Parameter Change in Engine Simulation and Performance Optimization of Diesel Engine

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Abstract. Diesel internal combustion engines have been widely used in automobiles, ships, power generation, and other fields, laying a foundation for modern science and technology. Due to the wide application of internal combustion engines, the working efficiency and exhaust gas generated by internal combustion engines have become issues of common concern. In order to optimize the working efficiency and emissions, simulations are carried out under different conditions by using Cantera IC Engine code. Through analysis, the relationship between similar factors and their effects on emissions and thermal efficiency are shown, thus obtaining the most effective method to improve efficiency and reduce emissions. On the one hand, it is found that factors, such as the compression ratio, have a very intuitive impact on the efficiency of the engine. On the other hand, the ambient temperature and air pressure have less influence on the engine operating within the controllable range. These results provide a general idea for diesel engine optimization under certain environments.

1. Introduction

The internal combustion engine is a type of heat engine that converts the chemical energy of fuel into mechanical energy. It is done through air and fuel mixed and combusted to generate heat energy, and the gas is heat-expanded and converted into mechanical energy by a mechanical device to do work externally [1].

Due to the fuel type, diesel engines often face a high greenhouse emission, but they also have higher thermal efficiency [2]. Given global warming, increasing population density, and deterioration of the ecological environment, engine emissions will gradually have higher requirements [3]. In recent years, through the improvement of processing technology, casting technology, and materials, the optimization of engines has also been a consistent process [4].

Recently, there has been a range of research in the field of gasoline engines. In contrast, there is still a lack of research on diesel engines and their optimization. The diesel engine used in this paper has a lower speed but higher torque than the gasoline engine, which has been widely used in automobile and heavy industries [5]. Because of the different application environments, the way of optimization of the diesel engine and the gasoline engine will be very different.

To optimize the engine, it is necessary to analyse each factor, which may affect the thermal efficiency and emissions of the engine. Similarly, because two similar factors will also affect each other, the direct relationship between each factor should also be carefully analysed. Currently, the common strategies used to study engine are using simulation and model machine experiment. The latter is often carried out after simulation mainly due to high cost and long-time consumption. At the initial stage of discovering relationships and optimal parameter range, simulation often has plenty of advantages, for example, it
allows researchers to obtain operational data with minimal cost. Although a few limitations exist for simulation, such as the engine is assumed operating under ideal conditions and few of the variables can be changed simultaneously, the simulation is still able to explore the relationship between factors and give reliable data on the favourable range for each parameter.

Though the digital simulation has been influential in the field, the limitation of this simulation is that it cannot consider too many external factors, such as screw wear, material hardness, and other details, because it is mainly simulated through code operation [7]. Therefore, the simulation will assume that the engine will operate under the most optimized conditions, but in practice, it will often be harsher. Further, due to the limitation of the simulation system and variable dimensions, the simulator can usually change only a few of the selected variables each time it simulates. However, through high reliable digital simulation and step-by-step adjustment of parameters, it can still be found that the relationship between factors and the favourable range for each parameter can be explored.

Through this study, this research is aimed to find out how similar factors of engines affect each other. After finding out the relationship, an ideal balance point can be found between efficiency and emissions with consideration of graphs. Finally, the research can give the ideal reference range of each factor. This study can provide a guide of thought for future diesel engine improvement and help researchers to understand which factors, if improved, can have the greatest effectiveness to optimize engine efficiency and emissions.

In the previous research in related fields, fuels, such as hydrogen and methane, have been extensively studied [8]. However, there is relatively little previous research on other macro-molecular chain fuel types for diesel engines. Similarly, because the molecular weight of diesel fuel is longer, the simulation is more difficult than that of a gasoline engine. In order to make up for the lack of research in the field of diesel engines, this paper will use relatively uncommon fuels.

For traditional internal combustion engines, the types of diesel fuels will also have different requirements for engines. The fuel type used in this research is n-Dodecane (NC12H26), which is one of the long chains, high molecular mass diesel fuel. This fuel is widely used in truck engines. The simulation of the diesel engine was done by using the Python Cantera Package “IC Engine” [9] with the model “SK54.cti”. With this fuel to simulate the engine, a deeper understanding of the operation of diesel engines under various conditions can be generated. Additionally, the relationship between factors will also be illustrated. Through the analysis of the relationship and data, the researcher can develop an intuitive optimization idea. This method will serve as a guide for the optimization of diesel engines in the future.

There are multiple important factors in the engine that can affect the operation and emissions of the engine. This research will mainly be focusing on the following factors: Engine Speed, Piston Diameter and Piston Displaced Volume, Engine Compression Ratio, Turbocharger Pressure and Turbocharger Air intake Temperature, Ambient Pressure and Temperature, Air Inlet and Exhaust Gas Outlet Time, Fuel Mass, and Air Inject Time. According to the existing models, it is hypothesised that with the increase of engine efficiency, the emissions of carbon monoxide and carbon dioxide will increase. Diesel engines, due to the fuel used, will have various types of exhaust gases, such as Ox, COx, HOx, NOx, SOx ROx, MOx, and POx [10]. In this paper, carbon monoxide and carbon dioxide are mainly used as the main measurement standards of exhaustion.

2. Methods

Different authors have measured engine efficiency and emission level in a variety of simulation models. Recently, a simpler, and more rapid model of “Cantera IC Engine” simulation model has been developed. In order to complete the experimental aim and reduce the interaction between distinct factors, there will only be one or two related parameters change at a time. Except for the selected variables, all parameters were set as default values. The main disadvantage of the experimental method is that it will demonstrate how one or two variables affected the internal combustion engine as a whole.

Firstly, for engine speed, since the operational speed for the diesel engine is relatively lower than that of the gasoline engine, the speed was set from 1000 rpm to 4000 rpm with each increment of 125rpm.
Secondly, the piston diameter and displace volume are bounded to form a 3D relation. The displaced volume is initially set to be 0.5×10⁻³ m³, with each increment of 1.875×10⁻⁵ m³. Similarly, the piston diameters were initially set to be 0.083 m, with each increment being 3.1125×10⁻² m. Additionally, the compression ratio was covered between the range 36 to 50. Each increment was 1 unit. Turbocharge pressure and temperature are two correlated variables. The temperature was between 300K to 1000K, with 17.5K per increment. The pressure was between 0.5 atm to 2 atm with 0.075 atm per increment. Next, the ambient properties contained ambient temperature and pressure. To imitate reality, the ambient temperature was set between 253K (-20°C) to 323K (50°C) with 3.5°C per increment. Similarly, the pressure was between 0.5 atm to 2 atm with 0.075 atm per increment. Subsequently, air inlet and exhaust are two processes that largely affect emission. Both of which were set with the unit as a degree to the crank angle. Therefore, both of their timing was between 136° to 216° with an increment of 2°. Lastly, fuel mass and air inlet time gave a good indication of the air to fuel ratio. Similar to the previous, the range and increment for inlet valve time were 136° to 216° and 2°, respectively. The fuel mass was set between 1.5×10⁻⁵ kg to 4.2×10⁻⁵ kg with 6×10⁻⁷ kg per increment. All the data obtained were then saved as notepad and graphed in MATLAB using inbuilt plotting functions. For the 2D plot, an additional trend line is obtained using the function “Polyfit” and “Polyval.”

3. Results

In order to investigate the different kinds of parameters effects on engine efficiency as well as CO and CO₂ emissions, both of them were separated into different groups according to their characteristic. Systematic scanning results are given in the following subsections for each group while setting other parameters to default values. Additionally, possible reasons behind the trends are discussed in details with reference to the diagram.

3.1 Engine Speed

As illustrated in Figure 1(a), the efficiency decreases as the engine speed increases. Diesel engines require the engine to provide higher torque than gasoline engines. With lower rotating speed, the engine will have a longer ventilation time, improve the ventilation quality, therefore, have a higher combustion time, thus improving its combustion efficiency.

The correlation between Carbon Monoxide (CO) and Engine rotational speed was tested. As shown in Figure 1(b) the CO Emission increased significantly once the engine speed reaches 3500 rpm. An explanation for the trend is that when the rotational speed becomes fast, the fuel and air in the combustion chamber cannot be completely combusted. As a result, the concentration of Carbon Monoxide, as the main product of incomplete combustion, increases. Similarly, in Figure 1(c), as the engine speed increases, the CO₂ emission also increases. However, once the Engine Speed reaches 3500 rpm, the CO₂ emission start to decrease. Compared with Figure 1(b), it can be reasonably inferred that as the CO Emission increase, CO₂ Emission decreases. Since most CO₂ gases are produced through complete combustion, while the CO gases are produced from incomplete combustion, with less complete
combustion reactions and more incomplete combustion reactions, less CO2 will be produced.

3.2 Piston Diameter and Displaced Volume

Figure 2. (a) The Engine efficiency, (b) the CO emission and (c) the CO2 emission as a function of T

Piston Diameter and Displaced Volume. The colour bar indicates the value on the vertical axis. It can be seen from the data in Figure 2(a) that the Piston Diameter, on the one hand, under the condition that other factors are fixed, will not have a great impact on engine efficiency. Its diameter has a greater relationship with the size and materials of the engine. On the other hand, when the compression ratio is fixed, the lower the displaced volume, the higher the efficiency. Since the efficiency is not directly affected by the displaced volume, instead, it is directly affected by the compression ratio. If a lower displaced volume can provide the same compression ratio, less energy will be needed to exert on the piston, thus, increases its efficiency. Moreover, with more air combined with the same amount of fuel, it disturbs the fuel to air ratio, which further explains the decrease in efficiency.

As can be seen from the Figure 2(b), as the displaced volume increases, the CO emission demonstrates a decreasing trend. This is correlated with the efficiency figure; as the efficiency decreases, the emission decrease. Similar to the trend of carbon monoxide emission, in Figure 2(c), since the efficiency decreases, the CO2 emission also decreases. The decreases in emission for both CO and CO2 shows that when displaced volume increases with other parameters constant, less combustion reaction happens during the combustion.

3.3 Compression Ratio

Figure 3. (a) The Engine efficiency, (b) the CO emission and (c) the CO2 emission as a function of engine speed. The red circle lines represent for simulation data while blue lines show the trend line which generated using MATLAB inbuilt function “polyfit”.

From the Figure 3(a), it can be seen that as the compression ratio increases, the efficiency also increases, respectively. A higher compression ratio directly indicates that the fuel/air mixture got compressed under a higher pressure, which, then, leads to higher fuel efficiency. Thus, the higher the compression ratio is, the higher the efficiency can be.

The CO Emission in Figure 3(b) decreases as the compression ratio gets higher. This is because under high compression ratio, fuel and air are fine mixed and fuel are utilized in the most optimal way. Therefore, most combustion process is complete combustion which does not produce Carbon Monoxide as its final products. As shown in Figure 3(c), in a larger scale, it could be determined that although
there is a slight increase in CO2 emission, this increase is less than 1% of its original emission value. Therefore, the CO2 emission is nearly independent of the Compression ratio.

3.4 Turbocharger

Figure 4. (a) The Engine efficiency, (b) the CO emission and (c) the CO2 emission as a function of Turbocharger Temperature and Pressure. The colour bar indicates the value on the vertical axis.

As can be seen from Figure 4(a), the highest efficiency occurs when the Turbocharger is at 300K with the highest turbocharger pressure. According to the formula

\[ pV = nRT \]  

where \( V \) represents the volume determined by the cylinder, and \( R \) is determined by the type of gas, the lower the temperature \( T \) is, the greater the amount of the intake air will be. Therefore, under the same condition, the lower the temperature, the greater the turbocharger pressure, the greater the intake air volume. And thus, this will lead to higher efficiency. There was a significant difference between the two conditions: High Temperature with Low Pressure, and Low Temperature with High Pressure. Under high pressure and low-temperature scenario, the CO emission reaches its lowest. This is due to under that condition, the amount of inlet air reaches its highest. With a sufficient amount of air, ECU would control the fuel to air ratios based on the environmental conditions obtained by the sensors; the combustion will occur under the most optimal condition. Thus, it gives a low Carbon Monoxide Emission.

Under normal working, the decrease in carbon monoxide often means the increase in carbon dioxide. Because ideally, carbon monoxide reacts with oxygen to produce carbon dioxide. This relation is shown through the comparison of Figure. 4(b) and Figure. 4(c)

3.5 Ambient Property

Figure 5. (a) The Engine efficiency, (b) the CO emission and (c) the CO2 emission as a function of Ambient Temperature and Pressure. The colour bar indicates the value on the vertical axis.

From the data in Figure 5(a), it is apparent that the ambient pressure does not have a visible effect on engine efficiency. The efficiency fluctuates as ambient temperature changes. As seen in the graph, the efficiency only fluctuates within a relatively small range, between 56.8%-57.6%. However, the maximum engine efficiency occurs at around ambient temperature at 300K. Nevertheless, the ambient temperature, as its own does not affect the efficiency largely.
Similar trends are also shown in Figure 5(b) and Figure 5(c). Both CO and CO2 emissions are fluctuating in such a small range that the ambient temperature and ambient pressure is not a great concern under this ideal case.

3.6 Air Inlet and Exhaust Gas Outlet Time

Figure 6. (a) The Engine efficiency, (b) the CO emission and (c) the CO2 emission as a function of Air Inlet Time and Outlet Valve Time. The colour bar indicates the value on the vertical axis.

The experimental data in Figure 6(a) shows that the greatest efficiency occurs with the maximum air inlet time and the maximum air outlet time. The maximum air inlet time allows more combustion-supporting gas present during the combustion. In this way, it enables the fuel to utilise in its most efficient way. Moreover, the pressure to the piston would also increases, which then, increases the torque and efficiency of the engine. Likewise, when the outlet valve time increases, all the exhaust gas can be emitted with little left in the combustion chamber. Exhausting more burnt gas increases the oxygen concentration in the chamber during each combustion, in other words, enabling fuel and oxygen to be reacted in the most efficient way, which increases the engine efficiency.

From Figure 6(b), the carbon emission level has a larger correlation with air inlet time than outlet time. As the air inlet time decreases, a significant increase in CO emission level is shown. As discussed, Carbon Monoxide, as the main products of incomplete combustion, concentration would increase when limit oxygens present. Therefore, when air inlet time is short, the oxygen concentration in the chamber is low, causing incomplete combustions and resulting increase in CO emission. When air inlet time is high, the outlet valve time starts to play a role in the emission level. Under that condition, the concentration of oxygen would not be a great concern. The carbon monoxide content concentration is already low. When outlet valve time increases, all carbon monoxide produced during the combustion will be released, which increases the CO emission. Contrastingly, with a lower outlet valve time, some of the exhaust gas will be left in the chamber to be reused, which would then form CO2, therefore, resulting in a lower CO emission. What is interesting in Figure 6(c) is that the CO2 emission did not show a strong relationship with the outlet valve time. However, as the air inlet time increase, the emission decreases. In Baskar and Senthilkumar’s study, it shows that under oxygen-rich condition, the combustion would produce less carbon emission [11].

3.7 Fuel Mass and Air Inject Time

Figure 7. (a) The Engine efficiency, (b) the CO emission and (c) the CO2 emission as a function of Fuel Mass and Fuel Inject Time. The colour bar indicates the value on the vertical axis.
The air inlet time is correlated with the amount of gas injected in the combustion chamber. In this case, the highest efficiency occurs is when $2.1 \times 10^{-5}$ kg fuel combined with air inlet valve time around $211^\circ$ of the crank angles. It is clearly shown in Figure 7(a) that there is an optimal gas to air ratio, which gives the highest engine efficiency. The reason behind is that for diesel engine, the equivalence ratio around 0.9 would be the most optimal combustion environment and thus gives the highest efficiency.

The results displayed in Figure 7(b) demonstrated the trend that the highest CO emission occurs when the greatest amount of fuel combines with the least amount of air. Besides, when the fuel to air ratio is approximately 1 (the most optimal combustion ratio), the CO emission would, therefore, be the lowest. This is because when fuel largely exceeds the amount of oxygen required, the rate of incomplete combustion grows rapidly and forms carbon monoxide as its product. In general, as the fuel mass increases, the CO2 emission increase. Once it reaches a maximum, it starts to decrease. This relation is clearly shown in Figure 7(c). When the fuel level is fixed, the higher the air inlet time is, the more amount present during combustion can be, which will then lead to a lower CO2 emission.

4. Discussion
The efficiency of the engine shows a decreasing trend as the engine speed increases. Also, the CO and CO2 emission increase at a fast rate once the engine speed reaches 3500 rpm. The optimal engine speed is between 1800-2200 rpm. Since CO is a toxic gas, as this speed range, both CO and CO2 are at an acceptable range with relatively high efficiency. For piston displaced volume, with a given compression ratio, a smaller displaced volume would be more desirable as it gives the highest efficiency. Although the carbon monoxide and carbon dioxide emission increase correspondingly, the emission level is still in the acceptable range if the displaced volume is greater than $5 \times 10^{-4}$ m$^3$. Piston diameter does not demonstrate a clear effect on the efficiency and emission, as it should varied based on the size of the IC engine.

As shown in Figure 8, higher compression ratio means more air in the combustion chamber. The trend is clear that efficiency has a positive relation with engine efficiency and a negative relation with both CO and CO2 emissions [13]. The relation between the engine thermodynamic efficiency and the compression ratio can be expressed in the equation

$$\eta_{th} = 1 - \frac{1}{\epsilon_c}$$

where $\eta_{th}$ is the thermodynamic efficiency, and $\epsilon_c$ is the compression ratio. As represented by the equation, a higher compression ratio will directly result in a higher efficiency, which explains the continued efforts for manufacturers to seek a higher compression ratio [14]. However, a higher compression ratio will have a higher restriction for the material chosen with the financial costs of the engine. Nevertheless, the engine should be chosen as the highest compression ratio under limited circumstances.

A turbocharger is a device fitted to a vehicle’s engine that is designed to improve the overall efficiency and increase performance [15]. A turbo is made up of two halves joined together by a shaft. On one side, hot exhaust gasses spin the turbine that is connected to another turbine, which sucks air in and compresses it into the engine. This compression is what gives the engine the extra power and efficiency because as more air can go in the combustion chamber, more fuel can be added for more
power [16].

Figure 9. A diagram shows how turbocharger work [17]

For the turbine intake air temperature and produced air pressure, the higher the air pressure produced, the higher the engine efficiency [18]. Since the air intake temperature is rarely lowered than room temperature, room temperature would be the optimal intake air temperature. With the highest turbine pressure and 300K air intake temperature, CO emission reaches its minimal level. While CO2 emission increased, since CO is more toxic than CO2 and the CO2 emission is still at an acceptable range, the highest turbine pressure possible, and room temperature are recommended for engine operation.

The ambient pressure, from the simulation results, does not show a strong impact on engine efficiency and emission. Therefore, on the one hand, it is not a great concern for improvement. On the other hand, the ambient temperature, between 250K-320 K, which is between (-23°C to 47°C), affects the engine efficiency and emission. For the peak at 309K, a possible explanation is that as the ambient temperature continually increases, the specific fuel consumption increases, which causes fuel losses [19]. However, in this simulation model, all these effects are small enough to be ignored. For the above reasons, the ambient conditions have minimal effects on the engine alone.

Both air inlet time and gas outlet time have a strong impact on the engine efficiency. The highest efficiency occurs when both inlet and outlet time are at their maximum position. The reason is clear, with the greatest exhaust time, the engine ensures the purity of air during each combustion [20]. With the greatest air inlet time, it ensures the concentration of oxygen to support the combustion. Therefore, by ensuring proper air intake and exhaust valve time, engine efficiency can be greatly improved [21]. Additionally, with the greatest air inlet time, it minimises the occurrence of incomplete combustion. Although the CO emission would be further reduced with a lower exhaust time, by doing so, it largely reduced the engine efficiency, only reduced the emission by a little. Furthermore, the CO2 emission is also at its low position. The recommended parameter is to have a high air inlet time with a reasonably high air outlet time.

Lastly, the injected fuel mass and air inlet time represent the fuel to air mix ratio. It is shown that there is an optimal ratio that gives the highest efficiency. In a common diesel engine, the highest efficiency occurs when fuel to air equivalence ratio is around 0.9. At this ratio, the engine ensures a fine chemical combustion condition with minimal ineffective reaction. Thus, by ensuring an ideal equivalence ratio, the engine would raise the volumetric efficiency [22]. At this ratio, both CO and CO2 emissions are at low levels. Although, by increase the air to fuel ratio, the CO emission would face a large decrease [23], this will also lead to a large sacrifice in engine efficiency. With the consideration of efficiency and emission, the optimal situation is that the air to fuel equivalence ratio is slightly below 1 (around 0.9).

5. Conclusion

In conclusion, the operation parameter effects are analysed on the efficiency and emission of the internal
combustion engine via the Cantera Python Code. On this basis, the recommended operating parameters are given and discussed through the simulation data. Significant effects and clear relationships are found for the engine speed, displaced volume, compression ratio, turbocharger pressure and temperature, outlet valve, fuel mass, and air inject time. This aspect of the research suggested that when adjusting these variables, the efficiency can increase largely. In terms of pollution emissions, this paper argued that, in most cases, carbon monoxide emissions gradually increase with the increase of internal combustion engine efficiency. Because the total amount of waste is relatively fixed and carbon monoxide can produce carbon dioxide by chemical reaction, the increase of carbon monoxide often means the decrease of carbon dioxide emissions. The two greenhouse gases are usually inversely proportional. Therefore, efficiency and carbon monoxide emissions often become two contradictory goals. It is an important finding in the understanding of the targets for carbon monoxide and carbon dioxide. In engine optimization, rather than seeking ways to minimize both, it is especially more important to find a balance between different exhaust gases.

The data provided in this paper offer valuable guides for future engine optimization. In addition, by giving the operation data of the engine under different parameters, engineers can have a reasonable expectation for the engine parameters. There is still much room for improvement in the simulation. The python simulation code used still only considers some environmental and ambient factors. Additionally, the reported emissions are measured by carbon monoxide and carbon dioxide, but other pollutants, such as nitrogen oxides, can also be included. Further research by using AI neural networks can be an effective tool to confirm this novel finding.

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