Artificial Neural Network Modeling and Numerical Simulation of Syngas Fuel and Injection Timing Effects on the Performance and Emissions of a Heavy-Duty Compression Ignition Engine

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ABSTRACT: The use of syngas as an alternative fuel in compression ignition engines is a potential way to curb the emission of pollutants and optimize the performance of these engines. The present research studied the effect of changing fuel injection timing and adding syngas on the output of a heavy-duty diesel engine. The optimal mode of the turbulence model, fuel spray model, combustion model, and pollutant emission model was used to solve computational fluid dynamics. Changing fuel injection timing from 70 to 10° before top dead center (BTDC) and diesel variants, including conventional diesel, diesel + 20% syngas, and diesel + 40% syngas, is the strategy studied here. It was found that the use of syngas could reduce emissions significantly. The in-cylinder mean effective pressure was the highest for diesel + 20% syngas. On the other hand, increasing the rate of syngas and retarding injection timing reduced the ignition period and in-cylinder temperature. The lowest rate of CO emission was obtained from diesel + 40% syngas at a fuel injection timing of 70° BTDC, whereas the lowest particulate matter emission was related to diesel + 40% syngas at 40° BTDC injection timing. The lowest rate of CO₂ emission was related to diesel + 40% syngas at a fuel injection timing of 10° BTDC, while the same timing for conventional diesel exhibited the lowest NOₓ emission rate. Finally, the performance parameters of the engine including indicated power, indicated fuel consumption, and indicated thermal efficiency were decreased with the increase in syngas fraction, so that their highest values were obtained from the conventional diesel at the injection timing of 40° BTDC. In addition, an artificial neural network (ANN) model based on a standard back-propagation learning algorithm was developed for modeling the performance and emissions of the engine. The results for the optimum ANN model showed that the optimal ANN has two hidden layers with 20−25 neurons and the transfer function of logsig−logsig for hidden layers 1 and 2, respectively, and can predict different parameters of the engine for different modes. The correlation coefficients (R-value) of optimal topology for training, validation, and testing are 0.99992, 0.96612, and 0.93424, respectively. The results for the optimum ANN model showed that the constructed model sufficiently predicts the performance and emissions of the CI diesel engine.

1. INTRODUCTION

It is projected that there will be a total of 2.8 billion vehicles in the world by 2036. The energy requirement of these vehicles will amount to 112 million barrels per day. Compression ignition engines account for 38 percent of energy converters that convert petroleum energy into work. These engines are generally used for power generation and heavy-duty users.1 In recent years, considerable attention has been drawn to the use of renewable energy resources in the transportation and energy generation sectors. Achieving a low-carbon future will be challenging and will require a comprehensive portfolio of technologies and policy measures. Modern bioenergy plays an essential role in the International Energy Agency (IEA) 2 °C Scenario (2DS), providing nearly 17% of final energy demand in 2060 compared to 4.5% in 2015. Bioenergy provides almost 20% of the cumulative carbon savings to 2060.

In this respect, research has been conducted on reactivity controlled compression ignition (RCCI) engines,2 homogeneous charge CI (HCCI) engines,3 and premixed charge CI (PCCI) engines.4 RCCI engines are used extensively because of their advantages including combustion phase control and a wide range of their operational types. These research reports present...
Table 1. Review of the Literature (R = Reduced; I = Increased)

| reference | engine specifications | fuel blends | operating mode | emission analysis | combustion analysis | performance analysis |
|-----------|-----------------------|-------------|----------------|------------------|---------------------|----------------------|
| 35        | Kirloskar TAF1         | biogas/diesel | hydrogen/diesel, CNG/diesel, hydrogen (H2), carbon dioxide (CO2), nitrogen (N2), and methane (CH4). | CO | NOX | CO2 | smoke | HRR | ID | CD | HC | BTE | BSFC/BSEC |
| 36        | Kirloskar TAF1         | hydrogen/diesel, CNG/diesel | hydrogen/diesel, CNG/diesel | CO | NOX | CO2 | smoke | R | I | R | I | I | R |
| 37        | CR17/7.1, 6,318 cc, SOI: 17° BTDC | hydrogen/diesel | hydrogen at 400 rpm | CO | NOX | CO2 | smoke | I | R | I | R | I | R |
| 38        | Perkins Prime M900, Inline-four cylinder engine, CR17.20.1394 cc | hydrogen/diesel | hydrogen at 400 rpm | CO | NOX | CO2 | smoke | R | R | I | R | I | R |
| 39        | Kirloskar TAF1, IT: 23° BTDC | hydrogen/diesel | hydrogen at 400 rpm | CO | NOX | CO2 | smoke | R | R | I | R | I | R |
| 40        | Caterpillar 3401 ESCOTE, Bowl type: CNG/diesel | hydrogen/diesel | hydrogen at 400 rpm | CO | NOX | CO2 | smoke | R | R | I | R | I | R |

strategies to accomplish maximum efficiency with minimum pollutant emissions using fuel injection timing control mechanisms. Other researchers have reported that the use of two fuels would be a promising way to control combustion and its duration. In their method, a lowly reactive fuel was charged along with air, and the second fuel, which was highly reactive, was injected directly. Also, a numerical and laboratory study on dual gas/diesel fuel for RCCI engines showed that the first fuel (with a low cetane number) was injected with the air intake into the combustion chamber, and then, the second fuel (with a high cetane number) was injected into the combustion chamber with high pressure. The authors experimented on both light- and heavy-duty engines. Their research results show that the high premix ratio and early pilot injection timing are necessary for the low-temperature combustion of the syngas/diesel RCCI engine. Based on the optimal fuel supply strategy, the NOX emissions can be controlled in a considerably low level, and the combustion efficiency of the syngas in the squish region is high. In conventional diesel engines, NOX emission directly depends on the rate of fuel injection, exhaust gas recirculation (EGR) fraction, and start-of-injection (SOI) timing. The combustion phase with dual fuel ratio and combustion duration is controlled by the classification of combustion delay. When injection has a delay versus the cycle (e.g., close to high dead center), combustion directly happens with fuel injection, and combustion control is not challenging anymore. The dual-fuel strategy using premixed fuel has some benefits such as improved performance and lower pollutant emission. As such, less soot is emitted and an optimal and shorter thermodynamic combustion is attained. Consequently, dual-fuel combustion strategies are advantageous over single-fuel strategies in both controlled and kinetic limits. One promising approach, especially for applications in industrial and agricultural stations, is the partial replacement of diesel with synthetic gas, or syngas. The gases generated during the burning of solid fuels are called syngas, which is generally a mixture of carbon monoxide (CO), hydrogen (H2), carbon dioxide (CO2), nitrogen (N2), and methane (CH4). The ratio of these compounds depends on the burning process and solid fuel structure and type. Experimentally investigated an RCCI diesel engine with iso-butanol/diesel fuel under different performance conditions. When they used an iso-butanol/diesel ratio of 29:71%, they found that the production of NOX and particulate matter (PM) was improved, but compared to the conventional diesel fuel, more unburned hydrocarbon and CO were produced. Studied the performance limits of a syngas–diesel dual fuel under different engine loading conditions from the perspective of the second law of thermodynamics. They revealed that cumulated work was increased with the increase in the hydrogen fraction in the syngas. Zhang et al. studied the effect of a diesel/natural gas dual fuel on engine performance and emissions. They found that as the natural gas fraction was increased, less nitrogen oxide and soot were emitted. There are various methods to reform fuels containing carbon and hydrogen, such as reforming with steam, auto thermal reforming along with partial oxidation, and dry reforming. Among syngas production technologies, biomass gas production is one of the recommended methods. Small-scale power plants generally rely on internal combustion engines for the conversion of the final energy of gaseous fuel into mechanical and then electrical energy. Susastriawan and Saptoadi reviewed conventional technologies used for small-scale gas production. Internal combustion engines are the best option for...
the use of syngases due to their high efficiency and strength.16 Diesel engines that are in the dual fuel mode have lower specific fuel consumption and emit lower PM.14 Ramalingam et al.5 also studied the effect of using syngas derived from biodiesel on the main parameters of engines. They reported that high hydrogen fraction in syngas composition would reduce the emission of nitrogen oxides. A numerical study using the AVL FIRE software package on the effect of using methane and moisture in syngas composition revealed that the oxides of nitrogen were increased and CO was decreased when the fraction of moisture in the syngas compositions was changed.18 Similarly, a research study on the effect of low H2−CO ratio versus high moisture ratio in syngas components on an HCCI engine under a fixed intake temperature showed an increase in the indicated efficiency and IMEP.19

From the perspective of the second law of thermodynamics, the (H2−CO) syngas has several benefits such as lower combustion energy destruction, meaning less entropy and more work generating potential per unit of fuel exergy.20 This type of combustion can prevent the formation of extremely hot flame fronts by premixing a considerable amount of fuel and given the time delay in its high combustion. This would reduce the emission of nitrogen oxides sharply on the one hand and increase thermal efficiency. Additionally, there will be more opportunities to mix fuel and air and prevent the development of locally fuel-rich zones, which cause particulate formation.

Castro et al.21 addressed the impact of H2 substitution for diesel on a dual-fuel engine. According to the experimental measurements, backfire took place at a hydrogen concentration higher than the downward flammability limit. The maximum hydrogen energy substitutions were 80, 60, and 40% corresponding to engine loads of 30, 60, and 100%, respectively. The maximum reduction of diesel consumption was 54.2% with respect to 100% diesel operation at 30% of engine load and 80% of hydrogen energy substitution. Brake fuel conversion efficiency decreased as hydrogen addition increased for all the engine loads tested. This decrease may be mainly caused by the steam formation during the hydrogen combustion. Their results revealed that the rate of direct injection fuel was higher at maximum engine loads than at lower loads, so the engine performance should be lower than the full load to minimize diesel intake. Guo et al.22 focused on specifying the effects of syngas and diesel in a dual-fuel engine for different compositions of syngas on achieving lower thermal efficiencies for the dual-fuel mode. Because H2 and CO fuels do not emit soot, diesel was responsible for the soot emission. They found that when the fraction of syngas was increased to 45%, more soot was emitted, but further increase in its fraction resulted in a decline in soot emission. Combustion with syngas/diesel fuel was accompanied by a decrease in combustion temperature, and this reduced soot generation. The reduced temperature of combustion leaves some CO nonoxidized and this increases its emission. Serrano et al.23 analyzed the effect of hydrogen/diesel fractions by using water injection on a compression ignition engine to figure out the performance trend and pollutant emissions. Their results revealed that as the fraction of hydrogen in fuel was increased, more oxides of nitrogen were produced, whereas at higher water injection, the emission of this pollutant exhibited a descending trend. Mobasher et al.24 explored the effect of hydrogen and nitrogen addition on the combustion of a diesel engine. They reported that H2 addition increased NOX and reduced CO and soot emission and vice versa. The trend of pollutant emissions was observed when nitrogen was added. The addition of H2 (alone or with N) reduced the maximum homogeneity factor (HF) and caused an increase in HF when N was added to the combustion chamber. HF is a major factor to predict combustion processes because it shows air/fuel-rich zones and vice versa. Syngas is usually produced from N-containing biomass. However, N species have not been considered due to the high energy concentration of syngas and oxidation complexities. Mahgoub et al.25 examined various compositions (H2, CO, N2, CO2, and CH4) for a dual-fuel diesel engine. They indicated that H2-rich syngas reduced CO and HC emission (up to 40% diesel replacement ratio), and then, these pollutants were increased. Also, recently, due to flexibility, accuracy, and fast response features of the artificial neural network (ANN), it has been selected as one of the attractive and positive methods in the context of modeling and to solve the complex problems.26 ANNs are computer systems that can automatically generate, form, and discover new knowledge without any help such as the human brain.27 An ANN model can accommodate multiple input variables to predict multiple output variables. It differs from conventional modeling approaches in its ability to learn about the system that can be modeled without prior knowledge of the process relationships.28 They used to solve a type of problems in science and engineering, especially where the conventional modeling methods cannot solve the problem.27 ANN is a powerful and nonlinear tool and an ANN model can be applied multiple input variables to predict multiple output variables.29 The ANN model includes three elements, namely, input layer, hidden layer(s), and output layer.30 The input neurons forward the values of the input variables to the hidden layer, and then, the final model is estimated by output neurons. The main characteristics that differentiate the various neural network architectures are the types of nodes in the hidden layer.31 Training and test are the two processes that are needed to develop an ANN model. When the network is trained to estimate output values relative to input data, its training and the testing process in the network are tested to stop training or save training data and used to estimate an output.32

In the following, several studies that used ANNs in the case of engines’ performance and emission with different fuels are presented. For instance, Rao et al. studied the IDI diesel engine performance and exhaust emission analysis using biodiesel with an ANN. They found that ANN was able to predict the engine performance and exhaust emissions with a correlation coefficient of 0.995, 0.980, 0.999, 0.985, 0.999, 0.999, 0.980, 0.999, and 0.999 for EGT, BSFC, BTE, HC, O2, CO2, CO, NOx, and smoke, respectively.33 In another study, Oğuz et al. examined the prediction of diesel engine performance using biofuels with ANN. They used diesel, biodiesel (B100 and B20), and biodiesel and bioethanol blends (E5−B20, E10−B20, and E15−B20) to use in developed ANN. Power, moment, hourly fuel consumption, and specific fuel consumption were estimated by using the ANN developed, and they found that the realized artificial intelligence model is an appropriate model to estimate the performance of the engine used in the experiments.27 Hosseini et al. studied the ANN modeling of performance, emission, and vibration of a CI engine using alumina nanocatalysts added to diesel−biodiesel blends. They reported that the ANN is a powerful application to predict the performance, emission, and vibration in CI and SI engines with reasonable accuracy.35 Karonis et al. applied the neural network approach for the correlation of exhaust emissions from a diesel engine with diesel fuel properties. They reported that the
predictions obtained were very good for all types of emissions (carbon monoxide, hydrocarbons, nitrogen oxides, and particulate matter). In this study, the ratio of H₂ in the syngas was considered to be less than 40% for the fuel replacement ratio in order to allow more use of syngas energy and optimization of combustion specifications. Because extensive research has addressed the use of syngas in diesel engines, Table 1 presents a brief review of the studies conducted in recent years. The review of the literature and the summary in Table 1 show that the preceding literature has dealt with the effect of mixed syngas with various compositions, but no research has focused on changing the parameter of fuel injection timing and its consequences. In addition, previous research has generally been laboratory analyses, which limits their domain, whereas the numerical analysis used here can provide a wider vision. Also, in the present study, changes in fuel injection timing and the addition of different fractions of syngas as an influential parameter were explored simultaneously, which has been impossible in previous works. In addition, the literature reviews show that no research has been reported on using ANNs to predict the performance and emission of a diesel engine using syngas fuels. The ANN can be trained by data obtained from experiments or numerical simulations. In the present work, the data obtained from these simulations have been used to train ANNs. Therefore, due to the lack of studies focusing on using syngas fuels, the objective of this study was to develop a neural network model for predicting the performance and emission of a diesel engine.

2. MODEL DESCRIPTION

The present research used the Converge CFD software package for numerical analysis. To maintain the accuracy and reduce calculation time, and due to the symmetry in the geometrical location of the fuel injection systems and its placement in the center of the cylinder, and because the injection nozzle had six holes, the calculations were performed on a 60° sector. The selected sector was meshed by software tools. Figure 1 displays the geometry of the selected sector at the top dead center. The computational step assumed for the calculations is 0.5 μs from the initiation until the onset of the combustion process and 0.01 μs for the combustion process until the end of the computations. Because the computational mesh factor,
which expresses the density of meshes, is assumed to be 1—1.4 for heavy-duty engines, the results independent of meshing were obtained for the value of 1.3. Figure 1 illustrates the selected computational mesh at the top dead center, the e-omission, and the calculation is finally performed for all regions just once.45 A decisive factor in compression combustion engines is the rate of fuel mixing. We used the Navier—Stokes equations to investigate the e-effects of grid size on in-cylinder mean pressure and rate of heat release. Because the combustion was simulated here by the precision chemistry method, the SAGE solver was applied.45 Also, the diesel combustion process was simulated by a heptane-reduced chemical kinetic mechanism composed of 29 species and 52 reactions.45 The process of soot formation and oxidation with 20 species and 139 reactions was simulated by the PAH-reduced chemical kinetic mechanism, and nitrogen oxides were predicted by the GRI NOX mechanism with 4 species and 12 reactions.44
particle decay to happen. When fuel particles are injected into the computational zone, a computational model will be required to convert liquid fuel particles into a gas stream. The research used the Frossling correlation model, improved by,46 to simulate the process of the evaporation of liquid fuel particles sprayed by the fuel injection system. Also, the research employed the physical specifications of the diesel, found in the software database, for direct injection fuel. To simulate the collision of the sprayed fuel particles, the no-time-counter (NTC) model presented by Rutland and Schmidt47 was used. This computational model is composed of a random sampling of particles in each computational cell, which accelerates the calculations of particle collisions. The computational model suggested by Naber and Reitz48 was used to simulate the collision of fuel particles with the wall.

2.1. Governing Equations. To simulate the process of compression ignition combustion in internal combustion engines, a series of mathematical models are solved for the phenomena. These models are robust and valid tools to study and analyze internal combustion engines. We used the Converge CFD software package for the simulations. This software automatically uses equations and solution methods for a problem and makes convergence possible. Converge CFD utilizes an integrated and fixed Cartesian network for the computational space and the finite volume method to solve fluid equations. To transport mass, momentum, and energy, network fluxes are calculated by second-order central difference. The equations of mass, momentum, and energy conservation and chemical species constitute the governing equations in the Converge code. To ensure the accuracy of the pressure gradient, partial differential equations of mass, momentum, and energy are solved simultaneously. The compressible equations of mass and momentum conservation are as follows41

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \tag{1}
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + \rho g_i + S_i \tag{2}
\]

\[
\sigma_{ij} \text{ which is the viscous stress tensor, is obtained from eq 3.}^{41}
\]

\[
\sigma_{ij} = \mu \left[ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] + \left( \mu' - \frac{2}{3} \mu \right) \frac{\partial u_k}{\partial x_k} \delta_{ij} \tag{3}
\]

Then, the energy equation is expressed as eq 4,\(^5\)

\[
\frac{\partial P e}{\partial t} + \frac{\partial u_i P e}{\partial x_i} = -P \frac{\partial u_i}{\partial x_i} + \rho \frac{\partial u_j}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \kappa \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_i} \left( \rho D \sum_m h_m \frac{\partial Y_m}{\partial x_i} \right) + S \tag{4}
\]

Finally, the species transport equation is solved individually and is defined by eq 5 as follows:\(^42\)

\[
\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m u_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Y_m}{\partial x_i} \right) + S_m \tag{5}
\]

Molecular mass diffusion based on the Schmidt number (Sc) is calculated by eq 7 as below

\[
D = \frac{\nu}{Sc} \tag{6}
\]

To analyze the combustion process with conventional diesel, 3D numerical simulation was performed with calibrated models for the conventional diesel mode and the syngas (2% v/v) mode. When the syngas was added, the amount of diesel was reduced and it was substituted by syngas. The indicated thermal efficiency is simulated by eq 8, and the lower heat value of the syngas is simulated by eq 9.

\[
\eta_{th} = \frac{\dot{m}_{\text{diesel}} \cdot \text{LHV}_{\text{diesel}} + \dot{m}_{\text{syngas}} \cdot \text{LHV}_{\text{syngas}}}{\text{IP}} \tag{8}
\]

\[
\text{LHV}_{\text{syngas}} = \text{LHV}_{\text{H}_2} \cdot x_{\text{H}_2} + \text{LHV}_{\text{CO}} \cdot x_{\text{CO}} \tag{9}
\]

Evaporation and mixing phase, especially fuel mixing rate, is a critical and determinant factor in compression ignition engines.
because the initial steps of ignition are strongly influenced by this process. This numerical research used the suppressed mixing rate of the reaction based on the time scale of RNG $K$ turbulence improved by through normalizing the Navier–Stokes equations to investigate the effect of smaller-scale effects of fluid motion in a standard $K$–$\varepsilon$ model, and viscosity vortex is determined by a longitudinal scale of turbulence. Therefore, the calculated turbulence dissemination occurs only for a certain scale, although, in the real world, all motion scales contribute to turbulence dissemination. Re-normalization group is a mathematical method that can be used to develop a turbulence model similar to the $K$–$\varepsilon$ model used here and results in a modified form of the $\varepsilon$ equation which tries to consider various scales of motion created during changes. The transport equation of $K$ is as below

$$\frac{\partial K}{\partial t} + \frac{\partial (\rho u_i K)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\mu}{\sigma_f} \frac{\partial K}{\partial x_i} \right) - \rho \varepsilon + S_K$$

(10)

The transport equation of $\varepsilon$ is given by

$$\frac{\partial \varepsilon}{\partial t} + \frac{\partial (\rho u_i \varepsilon)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\mu}{\sigma_f} \frac{\partial \varepsilon}{\partial x_i} \right) + C_{\varepsilon} \frac{\partial}{\partial x_i} \left( \frac{\partial K}{\partial x_i} \right)$$

+ \left( C_{\varepsilon} \frac{\partial u_i}{\partial x_j} \tau_{ij} - C_{\varepsilon} \varepsilon \right) \frac{\varepsilon}{K} - \rho R$$

(11)

In the RNG model, the term $R$ is defined by eq 13 shown below

$$R = \frac{C_{\varepsilon} \mu^3 \left( 1 - \frac{\varepsilon}{\eta} \right)}{(1 + \beta \eta^\nu) K}$$

(12)

The term $\eta$ in eq 12 is defined by eq 13:

$$\eta = \frac{K S_i}{\varepsilon} = \frac{K}{\varepsilon} \sqrt{2S_y S_\theta}$$

(13)

In eq 11, $Pr_\varepsilon$ defines the ratio of viscous penetration to $\varepsilon$ penetration and $C_{\varepsilon_f}, C_{\varepsilon_v}$, and $C_{\varepsilon}$ are the model constants. The RNG model is the modified form of the standard $K$–$\varepsilon$ model ($R = 0$) because the model constants can be analytically obtained from the interaction of isotropic turbulence, so there is no need to adjust the model constants.

### 3.2. Engine and Fuel

The engine selected for the study of the target parameters was of a heavy-duty diesel engine type whose specifications and model are given in Table 2. The engine uses a turbocharger-based aeration system.

Compression combustion engines usually need highly reactive diesel and air or a mixture of air and fuel for their combustion process. In this process, the fraction of premixed fuel can be considered to be 60%, whereas the fraction of substituted fuel energy is limited to, at most, 40%, to avoid the pressure rise inside the combustion chamber. This study made calculations for performance parameters and emissions under three modes of fuel mixing, that is, the use of conventional diesel, diesel + 20% syngas, and diesel + 40% syngas. Syngas was added to the primary fuel at two rates of 20 and 40% to derive results on its effects on the main performance parameters and emissions of the engine. Syngas is composed of $H_2$–CO whose minimum heat value is the sum of the minimum heat values of $H_2$ and CO. Table 3 presents the specifications of the fuel used, and Table 4 introduces the specifications of the fuel injection system.

### 3.3. Validation

To validate the results of the numerical simulation, Figure 2 depicts the trend of in-cylinder mean pressure variations and heat release rate in the experimental work as compared to the present research. The simulation of the comparison is for the pure diesel mode that is compared with the experimental results. After the selection of the model and the maximum matching of the experimental conditions, the results of changing fuel type and fuel injection timing parameters are discussed. The comparison was made for a fuel injection angle of $10^\circ$ before top dead center (BTDC) and at a fuel injection pressure of 1000 bars. As it is evident, the methodology and implementation of the present numerical work has close conformity with similar experimental work. The conformity is maximal at the medium values of the in-cylinder pressure. The difference reported in the results on the heat release rate between the numerical and experimental works can be ascribed to uncertainties in some initial conditions, such as the temperature of the wall and piston surface when air intake valves are closed.

The main objective of the present research was to simultaneously explore the effects of using additional compounds in diesel and fuel injection timing on the main parameters of an engine including performance, emissions, and combustion analysis. As is evident in Table 5, three fuel modes were used, and the results were derived for fuel injection timing from 70 to 10° BTDC.

### 3.4. ANN Modeling

In this study, the parameters, namely, type of fuel, injection timing, and fuel consumption have been used as input layer (three items) components of the ANNs that can affect diesel engine performance and emission characteristics. The output parameters (six items) were indicated power, indicated thermal efficiency (%), NOx, PM, CO, and CO2, respectively. The neural network architecture diagram is presented in Figure 3. Before training the model, the input–output parameters in data sets were arranged, and the data sets were normalized between 0 and 1 range by eq 14 using Excel 32. Because the output layer activation function is linear in all architectures, only the input parameters were normalized by eq 14.

$$I_{\text{norm}} = \frac{I - I_{\text{min}}}{I_{\text{max}} - I_{\text{min}}}$$

(14)

where $I_{\text{norm}}$ is the normalized data, "$I$" is the measured or input data, "$I_{\text{min}}$" is the minimum of measured data, and "$I_{\text{max}}$" is the maximum of measured data.

In the present work, the simulated data are applied to the ANN model. In this, the ANN model, 70% of the total data sets was arbitrarily selected for training the model, while the remaining 30% of data have been equally divided, 15% for validation and 15% for testing. Multilayer networks (MLP) with the feed-forward back propagation neural network model were employed. The Levenberg–Marquardt algorithm was used as the training algorithm. The log–sig, tan–sig, and purelin transfer functions were employed as an activation function in this research, which the relevant equations have been shown by eqs 15 and 16. In these equations, $x$ is the input data.

$$\text{logarithmic sigmoid} = \frac{1}{1 + e^{-x}}$$

(15)
tangentsigmoid = \frac{2}{1 + e^{-2x}} - 1 \tag{16}

To select the optimal network model (best number of neurons and hidden layers), the network was trained with the various number of hidden layers and neurons. The statistical methods of MSE and correlation coefficient (R-values) have been used for comparison. The optimal network model was obtained by a high maximum value of (R) and minimum value of MSE, which are computed by eqs 17 and 18, respectively.

\[ R = 1 - \left( \frac{\sum_{i=1}^{n} (T_i - O_i)^2}{\sum_{i=1}^{n} (T_i - O)^2} \right) \]  \tag{17}

\[ \text{MSE} = \frac{1}{n} \sum_{i=1}^{n} (T_i - O_i)^2 \]  \tag{18}

In eqs 17 and 18, “n” is the number of samples tested, “T_i” is the measured values (target), “O_i” is the predicted values (output), and “O̅” is the average of predicted values.

4. RESULTS AND DISCUSSION

4.1. Effect of Using H₂–CO on Combustion Characteristics. Figure 4 displays the variations in the combustion chamber pressure for three fuel modes (PDC, 20% syngas, and 40% syngas) at three angles BTDC in terms of degree crank. Also, the rate of heat release for these modes is depicted in this figure. As can be seen, the maximum peak pressure was for the injection angle of 70° BTDC. This, however, declined for the PDC + 40% syngas mode. On the other hand, when syngas was added to the main fuel, in-cylinder pressures decreased. The addition of H₂ and CO to the fuel retarded combustion and reduced the pressure inside the combustion chamber. This is related to the high auto-ignition of H₂ and the decline in diesel fraction. Therefore, when these gases are used in the fuel, the peak of the pressure curve is always lower than that of pure diesel. The lowest pressure decline happened at the injection angle of 40° BTDC for all three fuel modes. However, the conditions for the rate of heat release were effective too. H₂ addition reduced the volume efficiency and the amount of piloted fuel, resulting in a delay in combustion. However, after the combustion initiates, it goes on similar to the combustion in a fixed volume, and the released heat increases due to the presence of H₂ and its high flammability.

A look at the variations in the ignition delay period for different fuel injection angles shows that late injection of diesel into the combustion chamber increased the maximum of the heat release rate curve and its advancement and vice versa. As is evident in Figure 5, with the delay in fuel injection timing, the ignition delay period was shortened (angles close to TDC). In early fuel injection, because the pressure and temperature of the cylinder were not ready to evaporate all the injected fuel, combustion did not occur completely. Therefore, the in-cylinder pressure differed between the earlier injection and later injections (Figure 4). On the other hand, the addition of syngas itself retarded ignition due to the reduction of the ratio of diesel versus PDC, contributing to prolonging the ignition delay period. Figure 4 illustrates the differences in these values for three fuel modes. Accordingly, the ignition delay period was decreased with delaying fuel injection timing and less fuel was evaporated in this period.

Figure 6 displays the effect of fuel injection timing on the in-cylinder temperature. Delay in injection timing reduced the in-cylinder temperature for all three fuel modes. As already mentioned as to the relationship between delay period and fuel injection timing, the delay in fuel injection causes more fuel to burn in the cylinder, and less fuel is then accumulated. Consequently, the combustion rate is reduced and the length of the fuel particle evaporation period is increased, resulting in a decline in the in-cylinder temperature. It can be inferred from Figure 6 that the in-cylinder temperature was maximum at an injection timing of 70° BTDC and it declined up to 40 °C BTDC and then started to increase again. Finally, the minimum value was obtained from the injection timing of 10° BTDC. In
this injection timing, PDC, 20% syngas, and 40% syngas exhibited the lowest in-cylinder temperature, respectively.

Figure 7 shows the temperature counter for three modes of fuel injection timing at a crank angle of 40° after TDC (ATDC) and the use of three different fuel compositions. Clearly, at all fuel compositions, a delay in the injection time increased the temperature at the crank angle of 40° ATDC. On the other hand, when the rate of syngas in the fuel was increased, the temperature distribution across the cylinder surface was uniform. This is a result of better combustion (more efficient and more homogeneous) due to the use of H₂−CO.

4.2. Effect of Using H₂−CO on Emissions. NOₓ emissions are determined by the maximum in-cylinder temperature and controlled by oxygen availability. The maximum temperature itself depends on such factors as fuel composition, balance ratio, and initial air and fuel temperatures. When syngas is added,
oxygen is reduced and this increases emissions. On the other hand, the presence of syngas and the delay in combustion cause the temperature to rise when the exhaust valve opens, and this does not give enough chance for the formation of NO\textsubscript{X}. The quantity of NO\textsubscript{X} is dependent on in-cylinder temperature, oxygen concentration, and nitrogen residence duration at high temperatures.

Figure 8 displays the NO\textsubscript{X} emission rate for different fuels based on injection timing. The highest rate is for the injection timing of 40° BTDC when 20% syngas is applied. Based on Figure 6, this injection timing has the highest in-cylinder temperature too. Also, as the delay in the ignition is decreased,
less NO\textsubscript{X} is emitted. It can be drawn from Figures 6 and 8 that when 20% syngas is applied, temperature rises and this contributes to more emission of NO\textsubscript{X} versus 40% syngas and PDC.

Figure 9 demonstrates that the variations in CO emission with the delay in injection are higher for syngases, whereas it is finally reduced for PDC. In fact, PDC, 20% syngas, and 40% syngas had the highest CO emission rate at the injection timing of 10\textdegree BTDC, respectively. Figure 4 shows decreases in ignition delay with delaying injection time. This implies that a decrease in the ignition period does not give enough time for the oxidation of the carbon particles of the fuel, so CO emission ascends, whereas when the ignition time prolongs, there is enough chance for the oxidation of carbon particles and as a result, the CO emission
rate decreases. On the other hand, an increase in syngas fraction in the main fuel sharply increased CO emission when the fuel was injected at 10°. This is mainly ascribed to the escape of unburned CO particles in the syngas composition.

The trend of CO₂ emission at different fuel injection timings for three fuel compositions is displayed in Figure 10. It is observed that a delay in injection reduced CO₂ emission. In addition, 20% of syngas had higher CO₂ emissions than PDC, but 40% of syngas produced less CO₂ than PDC.

Figure 11 depicts PM emission for different fuel compositions at different fuel injection timings. PM emission for PDC did not differ from that of syngas significantly. The lowest emission was related to an injection angle of 40° BTDC and the highest to 10° BTDC. The comparison of NOₓ emission with PM reveals that delaying injection timing increased PM emission significantly and this had reverse consequences for NOₓ emission. As the ignition delay was reduced, most of the fuel mass was burned in the penetration mode, combustion and fuel evaporation period were extended, and consequently, the process of fuel particle oxidation was weakened. It should be mentioned that burning in the penetration mode reduced the combustion rate, maximum temperature point, and in-cylinder pressure. The decline in the in-cylinder temperature weakened soot particle oxidation and, as is evident in Figure 11, PM emission was increased with a delay in fuel injection timing.

Figure 12 displays the counter of the emission of (a) CO, (b) CO₂, (c) PM, and (d) NOₓ at fuel injection timing at the angles of 70, 40, 30, and 10° BTDC for the crank angle of 40° ATDC. According to Figure 7 and the counter in Figure 12a, which is specified at the angle of 40° ATDC, it can be explained that an increase in the syngas fraction of diesel to 20% escalated the emission of NOₓ, but its emission decreased with an increase in syngas fraction to 40%. The zones of maximum emission in the 20% syngas mode inside the combustion chamber are visible, whereas in the 40% syngas mode, NOₓ emission was reduced with the homogeneity of fuel composition and its more dispersion across the combustion chamber surface. The comparison of temperature counter in Figure 7 for the 40% syngas mode and NOₓ emission counter in Figure 12 indicates that an increase in syngas fraction to 40% reduced the effects of temperature rise versus the effect of an increase in the fraction of H₂—CO. Figure 12b shows the CO distribution counter at fuel injection timing at 10° BTDC at the crank angle of 40° ATDC. It is seen that when syngas fraction was increased in the diesel fuel, less unburned fuel zones were formed and the effect of fuel distribution became visible on the combustion chamber surface. The distribution of CO₂ at the injection timing of 70° BTDC at the crank angle of 40° ATDC is depicted in Figure 12c. Similar to the CO counter, this counter may show a more uniform distribution with an increase in H₂—CO fraction in the diesel fuel. Finally, Figure 12d shows the distribution of PM at the injection timing of 30° BTDC at the crank angle of 40° ATDC. It indicates that an increase in syngas composition in diesel reduced PM emission in the combustion chamber significantly.

4.3. Effect of Using H₂—CO on Engine Performance. Figure 13 shows the effect of incorporation of H₂—CO in main diesel on (a) indicated power, (b) indicated specific fuel consumption (ISFC), and (c) indicated thermal efficiency. Figure 13 demonstrates that delaying injection improved engine performance. Also, the use of syngas in the fuel reduced indicated power, indicated thermal efficiency, and ISFC. When diesel injection was delayed, the ignition delay period was reduced and subsequently less fuel was evaporated over this period. As the ignition delay period was reduced, most of the fuel mass was burned in the penetrative combustion state, the combustion rate was reduced, the ignition period was extended, the fuel particle evaporation process was weakened, and consequently, maximum temperature point and in-cylinder pressure were decreased. When the maximum temperature point was reduced and the combustion pressure impaired engine performance, ISFC was increased and indicated power and thermal efficiency were decreased (see Figure 13). In addition, the addition of syngas may reduce indicated power and indicated thermal efficiency, and increase fuel consumption.

4.4. ANN Modeling Result. To find the best prediction by the ANN model, various network models were applied. Summary of different model networks evaluated to yield the criteria of network performance is listed in Table 6. In this table, the trainlm algorithm, purelin transfer function for the output layer, and the transfer function of tan—sig, log—sig with two hidden layers are selected. The optimal network has two hidden layers with 20–25 neurons and transfer function of logsig—logsig for hidden layers 1 and 2, respectively. Figure 14 illustrated the performance of the optimal ANN model. The correlation coefficients (R-value) of optimal topology for training, validation, and testing are 0.99992, 0.96612, and 0.93424, respectively. Also, the MSE values of the optimal topology model for training, validation, and testing were obtained as 0, 0.0068, and 0.0118, respectively.

To investigate the network response in more detail, a regression analysis was performed between the network output and the corresponding targets. The results showed that the constructed model sufficiently predicts the performance and emissions of CI diesel engine. The ANN predicted outputs versus simulated values (the data were normalized between 0 and 1 range and then used in the modeling process) for performance, and emissions are shown in Figure 15. Performance regression coefficient's values using ANN are 0.9862 and 0.9922 for indicated power and indicated thermal efficiency (%), respectively. Also, emission regression coefficient's values using ANN are 0.9477, 0.9842, 0.9801, and 0.9975 for NOₓ, PM, CO, and CO₂, respectively. This indicates that the optimal ANN model has a high correlation between the predicted model and simulated data.
It can be concluded that the ANN is a powerful application to predict performance and emissions in engines with reasonable accuracy. The results for the optimum ANN model showed that the constructed model sufficiently predicts the performance and emissions of the CI diesel engine.

5. CONCLUSIONS

The present research focused on a heavy-duty compression ignition engine using three fuel modes, that is diesel, diesel + 20% syngas, and diesel + 40% syngas, at a fuel injection timing from 70 to 10\(^\circ\) BTDC. The results can be summarized as below:

1. When the syngas fraction was increased to 20\%, the in-cylinder average pressure was increased, but further increase in the syngas to 40\% reduced the pressure. In addition, the addition of syngas had no significant impact on shortening the ignition period versus conventional diesel, and only the minimum value of this parameter occurred at fuel injection timing of 10\(^\circ\) BTDC for the syngas compositions. On the other hand, delaying injection timing of the control fuel reduced in-cylinder temperature whose minimum value was related to 40\% syngas.

2. All in all, the addition of syngas did not reduce NO\(_X\) emissions. Delaying injection from 70 to 10\(^\circ\) BTDC first increased NO\(_X\) emission, but it then started to decrease and its minimum was obtained for the conventional diesel. Also, the addition of syngas at fuel injection timing of 70–40\(^\circ\) BTDC reduced CO, although as moving from 40 to 10\(^\circ\) BTDC, syngas suddenly increased the CO emission. The lowest CO emission was obtained from an injection timing of 70\(^\circ\) BTDC and the highest from 10\(^\circ\) BTDC for 40\% syngas. Also, it was found that the application of 20\% syngas maximized CO\(_2\) emission, whereas 40\% syngas

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**Figure 15.** Prediction of ANN and simulation values for the performance and emissions of engine.
minimized it. The lowest CO₂ emission was related to the injection timing of 10° BTDC. However, when syngas was increased, PM emission was sharply decreased versus conventional diesel. The lowest PM emission occurred at 40° BTDC injection timing for 40% syngas.

3. The results reveal that the indicated power and indicated thermal efficiency were decreased and indicated that fuel consumption increased when syngas was applied either at a 20 or 40% rate. The highest of these parameters were obtained from the injection timing of 40° BTDC, whereas the lowest was related to the timing of 60° BTDC.

The study shows that the addition of H₂–CO as syngas at the rates of 20% or 40% to the base diesel reduced CO, CO₂, and PM emissions significantly, whereas NOₓ emission was increased at fuel injection timing of 40° BTDC. Also, the highest output for the indicated power, indicated fuel consumption, and indicated thermal efficiency occurred at this injection timing (40° BTDC). Also, the results showed that the optimal network has two hidden layers with 20–25 neurons and transfer function of logsig–logsig for hidden layers 1 and 2, respectively. The correlation coefficients (R-value) of optimal topology for training, validation, and testing are 0.99992, 0.96612, and 0.93424, and the MSE values of the optimal topology model for training, validation, and testing are obtained as 0, 0.0068, and 0.0118, respectively. Also, performance and emissions of engine regression coefficient’s values using ANN are 0.9862, 0.9922, 0.9477, 0.9842, 0.9801, and 0.9975 for indicated power, indicated thermal efficiency (%), NOₓ, PM, CO, and CO₂, respectively. It can be concluded from the present study that the ANN is a powerful application to predict performance and its emissions in engines with a high correlation between the predicted model and simulated data.

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Notes
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■ NOMENCLATURES

ρ, density
LHVₜₜₜₜ, lower heat value of the syngas
uᵢ, velocity component
LHV₃ₜₜₜₜ, lower heat value of the H₂
Pᵢ, pressure
LHVₔₐₜₜₜₜ, lower heat value of the CO
Sₑ, Schmidt number
LHV₃ₜₜₜₜ, lower heat value of the diesel
µ, dynamic viscosity
mₜₜₜₜ, the mass flow rate of diesel
µᵢ, dilatational viscosity (usually assumed zero)
mₜₜₜₜ, the mass flow rate of syngas
gᵢ, mass force acceleration component
Pᵢ, indicator power
δᵦ, Kronecker delta
Zᵢ, the rate of diesel substitution
eᵦ, specific internal energy
Prᵦₑ, Prandtl number
Kᵦ, heat conductivity
θₜₜₜₜ, hydrogen molar fraction in the syngas
Tᵦ, temperature
θₜₜₜₜ, carbon monoxide molar fraction in the syngas
Dᵦ, mass diffusion
ISPₚᵦₑ, indicated specific fuel consumption
θₜₜₜₜ, specific enthalpy of species m
CAᵦ, crank angle
Yₜₜₜₜ, mass fraction of species m
CIᵦₑ, compression ignition
Sᵦ, term for the energy source
DIᵦₑ, direct injection
ρₜₜₜₜ, density of species m
EVOᵦₑ, exhaust valve opening
θₜₜₜₜ, energy source term of species m
EVCᵦₑ, exhaust valve closing
ηₜₜₜₜ, indicated thermal efficiency
HRRᵦₑ, heat released rate
IVOᵦₑ, inlet valve opening
IVCᵦₑ, inlet valve closing
LHVᵦₑ, lower heating value
TDCᵦₑ, top dead center
BTDCᵦₑ, before top dead center
ANNᵦₑ, artificial neural networks
PMᵦₑ, particulate matter
COᵦₑ, carbon monoxide
H₂ᵦₑ, hydrogen
CO₂ᵦₑ, carbon dioxide
CH₄ᵦₑ, methane
NCTᵦₑ, no-time-counter
MLPᵦₑ, multilayer networks
PDCᵦₑ, pure diesel combustion

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