of the diesel and natural gas jet development process and the results are very consistent with the experimental. Because diesel is in a liquid phase and natural gas is in a gas phase, the density and momentum of diesel is much larger than the density and momentum of natural gas, resulting in the consequence that diesel is growing much faster than natural gas in simultaneous injection of two fuels. Backpressure has a great impact on the development of diesel jets and natural gas jets.

The Chemical Kinetics Model Prediction using Chemkin II software:

By utilizing the surface reactions dynamics theories for the dual fuel reactions applying the multi-step reaction; a mechanism of 5125 step with 1194 species were obtained. The dual fuel reaction prediction was simulated using Chemkin II software; the predicted dual fuel selected 50 first dual fuel reaction pathways were to indicate the whole reaction's paths are illustrated in the supporting material Table. 1S Which were adopted from Zhang et al. dual fuel mechanism [26].
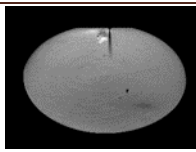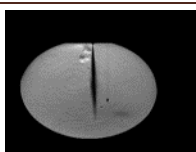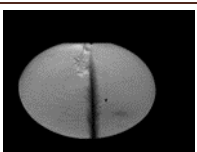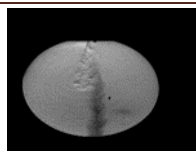
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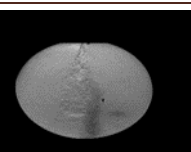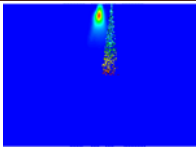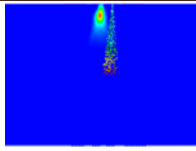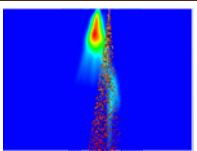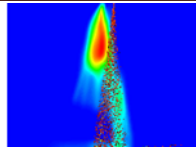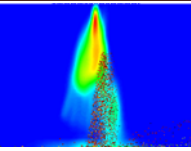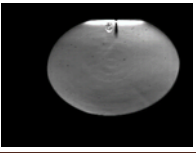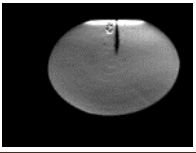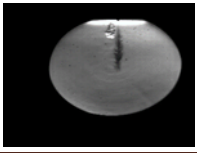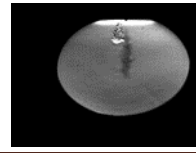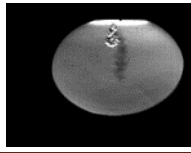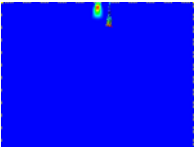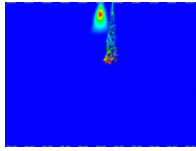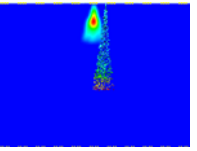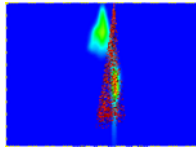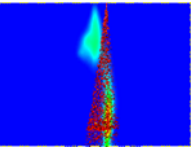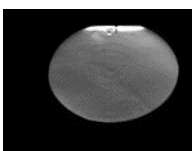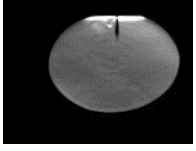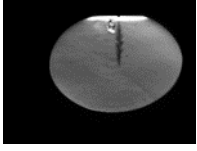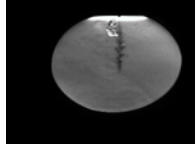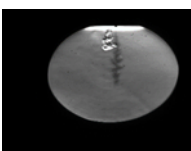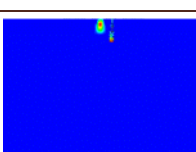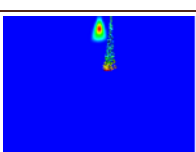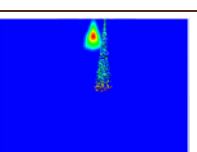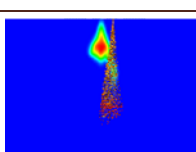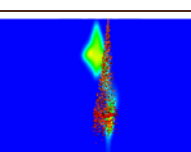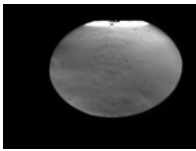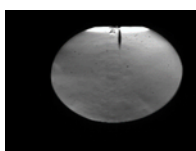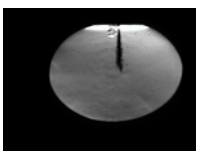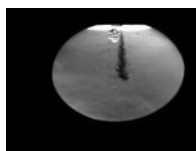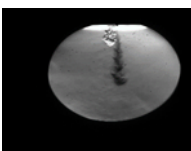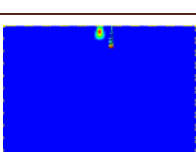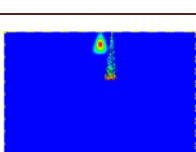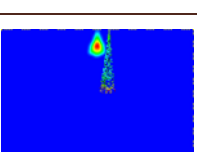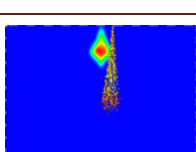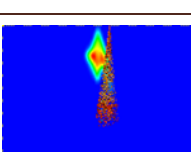
Reflected shock tube ignition is chosen to validate the combustion reaction mechanisms. This choice was made from several measurements using a range of diagnostics and a variety of shock tubes, fuels, and initial conditions. With the wide selection of the mechanisms available, it is useful to realize that not all of the data are of all the same type or quality, nor are all the mechanisms suitable for simple, direct comparison with the predictions of reaction paths. We apply a comparison of some guidelines for the shock tube ignition with reaction mechanism modeling; shock tube constant-volume behavior; shock tube diameter and boundary layer effects; carrier gas and impurity effects; and future needs and challenges in shock tube research.

Shock Tube Constant Volume Behavior

In comparing modeled ignition data with experimental data, the model calculations are usually done with a constant volume or constant density constraint. One measure of the validity or suitability of this assumption is a comparison of modeled and experimental pressure jump and plateau pressures during and after ignition.

The Shock tube pressure has a range of traces of fuel concentrations from literature review [14]. These traces have a several identifiable features. The first plateau is the filling pressure P1, the second plateau is the pressure behind the incident shock P2. The pressure transducer in these experiments was placed2 cm from the end wall of the shock tube, resulting in a short intervals represented in 65s order where this incident shock pressure can be measured. The third plateau is the reflected shock pressure P5. The rapid raise in the pressure at ignition in the highest concentration examples, 0.5% and 0.25% fuel and 0% is the constant volume ignition pressure increase. The ragged form of the

Table 1. The dual fuel jet images under different injection time and back pressure compared from the results from Fire software.

Spray time The Exp. And Simulation.	0. 3ms	0.5ms	1.0ms	1.5ms	2.0ms
The experiment at 0.1 Mpa					
The simulation at0.1 Mpa					
The experiment at 0.3Mpa					
The simulation at 0.3Mpa					
The experiment at 0.5Mpa					
The simulation at 0.5Mpa					
The experiment at 0.7Mpa					
The simulation at 0.7Mpa					
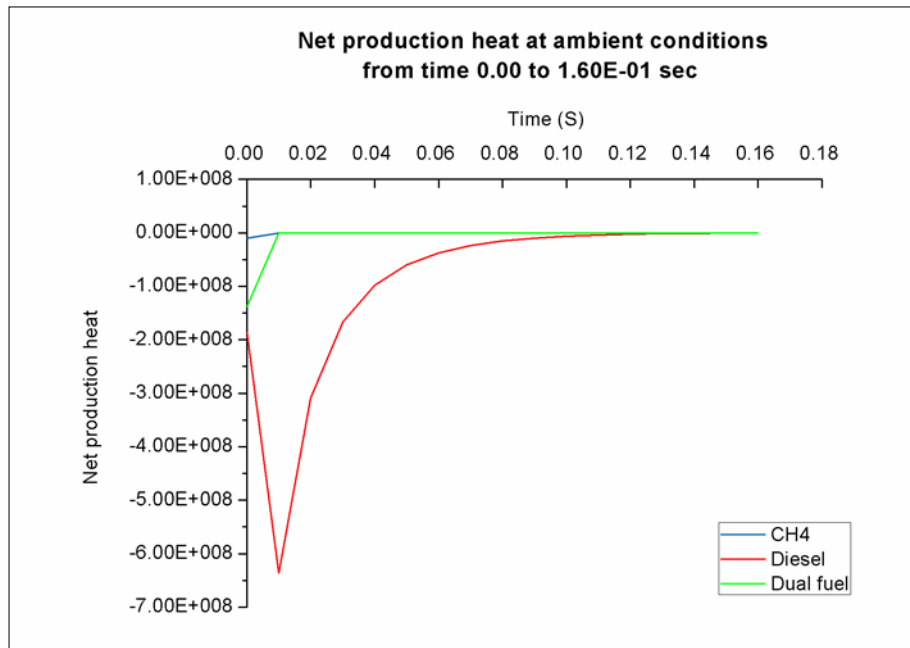
Figure 3. Comparison of predicted net production heat using different types of fuels at the beginning of the combustion from time 0.00 till 1.60E-01 second when p=1 atm, T= 297.

Table 2. Basic parameters of experimental and simulation.

The parameters name	The parameters value
Diameter of diesel nozzle /mm	0.16
Diameter of nature gas nozzle/mm	1
Ambient gas	N2
Ambient temperature/k	293
Ambient pressure/MPa	0.1,0.3,0.5,1
Injection pressure of nature gas/MPa	5
Injection duration of nature gas/ms	1.5
Injection pressure of diesel/MPa	40
Injection duration of diesel/ms Phase difference of nature gas and diesel/ms	0.7

experimental pressure data after this time is evidence of a blast wave or detonation that occurs after this pressure jump. In the lower concentration examples, the post-ignition plateau pressures are similar to P5 and the ignition pressure jump is barely noticeable. At times longer than 2 ms in all of these traces, the pressure begins to fall because of the interaction of the driver wave with the reflected shock region[27].

If the shock tube reactor were an ideal constant volume reactor, then even with the energy release process occurring during ignition, the modeled pressure along with the measured pressure would achieve the same levels during the initial ignition pressure jump and the final resting plateau. The ignition pressure jump there for can be determined by the energy release rate of the ignition process, and the final resting pressure is determined by the energy that is released. A comparison of the experimental and modeled ignition pressure indicates that at higher fuel concentrations; the pressure jump is substantially less than that predicted by the constant volume model, which is indicative of a failure of the constant volume constraint during the last stages of these energetic ignition events.

Results and Discussion

The results of the numerical simulation using Chemkin software investigating the mechanism of natural gas fuel, diesel fuel and dual fuel combustion as investigating the net heat production of combustion paying great attention to the effect of both initial temperature and pressure along with their related pollutant emissions behavior are reported as follow:

The Net Heat Produced Applying the Three Types of Fuels:

Unlike the in-cylinder pressure estimation based on diesel mechanism and Zheng and Yao mechanism, diesel mechanism equivalent ratio variety range might not be sufficient to model the diffusion combustion[28]. From previous studies it is stated that the diesel mechanism is the only applicable mechanism at the standard equivalent ratio 1.0[29], however Zheng and Yao provided a modified mechanism that is applicable even when the equivalent ratio is 1.5 which gives more flexibility in modeling the diffusion combustion[29].

In the continuous flow device; at relatively high temperature, the liquid fuel is injected directly to the air flow, the combined stream ignites as it flows through the combustion chamber[30]. After the ignition; a massive temperature increase occurs under constant pressure which produces the heat of production. The net production heat is thus defined as the net heat produced from burning the fuel inside the internal combustion engine [8]. The heat transferred from higher temperature regions to lower temperature regions is converted to mechanical work [8, 30, 31].

The predicted behavior of methane, diesel and dual fuel is verified in Fig.4. Using each fuel mechanism applied individually in Chemkin II software[32], with estimated experimental end time at 1 second. The associated operating conditions of the dual fuel are given in Table.3. Fig.4. illustrates different types of fuel: methane, diesel and the dual. The figure agrees with the previous studies that at ambient conditions CO emissions is maximized and NO_2 emission are negligible [10, 16, 17]. The model was predicted by varying the initial pressure, furthermore; the temperature was varied in cases 5, 6, 7 and 8. Generally, an increase in the engine's heat production leads to an improvement in the performance of the engine. Moreover, increasing the initial pressure results in a swift delay in the spark fire that leads to shorter burn duration.

The striking feature of the graph is that contrasting other cases: cases 1 and 2 correspond to a high similarity between dual fuel and methane fuel where as in cases 3 and 4, the prediction changes to show an obvious oscillation in the dual fuel behavior between the diesel fuel response and methane fuel response. However, the diesel fuel tends to have identical prediction with methane after the starting of combustion in case 4. On the other hand, increasing the initial temperature in Fig.5. Cases 5, 6, 7 and 8;Converts the engine behavior to act as energy consumer rather than an energy producer. Incases 5 and 6, the behavior of the methane, diesel and dual fuel is quite stable: diesel fuel consumes heat in order to start the combustion. However; there is a small amplitude oscillation in dual fuel in case 5. Furthermore, there is a small amplitude oscillation in methane and diesel in case 6. As the initial temperature increases in cases 7 and 8 diesel fuel becomes inapplicable o produce net heat production. In fact, the endothermic behavior of all fuels becomes quite obvious revealed in consuming a lot of energy at the beginning of the combustion rather than

Table 3. The operating condition for combustion simulation for methane, diesel and Dual-fuel.

Combustion mode	Methane	Diesel	Dual-Fuel
Mach number BIS (from simulation results)	284	3.43	2.91
Initial Temperature at ambient conditions (K)	297	297	297
Initial Pressure at ambient conditions (atm)	1	1	1
Fluid velocity BIS (cm/s)	10,000	10,000	10,000
Enthalpy BIS (from simulation results) (erg/g)	-2.71E+09	-5.25E+09	-3.03E+09
Entropy BIS (from simulation results)	7.25E+07	6.23E+07	7.14E+07

Table 4. Chemkin II software simulation bases.

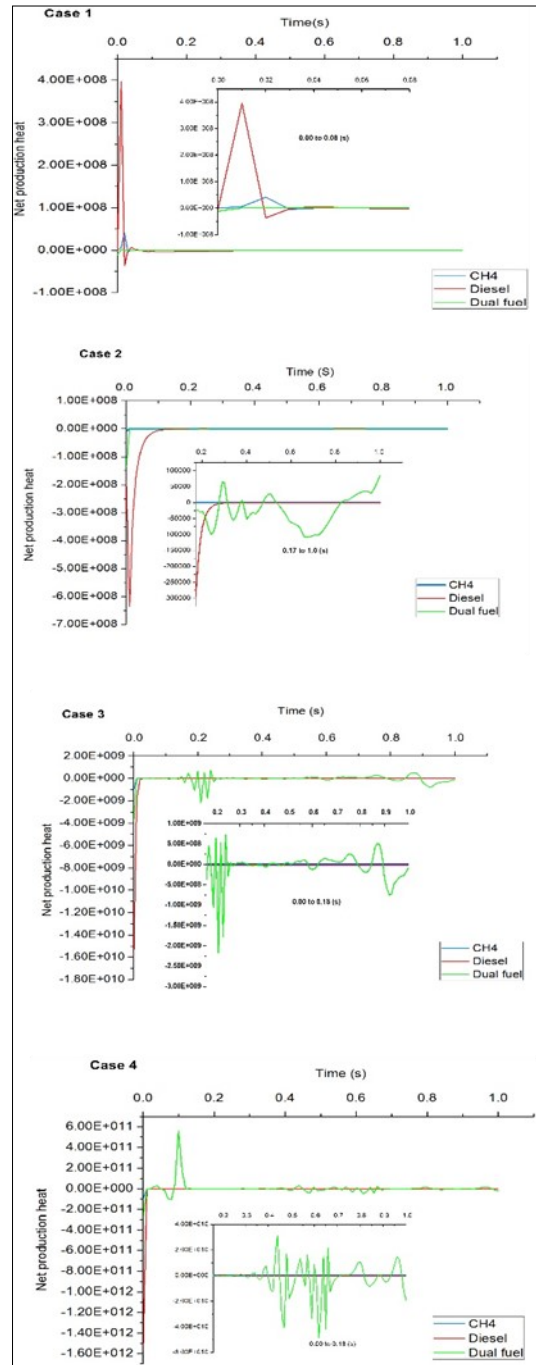| Reaction type	Normal Reflected Shock reactor
The Reactor End time	1 second
The reactor incident velocity	100,000 cm/sec
Percentage of N_2 in the reaction	0.7
Percentage of O_2 in the reaction	0.2
Reactant species in Methane fuel case	CH4 : 0.1
Reactant species in Diesel fuel case	Diesel : 0.1
Reactant species in Dual fuel case	CH4:0.09 (90%) Diesel: 0.01 (10%)

Figure 4. Comparison of predicted net production heat using different types of fuels for cases 1, 2, 3 and 4 representing pressures 0.1, 1, 10 and 100 respectively.
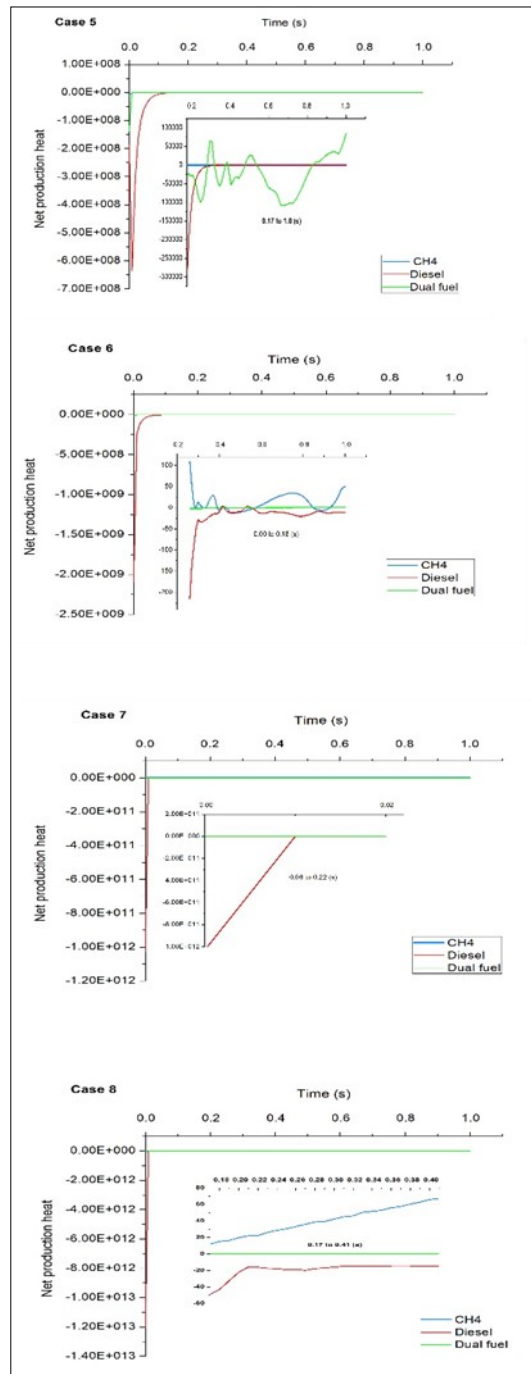
Figure 5. Comparison of predicted net production heat using different types of fuels for cases 5, 6, 7 and 8representing temperatures 297, 500, 900 and 1100 respectively.

producing any. According to the initial temperature effect; increasing the initial temperature doesn't clearly affect the behavior of the dual fuel but it destroys the trend of diesel fuel to become heat consumer at relatively high initial temperature. In each case 10% of combustion energy is obtained from diesel when applying the methane/diesel dual fuel mode.

As the engine works as dual fuel, more premixed fuel and oxidizers exist [8].The model results generally show some similarities when changing the fuel type. Moreover, in Fig.4. Case 1, the highest net heat produced were obtained by diesel caused by the cylindrical combustion. From cases 3 and 4 it's clear that the net heat produced reaches its peak in the dual fuel combustion case while in Fig.5. Cases 5, 6, 7 and 8. The effect of changing the initial temperature doesn't really change the behavior of the dual fuel. Furthermore, in the dual fuel combustion case 2, the peak is delayed to 2.90E-01 second where the auto ignition begins. Emissions were taken under different initial pressures and temperatures.

The prediction of COx and NOx Exhaust Emissions using Methane, Diesel and Dual of Fuel at various Pressures and Temperatures:

The combustion net production heat among the different types of fuel are illustrated in Figs. 4 and 5.

Which agrees to some extent with the literature data [8, 21, 33]. The model predicts COx and NOx emissions with higher accuracy compared to previous literature studies. The exhaust simulation results of COx and NOx at standard conditions for different types of fuel are shown in Figs. 6, 7 and 8. Illustrate the dual fuel emissions at different initial pressures and temperatures. However, the input energy, fuel flow rate as well as all the initial thermodynamics; all are kept constant in order to perform the dual fuel injection as shown in Figs. 7 and 8. At ambient initial conditions as illustrated in Fig. 6. However, Considering CO_2 emissions and the peak amount was caused by both methane and dual fuel; CO_2 emissions were quite negligible when burning the diesel fuel. However the emissions of CO were reduced when using the dual fuel engine. The peak emissions of NO were caused by the dual fuel. It is also implied that burning diesel doesn't release any NO emissions. There is no NO_2 emission in all cases.

It is observed that varying the initial pressure greatly influences the outlet emissions of the engine. For example, in Fig.7. Case (A) at ambient conditions, CO_2 emissions intensity is maximized in case of dual fuel. This initial pressure varies either increasing or decreasing. As the initial pressure increases the CO_2 emissions of
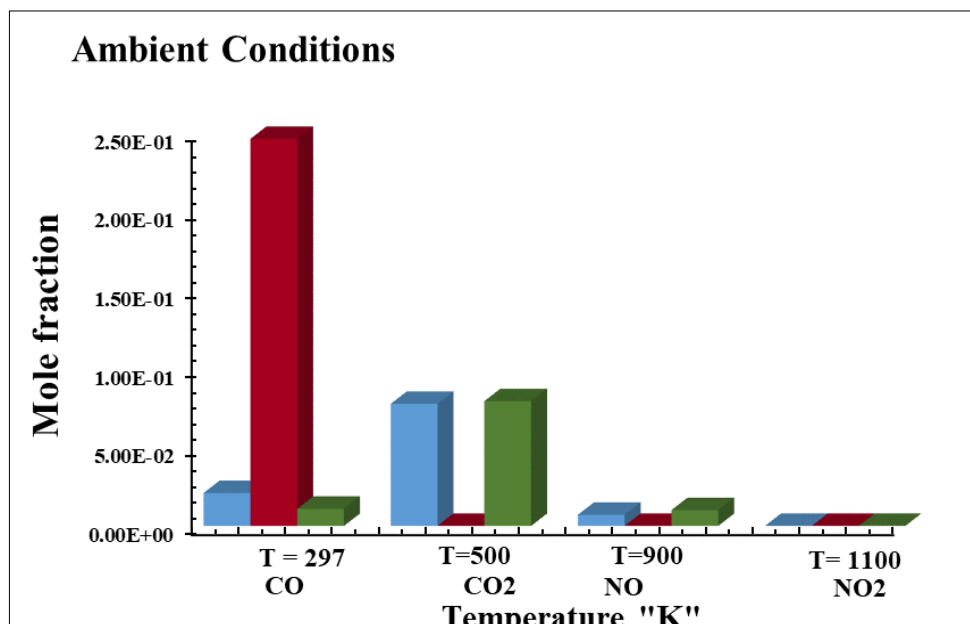
Figure 6. The exhaust simulation results of CO, CO2, NO and NO2at ambient conditions for different types of fuels. ( ) Methane fuel; ( ) diesel and ( ) dual fuel.
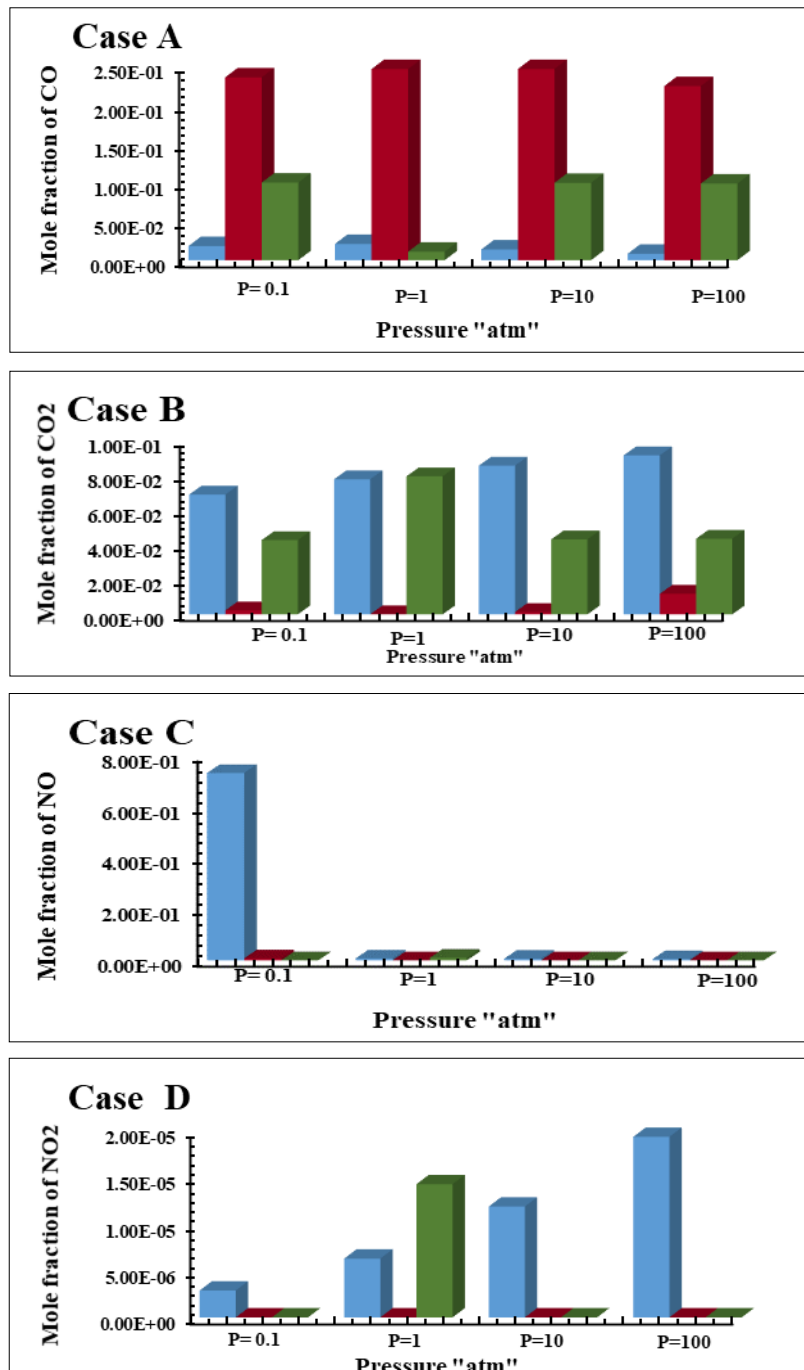
Figure 7. Illustrates the different types of fuel emissions CO, CO2, NO and NO2 at different initial pressures;(▢) Methane fuel; (▮ () diesel and (▮) dual fuel.
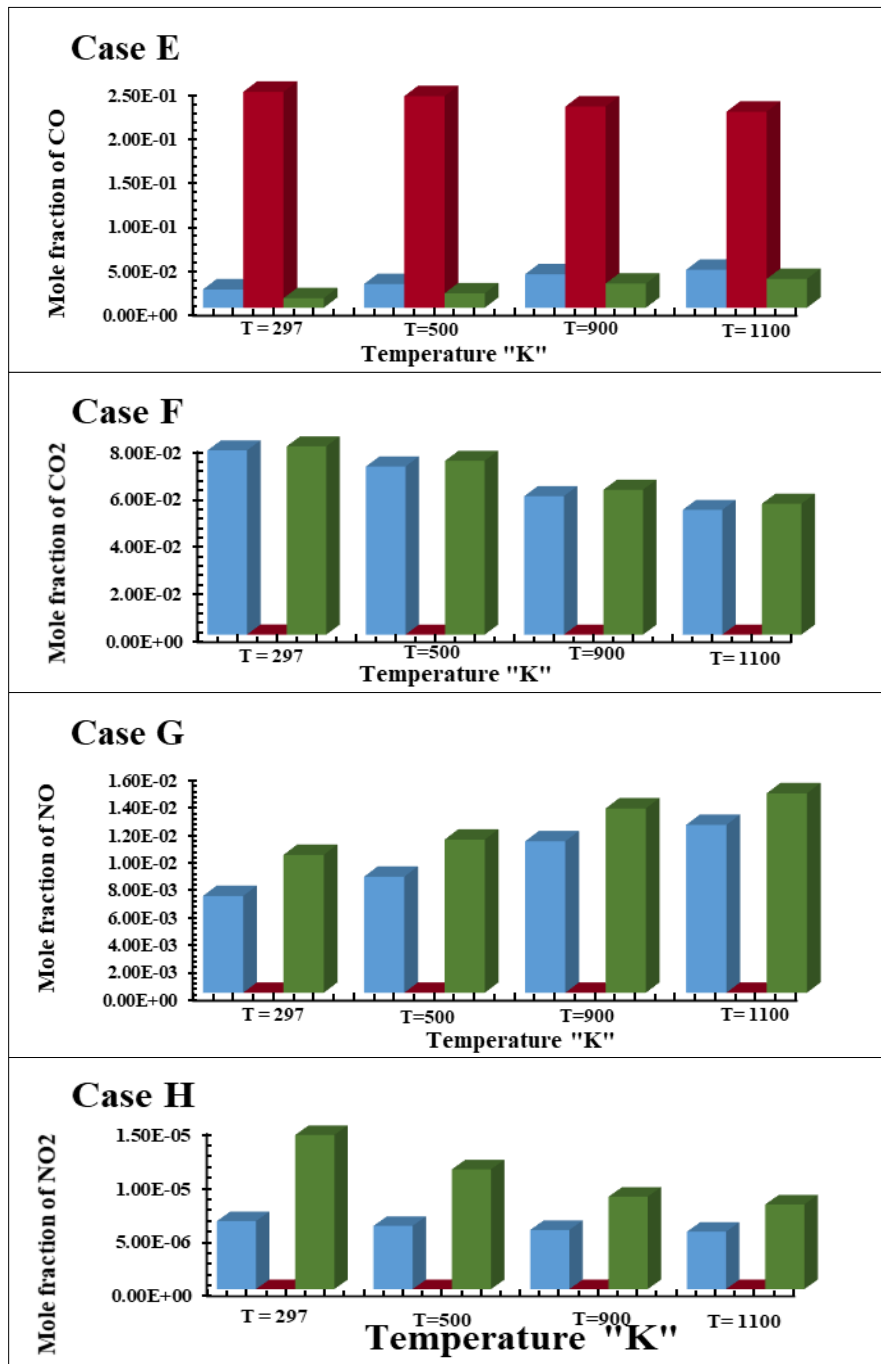
Figure 8. Illustrates the different types of fuel emissions CO, CO2, NO and NO2 at different initial Temperatures; (■) Methane fuel; (■) diesel and (■) dual fuel.

methane and diesel increases. In contrast to the reduction of the initial pressure where methane and diesel behave differently; at low pressures diesel emissions increases while methane emissions decreases. CO emissions jump to reach its peak at an estimated mole fraction of 0.1 in the case of dual fuel combustion , as the initial pressure skew from the ambient conditions.

A Diesel emission remains high and unaffected by the pressure variations. However, methane CO emissions are reduced slightly as the pressure increase or decrease as illustrated in Fig. 7. Case (B). The striking feature of Fig 7. Cases (C) and (D) is that as the initial pressure either increase or decrease; dual fuel NOx emissions are completely vanished. However, varying the initial temperature has no effect on CO_2 emissions in case of diesel fuel combustion. Varying the initial temperature has no effect on CO_2 emissions in case of diesel fuel combustion.

Case (F) illustrates that in the highest initial values of CO emissions from both methane and dual fuel but the dual fuel rise at a lower rate than that when the initial pressure changes. In addition, the temperature effect on the diesel fuel is negligible. Methane and dual fuel NO emissions. A reverse trend appears in dual fuel NO_2 emissions characterized by obvious NO_2 reduction as the initial temperature increase.

As a conclusion, using the dual fuel at ambient conditions increases the engine's efficiency and causes less CO_x emissions, however it causes a considerable increment in NO_x level. As the initial pressure varies -either increase or decrease- the performance of the dual fuel improves. Increasing the engine's initial temperature will result in lower CO_2 and NO_2 emissions and higher CO and NO emissions. Simultaneously; varying the initial pressure largely reduces CO_2 emissions and eliminates NO_x emissions. CO emissions are at the peak when the initial temperature and pressure are varied from the ambient conditions in either an increase or a decrease manner.

Modifying the conventional diesel engine to serve as dual fuel engine increases its efficiency at relatively higher initial pressure. However, changing the initial temperature doesn't really affect the performance of the dual fuel engine.

Conclusions

After obtaining the model results, the main conclusions are as follow;

- Diesel is injected first inside the combustion chamber then followed by Natural gas through separate injectors. The fuel mixes inside the chamber and ignites.

- Dual fuel mechanism is capable of producing different heat production behaviors when either increasing or decreasing the initial pressure and temperature.

- The scientific values added of this field include;

1. At low initial pressures, the performance of diesel is at its maximum but as the initial pressure increases the behavior of dual fuel becomes more favorable.

2. Increasing the initial temperature enhances the endothermic behavior of all types of fuel where it becomes heat consumer instead of heat producer.

3. CO_2 emissions are minimized by changing the initial pressure above or below the atmospheric value. However, CO emissions are peaked when diesel fuel is used. The dual fuel engine minimizes the CO emissions amount caused by diesel fuel. Increasing the initial pressure eliminates dual fuel CO_2 combustion emissions.

4. Increasing the initial pressure reduces the dual fuel NOx emissions. However methane NO emissions are minimized by increasing the initial pressure.

5. The results indicate that NO and NO_2 emissions have a reverse behavior when it comes to temperature variations; as the initial temperature rises, the NO emissions production from methane and dual fuel increases contrasting NO_2 emissions that gets lower as dual fuel burns.

6. There are no diesel NOx emissions in all cases for the development of the engine output high initial pressure is preferred in order to obtain high efficiency as well as low CO_2 emissions.

El-Fatah Abomohra (School of Energy and Power Engineering, Jiangsu University) during paper revision.

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