Effect of Steam on the Adiabatic Flame Temperature and Specific Heat of Equilibrium Combustion Products of Conventional Diesel Fuel and Biodiesel

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Abstract: When compression ignition engines operate with biodiesel, emissions of carbon monoxide (CO), particulate matter, and hydrocarbons are significantly reduced, whereas emissions of nitric oxides (NO_x) increase substantially. Steam injection was used in this study to reduce NO_x emissions and for its effects on the chemical equilibrium of combustion products. Variations in the thermodynamic properties of the combustion products at chemical equilibrium, as well as changes in the temperature of the adiabatic flame and the combustion products at chemical equilibrium, were studied during combustion of both conventional diesel fuel and biodiesel, with and without 5% steam injection. These variations were analyzed at different pressures, equivalence ratios, and temperatures of the unburned mixture. The results showed that when the flame temperature exceeded 1800 K, a decrease of 103 K in the maximum flame temperature due to steam injection reduced thermal nitric oxide (NO) production by 73%. The results also indicated that while NO emissions and adiabatic temperature decrease significantly, specific heat values increase as the steam injection rate was raised. At chemical equilibrium, combustion products contain only the most stable species in substantial quantities below 1300 K. The emission of CO and NO_x by lean combustion systems indicates that chemical equilibrium is not maintained when the combustion products are cooled.

Keywords: Chemical Equilibrium Products, Combustion, Biodiesel, Conventional Diesel Fuel, Steam Injection Method

1. Introduction

Since green plants absorb solar energy for photosynthesis and store it in biomass, combustion of biomass is an example of indirect solar energy. Biomass, one of the earliest energy sources utilized by humans, consists of various organic materials, including wood, algae, fast-growing plants, agricultural residues, sawdust, wood shavings, and animal waste. It includes chemical energy derived from the sun's rays, which is used by photosynthetic organisms to create organic molecules.

With the world's fossil fuel reserves dwindling, an energy crisis is imminent. In addition, scientists are searching for alternative fuel sources due to factors including growing fossil fuel prices, greenhouse gas emissions, energy security, and diversification of energy. Methanol and ethanol are the two main liquid fuels that can be produced from biomass and utilized in internal combustion engines as well as for the production of biodiesel. Some energy companies are interested in the commercial conversion of agricultural waste into ethanol, while others turn wood, corn, or sugarcane into alcohol. Several companies are now developing plants that convert biomass into ethanol; using maize stubble, rice straw, fibrous leftovers from sugarcane processing, and sewage products. One of the greatest sources of alternative fuels is biodiesel, which has several benefits over fossil fuels [1, 2]. Biodiesel, derived from vegetable or animal oils, is increasingly being adopted as an alternative fuel for compression ignition engines, powering vehicles, agricultural machinery, and marine vessels. After being used in restaurants,

the oil is frequently refined; for example, frying oil; biodiesel burns much cleaner than conventional diesel fuel. Biodiesel production involves various feedstocks and employs methods such as transesterification, microemulsification, dilution, and pyrolysis. The viscosities of vegetable oils are significantly higher than those of fossil fuels, so chemical processing is needed to turn vegetable oils into biodiesel fuel [3, 4]. Because biodiesel is nontoxic, biodegradable, free from sulfur and aromatic contents, and produces fewer greenhouse gases than other conventional fuels, it is environmentally friendly [5]. The combustion is generally the main sources of pollution emissions. Climate change and global warming have led to the implementation of stricter environmental regulations. Furthermore, a significant factor in the scarcity of fossil fuels is the widespread usage of fossil fuels in these engines, even though the supply of these fuels is rapidly depleting. As a result, researchers are studying combustion with alternative fuels and internal combustion engines. In this regard, biodiesel may be seen as a fossil fuel substitute that could meet both the stringent environmental regulations and the expanding fuel demand. Conventional diesel fuel and biodiesel have very similar physical properties. The utilization of biodiesel has the potential to mitigate the adverse effects of air pollution and human health by lowering the emissions of harmful pollutants such as carbon dioxide and particulates. Furthermore, the geopolitical issues surrounding the extraction and distribution of oil, gas and coal are driving the exploration of sources of alternative energy, as their usage is increasing at a rapid rate and contributing to their depletion [6].

The process's thermodynamic boundary conditions are constantly changing as a result of the piston's movement and the cooling of the combustion chamber's walls caused by the impact and evaporation of the fuel injection. The local equivalent ratio is further influenced by the mixture's spatial mobility, diffusion, and the injected fuel's evaporation. In the time scale of combustion, very little heat or work transfer occurs and the combustion reaction happens quickly about 1 ms. Because of this, the highest temperature that may be reached during combustion is frequently close to a temperature of adiabatic flame. Since the equilibrium state is what would be reached for chemical processes to happen, chemical equilibrium provides a good estimate to the composition of the combustion products at high temperatures. The chemical equilibrium model offers a good approximation for a combustion model. Under the present conditions, the net change in species composition remains the same because the products of combustion react collectively to generate and eliminate each species at comparable rates [7]. Models of chemical equilibrium are employed [8, 9]. A basic model with just six product species was established to examine the effect of steam injection on the operation and NO emissions of a diesel engine operating on a blend of ethanol and conventional diesel fuel [10], Chaudhari et al. [11] conducted a numerical research. They used a formed solution approach based on chemical equilibrium to assess different ethanol-diesel blends as a function of their steam/air ratios. To forecast the chemical equilibrium of combustion products, enthalpy, and specific heat of ten combustion products in an H_2O injected combustion system at different H_2O rates, Yeliana [12] employed a chemical equilibrium model. They created different equation systems for rich and lean mixes, ignoring the production of CO and H_2 in lean mixtures. Sun et all. [13] concluded that engine performance could be improved by manipulating the thermophysical properties of steam injection. Hellier et al. [14] used a chemical equilibrium model to examine the combustion of jatropha and biodiesel/diesel blends in a diesel engine. Tamilselvan et al. [15] developed a multifeatured model to estimate the mole fractions of combustion products at chemical equilibrium, the thermodynamic characteristics of fuels, and the temperature of adiabatic flame of fuel additives. Their equations for lean and rich mixes were developed separately.

A comparison of past researches versus the current study is shown in Table 1.

Table 1. Comparison table of previous researches with the present research.

Previous researches
1) Investigation of the effect of biofuel combustion with steam injection on the equilibrium combustion products and thermodynamic properties such as specific heat of the exhaust mixtures and adiabatic flame temperatures [12].
2) Investigation of the effects of steam injection on performance and NO emissions of a diesel engine running with ethanol-diesel blend [10].
3) Thermophysical and chemical effects of in-cylinder steam injection on gasoline engine performance was investigated using a computational fluid model established. A premixed laminar flame model was developed to examine the influence of steam injection on laminar flame speed and the characteristics of engine with steam injection [13].
Current research
This study investigates not only the effect of conventional diesel fuel and biodiesel combustion with steam injection on the equilibrium combustion products and thermodynamic properties such as specific heat of the exhaust mixtures and adiabatic flame temperatures but also its effect on enthalpy and entropy for a range of equivalence ratios. It is not the case of the previous researches.
Thermal NO is calculated based on the equilibrium combustion products.
This study investigates equally the effect of unburned temperatures of reactants and pressure on the equilibrium combustion products and thermodynamic properties.

Equilibrium computer programs exist, such GASEQ [16] and NASA CEA [17]. There could be considerable errors in engine performance calculations due to the neglect of the impact of dissociations on the specific heat of combustion products by GASEQ software. In contrast, computer software CEA requires a temperature of adiabatic flame or enthalpy of combustion as an initial parameter before beginning computations. There are significant discrepancies between the specific heat values produced with the CEA and GASEQ codes, particularly at high temperatures. This research investigates the effect of steam injection on the combustion products at chemical equilibrium, NO production, thermodynamic properties of the combustion products and temperatures of adiabatic flame of conventional diesel fuel and biodiesel. The study investigates also the effect of unburned mixture temperature and pressure on adiabatic flame temperatures and thermodynamic properties. The model accounts for the influence of temperature-dependent dissociations of combustion products on the specific heat of combustion products at chemical equilibrium.

Steam injection into combustion systems can have significant effects on the chemical equilibrium of combustion products. It is important to understand the mechanisms of action and the specific applications to optimise the benefits. The aim is to understand and control the products of chemical equilibrium during combustion in order to improve the efficiency, safety and durability of combustion systems. To date, there are no studies in the literature that investigate the combined effects of conventional diesel fuel and biodiesel combustion with steam injection on thermodynamic properties such as entropy and enthalpy. Additionally, there is a lack of research examining the influence of unburned mixture temperature and pressure on adiabatic flame temperature and thermodynamic properties. Therefore, this study presents notable novelty and originality.

2. Methods

2.1. Equilibrium Combustion Products

The combustion model is developed by incorporating the equilibrium constants of the dissociation reactions. The combustion products are computed as a function of temperature, pressure, and equivalence ratio. The principal assumption is that all phase species exist as ideal gases, with their thermodynamic properties, excluding entropy, varying with temperature. The species are defined based on dissociation considerations, and this model is deemed sufficiently accurate for internal combustion engines, where equivalence ratios are typically less than 3 and α/γ ratios are below one.

$$\frac{1}{2}H_2 \rightleftharpoons H \qquad\qquad K_{P,1} = \frac{y_7 p^{1/2}}{y_6^{1/2}} \qquad (1)$$

$$\frac{1}{2}O_2 \rightleftharpoons O \qquad\qquad K_{P,2} = \frac{y_8 p^{1/2}}{y_4^{1/2}} \qquad (2)$$

$$\frac{1}{2}H_2 + \frac{1}{2}O_2 \rightleftharpoons OH \qquad K_{P,3} = \frac{y_9}{y_4^{1/2} y_6^{1/2}} \qquad (3)$$

$$\frac{1}{2}O_2 + \frac{1}{2}N_2 \rightleftharpoons NO \qquad K_{P,4} = \frac{y_{10}}{y_3^{1/2} y_4^{1/2}} \qquad (4)$$

$$H_2 + \frac{1}{2}O_2 \rightleftharpoons H_2O \qquad K_{P,5} = \frac{y_2}{y_4^{1/2} y_6 p^{1/2}} \qquad (5)$$

$$CO + \frac{1}{2}O_2 \rightleftharpoons CO_2 \qquad K_{P,6} = \frac{y_1}{y_4^{1/2} y_5 p^{1/2}} \qquad (6)$$
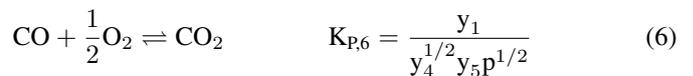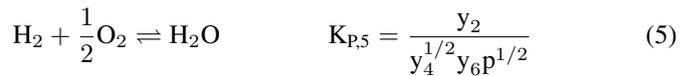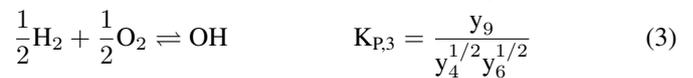
where the unit of pressure p is in atmospheres and $K_{P,1}$ to $K_{P,6}$ are the equilibrium constants of the dissociation reactions.

The chemical reactions describing combustion ($\phi < 3$) and for α/γ ratios less than one are as follows :

$$\epsilon\phi C_\alpha H_\beta O_\gamma N_\delta + (0.21O_2 + 0.79N_2) + \zeta H_2O \rightarrow$$
$$\nu_1 CO_2 + \nu_2 H_2O + \nu_3 N_2 + \nu_4 O_2 + \nu_5 CO + \nu_6 H_2 + \nu_7 H + \nu_8 O + \nu_9 OH + \nu_{10} N \qquad (7)$$

where ν_i denotes the number of moles for each product, α, β, γ, and δ represent the atom numbers of carbon, hydrogen, oxygen, and nitrogen in the used fuel, respectively. ζ is the number of mole for steam injection. The percentage of steam can be varied in order to lower the adiabatic flame temperature. It is possible to determine an optimal amount of steam to inject based on the combustion conditions. In this study, we maintained a 5% steam injection. The percentage of steam injection is the ratio of the steam mass to the air mass, expressed as a percentage.

The atom balance for various elements in Eq. (7), the constraint that the mole fraction of all the products adds up to 1, the unknown total product moles N and the 6 dissociation equations provided by the criteria of equilibrium among combustion products Eqs. (1) - (6) yield to 11 equations for 11 unknowns namely unknown mole fractions y_i and the unknown total product moles N. After writing the mole fractions of the other equilibrium combustion products with respect to the mole fractions of 4 independent variables y_3, y_4, y_5, and y_6, the following nonlinear equations are obtained.

$$f_1 = C_6 y_4^{1/2} y_5 + C_5 y_4^{1/2} v_6 + y_3 + y_4 + y_5 + y_6 + C_1 y_6^{1/2} + C_2 y_4^{1/2} + C_3 y_4^{1/2} y_6^{1/2} + C_4 y_3^{1/2} y_4^{1/2} - 1 = 0 \qquad (8)$$

$$f_2 = 2C_5 y_4^{1/2} y_6 + 2y_6 + C_1 y_6^{1/2} + C_3 y_4^{1/2} y_6^{1/2} - \eta(C_6 y_4^{1/2} y_5 + y_5) = 0 \qquad (9)$$

$$f_3 = 2C_6 y_4^{1/2} y_5 + C_5 y_4^{1/2} y_6 + 2y_4 + y_5 + C_2 y_4^{1/2} + C_3 y_4^{1/2} y_6^{1/2} + C_4 y_3^{1/2} y_4^{1/2} - \sigma(C_6 y_4^{1/2} y_5 + y_5) = 0 \tag{10}$$

$$f_4 = 2y_3 + C_4 y_3^{1/2} y_4^{1/2} - \xi(C_6 y_4^{1/2} y_5 + y_5) = 0 \tag{11}$$

where

$$C_1 = \frac{K_{P,1}}{p^{1/2}} \tag{12}$$

$$C_2 = \frac{K_{P,2}}{p^{1/2}} \tag{13}$$

$$C_3 = K_{P,3} \tag{14}$$

$$C_4 = K_{P,4} \tag{15}$$

$$C_5 = K_{P,5} p^{1/2} \tag{16}$$

$$C_6 = K_{P,6} p^{1/2} \tag{17}$$

$$\eta = \frac{\varepsilon\phi\beta + 2\zeta}{\varepsilon\phi\alpha} \tag{18}$$

$$\sigma = \frac{\varepsilon\phi\gamma + 0.42 + \zeta}{\varepsilon\phi\alpha} \tag{19}$$

$$\xi = \frac{\varepsilon\phi\delta + 1.58}{\varepsilon\phi\alpha} \tag{20}$$

The equivalence ratio ϕ and the molar fuel/air ratio ε are expressed as follows :

$$\phi = \frac{FA}{FA_S} \tag{21}$$

$$\varepsilon = \frac{0.84}{4\alpha + \beta - 2\gamma} \tag{22}$$

By setting a vector for unknowns $Y = (y_3, y_4, y_5, y_6)^T$, the correction vector $\delta Y = (\delta y_3, \delta y_4, \delta y_5, \delta y_6)^T$, and f_1, f_2, f_3, f_4 the coordinate functions of F.

$$F(Y) = [f_1(Y), f_2(Y), f_3(Y), f_4(Y)] = 0 \tag{23}$$

If the exact solution of the problem is $Y = Y^{(0)} + \delta Y$, then in the neighbourhoods of $Y^{(0)}$, each of the functions f_i can be expanded in Taylor series and by neglecting terms in δy_j^2 and higher, we get:

$$f_i(Y^{(0)} + \delta Y) = f_i(Y^{(0)}) + \sum_{j=3}^{6} \frac{\partial f_i(Y^{(0)})}{\partial y_j} \delta y_j = 0, i = 1, 2, 3, 4 \tag{24}$$

where $Y^{(0)}$ is a given rough initial guess and δY is the correction term. We obtain a set of linear equations for the correction δY that move each function closer to zero simultaneously. The set of linear equations obtained is solved for δY using a numerical approach.

2.2. Thermodynamic Properties

Gordon and McBride [18] proposed expressions, at constant pressure, for the molar specific heat $\bar{c}_{p,i}$, molar enthalpy $\bar{h}_i^{\,0}$, and molar entropy $\bar{s}_i^{\,0}$ of each species. These expressions have been fitted to the JANAF thermochemical tables [19].

At constant pressure, the molar enthalpy of the gas mixture changes due to dissociations because the molar fractions of the species change with temperature.

$$\bar{h} = \sum_{i=1}^{10} y_i \bar{h}_i^{\,0} \tag{25}$$

$$\bar{s} = R \sum_{i=1}^{10} y_i \left(\frac{\bar{s}_i^{\,0}}{R_u} - \ln\left(\frac{y_i p}{p_0}\right) \right) \tag{26}$$

$$M = \sum_{i=1}^{10} y_i M_i \tag{27}$$

$$h = \frac{1}{M} \sum_{i=1}^{10} y_i \bar{h}_i^{\,0} \tag{28}$$

$$s = \frac{R}{M} \sum_{i=1}^{10} y_i \left(\frac{\bar{s}_i^{\,0}}{R} - \ln\left(\frac{y_i p}{p_0}\right) \right) \tag{29}$$

At constant pressure, temperature variation has effect on specific heat due to the dissociations of species at high temperature.

$$c_p = \frac{1}{M} \sum_{i=1}^{10} \left(y_i \bar{c}_{p,i} + \bar{h}_i^{\,0} \left(\frac{\partial y_i}{\partial T}\right)_p - y_i \bar{h}_i^{\,0} \frac{\Lambda}{M} \right) \tag{30}$$

where

$$c_p = \left(\frac{\partial h}{\partial T}\right)_p \quad and \quad \Lambda = \left(\frac{\partial M}{\partial T}\right)_p = \sum_{i=1}^{10} M_i \left(\frac{\partial y_i}{\partial T}\right)_p \tag{31}$$

2.3. Validation of the Model

The results are compared with those obtained using software CEA [22], a chemical equilibrium application developed by NASA, as well as as with GASEQ [23]; CEA requires the flame temperature to be provided as an initial condition. The discrepancy between the specific heat results of GASEQ and those from our model and CEA arises because GASEQ does not account for the dissociation of product species that occurs at high temperatures. When dissociation effects are ignored, our model yields specific heat values consistent with those from GASEQ, although the equilibrium products, enthalpy, and entropy values remain comparable in both cases. The

specific heat values produced by our model are in excellent agreement with those from NASA's CEA. This validation demonstrates that the results presented in this study are both reliable and in good agreement with well-established codes such as CEA and GASEQ. Experimental studies [24–28] can be used to validate the model. The percentage of steam can be varied in order to lower the adiabatic flame temperature. It is possible to determine an optimal amount of steam to inject based on the combustion conditions. In our study, we maintained a 5% of steam injection because it results in a reduction of approximately 73% in thermal NO emissions due to the decrease in the temperature peak. We considered this reduction to be satisfactory.

The comparison results are shown in Tables 2 and 3. From the Tables, it can be known that the relative deviations of the components except NO are within 1.3%, which verifies the correctness of our mathematical model. For NO, the relative deviations are 4.83% (for $\phi = 0.5$) and 4.57% (for $\phi = 1$). When the combustion temperature is high, a higher amount of NOx is produced due to higher thermal energy available for nitrogen reactions.

3. Results and Discussion

3.1. Mole Fraction of Combustion Products

Figures 1a and 1b illustrate the variations in the mole fractions and specific heat of the combustion products of biodiesel fuel and conventional diesel fuel. These figures illustrate that nearly no O_2 remains at $\phi = 1.12$, exactly as the mole fractions of OH and CO_2 reach their maximum at $\phi = 0.976$ and $\phi = 0.964$, respectively. The mole fraction of NO

reaches a peak around $\phi = 0.85$, when CO and H_2 begin to develop. The highest mole fraction of O is seen at $\phi = 0.94$. The mole fractions of H_2O and H reach their peak at $\phi = 1.13$, while the mole fraction of N_2 declines steadily with ϕ. The mole fractions of CO and H_2 do not have a maximum value, but rather grow with ϕ and are formed at ϕ of approximately 0.85.

The equilibrium mole fractions of H_2O rise with the amount of steam injection. As a result, the steam injection promotes the creation of H_2 and O_2. The equilibrium mole fractions of N_2 drop as the amount of steam introduced rises. For $\phi = 1.2$, the equilibrium mole fractions of CO drop as the amount of steam injection grows. Because the injected steam promotes H_2 generation, the equilibrium mole fractions of H_2 also increase. Due to the absence of O_2 caused by lean combustion, the equilibrium mole fractions of O_2 drop with the amount of steam injection at $\phi = 0.2$. The trends in independent equilibrium mole fractions can explain the rest of the equilibrium mole fraction changes. The equilibrium composition of combustion gases is strongly temperature-dependent. As the temperature rises, the degree of dissociation decrease increases dramatically. Even if there is enough oxygen for complete combustion, significant amounts of CO_2, H, and other partially oxidized products may be present at the temperature of adiabatic flame. As the temperature drops, chemical equilibrium favours the synthesis of stable products like CO_2, H_2O, N_2, and O_2, while destroying less stable species like CO, H_2, NO, O, H, and OH, as seen in Figure 1. At chemical equilibrium, the combustion products contain only the most stable species in substantial quantities below 1300 K. The emission of carbon monoxide and nitrogen oxides by lean combustion systems indicates that chemical equilibrium is not maintained when the combustion products cool.


(a) Biodiesel fuel   *(b) Conventional diesel fuel*
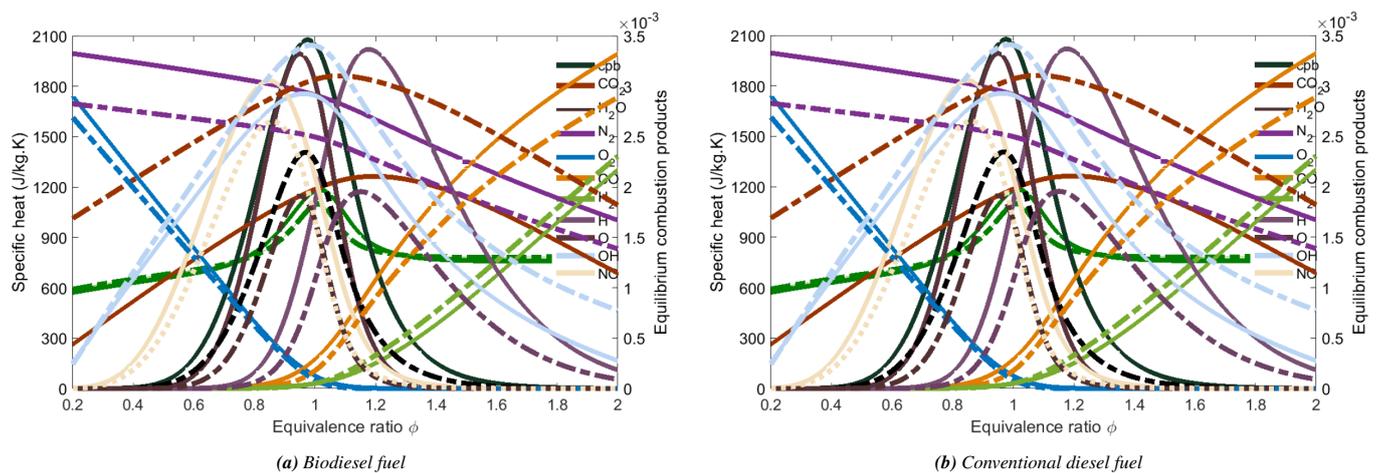
Figure 1. *Effect of steam injection on the equilibrium combustion products and specific heat of equilibrium combustion products under atmospheric pressure with equivalence ratios.*

When 0.533 kg of steam is injected for each kilogram of biodiesel fuel burned under stoichiometric conditions, the temperature of adiabatic flame decreases by 99 K, 2247 K to 2148 K. Adding 0.533 kg of steam for every kilogram

of biodiesel fuel burned reduces NO emissions by 73.5%. The specific heat c_p is reduced from 2.258 $kJ.kg^{-1}.K^{-1}$ to 2.107 $kJ.kg^{-1}.K^{-1}$, a reduction of 0.151 $kJ.kg^{-1}.K^{-1}$. NO formation rate decreases by 2.395 $mol.m^{-3}.s^{-1}$, from 3.258

mol.$m^{-3}.s^{-1}$ to 0.8629 mol.$m^{-3}.s^{-1}$.

When 0.716 kg of steam is injected for each kilogram of conventional diesel fuel burned under stoichiometric conditions, the temperature of adiabatic flame decreases by 103 K, from 2305 K to 2202 K. The addition of 0.716 kg of steam for every kilogram of conventional diesel fuel burned reduces NO emissions by 73%. The specific heat is reduced from 2.353 kJ.$kg^{-1}.K^{-1}$ to 2.190 kJ.$kg^{-1}.K^{-1}$, a reduction of 0.163 kJ.$kg^{-1}.K^{-1}$. NO generation rate decreases from 6.716 mol.$m^{-3}.s^{-1}$ to 1.809 mol.$m^{-3}.s^{-1}$, a reduction of 0.163 mol.$m^{-3}.s^{-1}$.

The reduction of temperature slows the rate of N_2 destruction, resulting in a slower rate of NO production. This reduction in temperature reduces NO emissions. Figures 2a and 2b depict the effect of steam injection on temperature of adiabatic flame and specific heat of combustion products at chemical equilibrium under atmospheric pressure. According to these results, the injected steam lowers the temperature of

adiabatic flame. However, we can see that the temperature of adiabatic flame and specific heat increase with the equivalence ratio, then change abruptly after the equivalence ratio reaches approximately 1.2 and decreases. Specific heat reaches its peak at $\phi = 1.0165$ for conventional diesel fuel without steam injection and at $\phi = 1.0105$ for conventional diesel fuel with steam injection. Steam injection reduces specific heat only between $\phi = 0.7490$ and $\phi = 1.2845$ for conventional diesel fuel. The specific heat peaks at $\phi = 1.0570$ for biodiesel fuel without steam injection and $\phi = 1.0420$ for biodiesel fuel with steam injection.

Steam injection reduces the value of specific heat for biodiesel fuel only between $\phi = 0.7530$ and $\phi = 1.2740$. In all condtions, the temperature of adiabatic flame and specific heat reach their maximums as the equivalence ratios approach unity, after which they both decrease. Tables 4 and 5 provide the exact value of ϕ for maximum temperature of adiabatic flame that are somewhat higher than stoichiometric conditions.

(a) Biodiesel fuel

**(b) Conventional diesel fuel**
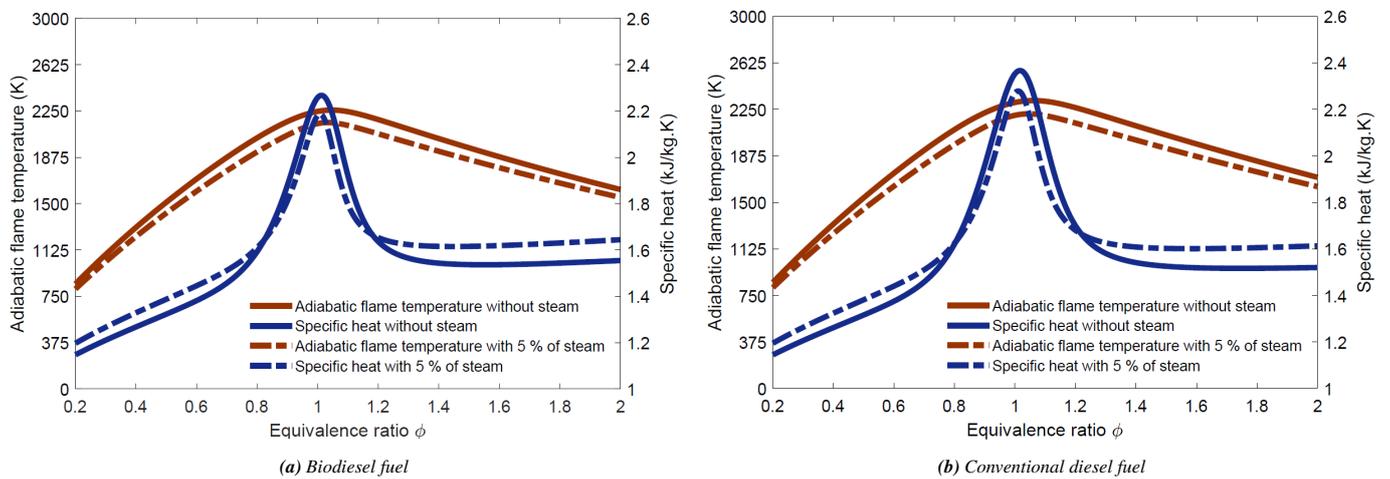
Figure 2. *Effect of steam injection on the adiabatic flame temperature and specific heat of equilibrium combustion products under atmospheric pressure with equivalence ratios.*

Table 2. *Tabulated equilibrium combustion products and thermodynamic properties corresponding to the equivalence ratio of the highest adiabatic flame temperature at atmospheric pressure (biodiesel at p = 1 atm and T_u = 300 K).*

	0% of steam	5% of steam	Variation Δ
CO_2	0.1183291	0.1145245	3.22%
H_2O	0.1212650	0.1845955	- 52.2%
N_2	0.7260302	0.6750476	7.02%
O_2	0.0073055	0.0018380	74.8%
CO	0.0164881	0.0159330	3.37%
H_2	0.0030540	0.0049338	- 61.6%
H	0.0005495	0.0003952	28.1%
O	0.0004363	0.0001154	73.6%
OH	0.0035449	0.0020612	41.9%
NO	0.0029973	0.0011563	61.4%
c_p(kg/kJ/K)	2.371554	2.098404	11.5%
s_b(kg/kJ/K)	9.787615	9.786633	0.010%
h_b(kg/kJ)	- 77.2703	- 701.380	807.69%
ϕ	1.0570	1.0420	1.42%
T_{ad} (K)	2305.959	2200.460	4.58%

Table 3. *Tabulated equilibrium combustion products and thermodynamic properties corresponding to the equivalence ratio of the highest adiabatic flame temperature at atmospheric pressure (conventional diesel fuel at p = 1 atm and T_u = 300 K).*

	0% of steam	5% of steam	Variation Δ
CO_2	0.1153313	0.1149529	0.328%
H_2O	0.1169065	0.1769658	- 5.68%
N_2	0.7259531	0.6808807	6.21%
O_2	0.0029218	0.0019240	34.2%
CO	0.0278787	0.0171555	38.5%
H_2	0.0050667	0.0050318	0.689%
H	0.0007641	0.0004309	43.6%
O	0.0003006	0.0001287	57.2%
OH	0.0029233	0.0021563	26.2%
NO	0.0019538	0.0012249	37.3%
c_p(kg/kJ/K)	2.264087	2.114136	6.62%
s_b(kg/kJ/K)	9.592072	9.764400	- 1.80%
h_b(kg/kJ)	- 33.8045	- 627.045	1754.9%
ϕ	1.0615	1.0445	1.60%
T_{ad}(K)	2320.887	2214.081	4.60%

Figures 3a and 3b show how steam injection affects the temperature of adiabatic flame and the specific heat of combustion products. According to the figures depicting the effect of steam addition, steam injection lowers the temperature of adiabatic flame and specific heat. The temperature of adiabatic flame and specific heat decrease as the amount of steam injected rises. Figure 3 illustrates that the temperature of adiabatic flame increases with pressure, and that this increase is more rapid for pressures below around 10 atm. The same applies to specific heat, but the pressure at which the decrease in specific heat slows down is lower than the adiabatic flame temperature.


(a) Biodiesel fuel   *(b) Conventional diesel fuel*
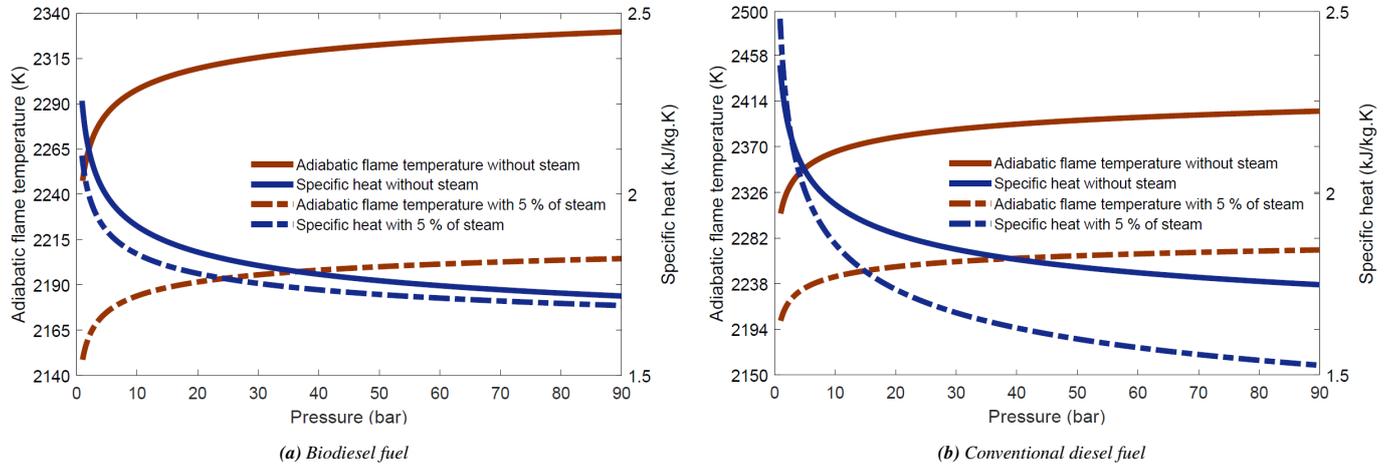
Figure 3. *Effect of steam injection on the adiabatic flame temperature and specific heat of equilibrium combustion products with pressure at $\phi = 1$.*

Figures 4a and 4b illustrate the influence of steam injection on adiabatic flame temperature and on the specific heat of combustion products. As the flame temperature approaches 1800 K, a 103 K drop in maximum flame temperature reduces NO production by around 73%. These curves show that temperature of adiabatic flame and specific heat increase linearly with increasing unburned mixture temperature. Figures 4a and 4b demonstrate that for both biodiesel fuel and conventional diesel fuel, the temperature of adiabatic flame increases by 10.7% for every 500 K increase in the initial unburned mixture temperature. Steam injection lowers the temperature of adiabatic flame and increases the specific heat.


(a) Biodiesel fuel   *(b) Conventional diesel fuel*
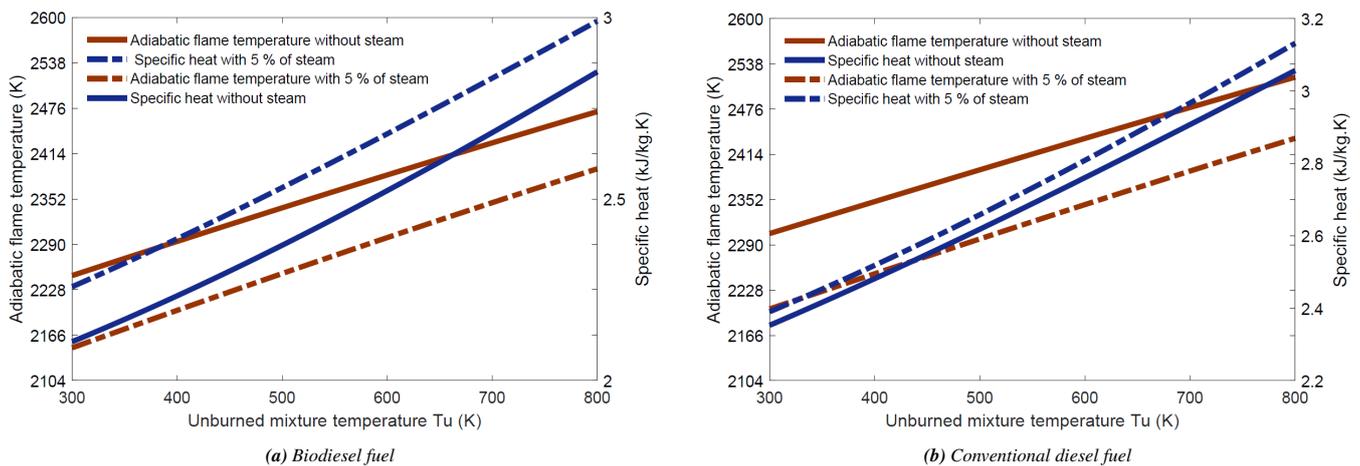
Figure 4. *Effect of unburned mixture temperature on the adiabatic flame temperature and specific heat of equilibrium combustion products under atmospheric pressure at $\phi = 1$.*

3.2. Thermodynamic Properties of Combustion Products

Because superheated steam has a larger specific heat than air at this temperature, the specific heat and enthalpy of the gases in the mixture increase as more steam is injected.

Figures 5a and 5b depict the influence of steam injection on the equilibrium products of combustion and the enthalpy of the products of combustion. To show the differences, some curves are fitted using the values shown in the legends. The specific heat reaches its maximum at $\phi = 1.0165$ for conventional diesel

fuel without steam injection and at $\phi = 1.0105$ for conventional diesel fuel with steam injection, However, the specific heat hits its peak at $\phi = 1.0570$ for biodiesel fuel without steam injection and at $\phi = 1.0420$ for biodiesel fuel with steam injection.

Entropy always rises with ϕ, but falls slightly with the amount of steam injected. Steam injection reduces with ϕ, but only marginally with amount injected. In contrast, enthalpy drops as ϕ and amount of steam injected increase.

*(a) Biodiesel fuel*   *(b) Conventional diesel fuel*
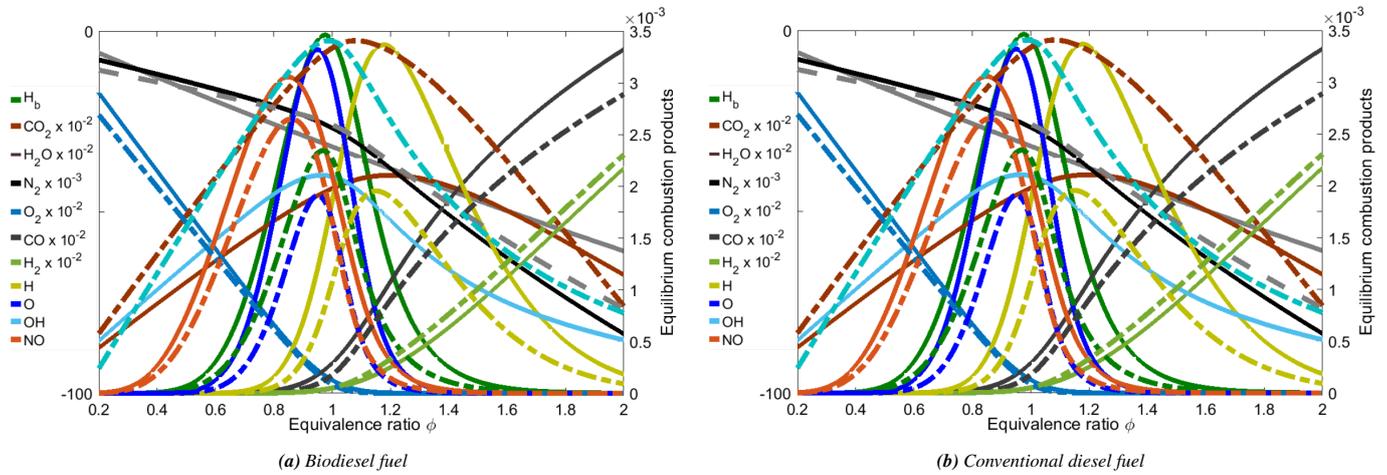
Figure 5. *Effect of steam injection on the products combustion and specific enthalpy of equilibrium combustion products under atmospheric pressure with equivalence ratios.*

Figures 6a and 6b show how steam injection affects the products of combustion in chemical equilibrium, as well as the entropy of gases. To show the differences, some curves are fitted using the values shown in the legends. Entropy always rises with ϕ and very marginally with the amount of steam injected.

*(a) Biodiesel fuel*   *(b) Conventional diesel fuel*
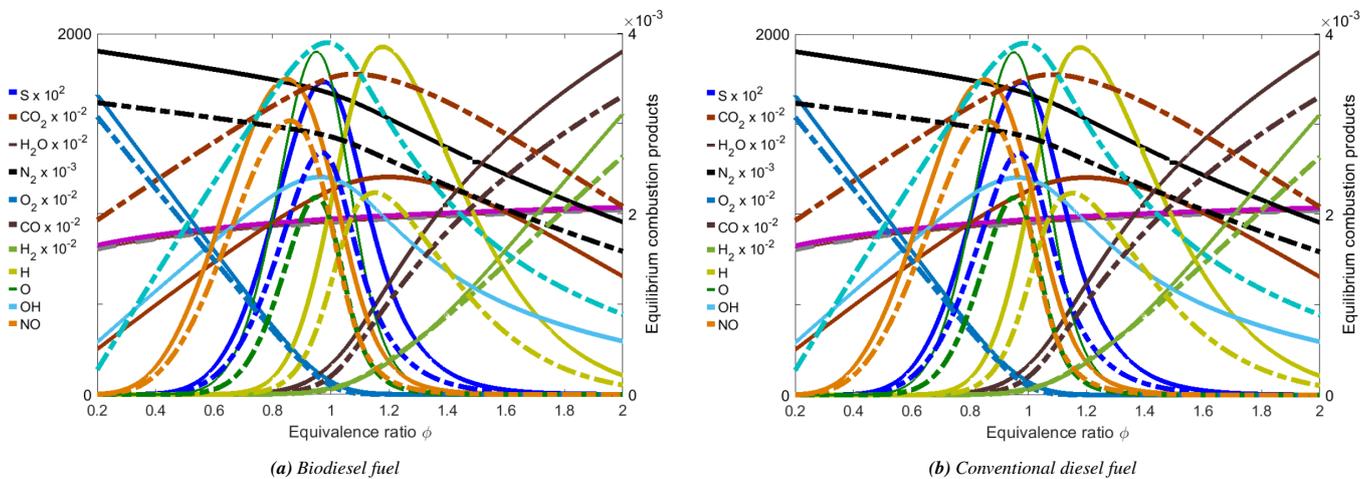
Figure 6. *Effect of steam injection on the products combustion and specific entropy of burned gases under atmospheric pressure with equivalence ratios.*

4. Conclusion

In this research, the chemical equilibrium combustion model is used to investigate the effect of steam injection on the chemical equilibrium combustion products, the temperature of adiabatic flame, and the thermodynamic properties of combustion products of biodiesel and conventional diesel fuel. The model determines the temperature of adiabatic flame and the values of specific heat, enthalpy and entropy, while determining the chemical equilibrium mole fractions of the combustion products. Chemical equilibrium products are crucial in combustion, as they determine the characteristics and performance of combustion. They influence the energy efficiency of combustion by determining the amount of energy released or absorbed during combustion. They determine the composition of exhaust gases, including emissions of pollutants such as carbon monoxide (CO) and nitrogen oxides (NO_x). They also influence combustion temperature, which in turn affects combustion performance and nitrogen oxide (NO_x) emissions. Furthermore, They contribute to

flame stability by determining reaction rates and radical formation. The results of this work can help not only those carrying research on biodiesel fuel and conventional diesel fuel, but also those modeling internal combustion engines, as the mole fractions of each product species are essential data for calculating pollutants such as thermal NO using chemical kinetics concepts. Steam injection is vital not only for performance but also for environmental reasons. The practical implications of chemical and steam injection in compression ignition engines using conventional diesel fuel and biodiesel are profound.The role of chemical equilibrium in determining the combustion products and the influence of steam injection on reducing emissions, enhancing combustion stability, and improving thermal efficiency offer valuable insights for developing cleaner and more efficient engines. By optimizing steam injection strategies, it is possible to reduce harmful emissions like (NO_x), improve engine performance, and reduce the environmental impact of both conventional diesel fuel and biodiesel.

Abbreviations

AF	Fuel/air Ratio
AF_s	Stoichiometric Fuel/air Ratio
CEA	Chemical Equilibrium Application
NASA	National Aeronautics and Space Administration
α	Atomic Number of Carbon for Fuels
β	Atomic Number of Hydrogen for Fuels
γ	Atomic Number of Oxygen for Fuels
δ	Atomic Number of Nitrogen for Fuels
ε	Molar Fuel-air Ratio
ϕ	Equivalence Ratio
ν_i	Number of Moles for Product Species i
a	Air
f	Fuel
s	Stoichiometric
u	Unberned

Conflicts of Interest

The author declares no conflicts of interest.

References

[1] Veza I, Spraggon M, Fattah IMR, Idris M. Response surface methodology (RSM) for optimizing engine performance and emissions fueled with biofuel: Review of RSM for sustainability energy transition. Results in Engineering 2023; 18: 101213.

[2] Rizwanul Fattah IM, Ong HC, Mahlia TMI, Mofijur M, Silitonga AS, Rahman SMA, et al. State of the Art of Catalysts for Biodiesel Production. Front Energy Res 2020; 8.

[3] Fayad MA, Abed AM, Omran SH, Jaber AA, Radhi AA, Dhahad HA, Chaichan MT, Yusaf T. Influence of renewable fuels and nanoparticles additives on engine performance and soot nanoparticles characteristics. Int J Renew Energy Dev. 11 (4) (2022) 1068-1077.

[4] Fayad MA, Ibrahim SI, Omran SH, Martos FJ, Badawy T, Al Jubori AM, Dhahad HA, Chaichan MT. Experimental effect of CuO_2 nanoparticles into the RME and EGR rates on NO_x and morphological characteristics of soot nanoparticles, Fuel 331 (Part 1) (2023) 125549.

[5] Xu H, Ou L, Li Y, Hawkins TR, Wang M. Life Cycle Greenhouse Gas Emissions of Biodiesel and Renewable Diesel Production in the United States. Environ Sci Technol 2022; 56: 7512-21.

[6] L. Marousek J, Strunecky O, Bartos V, Vochozka M. Revisiting competitiveness of hydrogen and algae biodiesel. Fuel 2022; 328: 125317.

[7] A. Parlak, Comparative performance analysis of irreversible Dual and Diesel cycles under maximum power conditions, Energy Conversion and Management 46 (3) (2005) 351-359.

[8] S. Hou, Heat transfer effects on the performance of an air standard Dual cycle, Energy Conversion and Management 45 (2004) 3003-3015.

[9] O. Ozsoysal, Heat loss as a percentage of fuel's energy in air standard Otto and Diesel cycles, Energy Conversion and Management 47 (2006) 1051-1062.

[10] Gonca G. Investigation of the effects of steam injection on performance and NO emissions of a diesel engine running with ethanol-diesel blend. Energy Convers Manag 2014; 77: 450-7.

[11] Chaudhari AJ, Sahoo N, Kulkarni V. Simulation models for spark ignition engine: a comparative study. Energy Procedia 2014; 54: 330-41.

[12] Y. Yeliana, C. Cooney, J. Worm, D. Michalek, J. Naber, Wiebe function parameter determination for mass fraction burn calculation in an ethanol-gasoline fuelled SI engine, Journal of Kones, Powertrain Transportation 15(No. 3) (2008) 567-574.

[13] Sun X, Zhao P, Liang X, Zhou Z, Chen G. Investigation of thermo-physical and chemical effects of in-cylinder steam injection on gasoline engine performance. Fuel 334(2023)126625.

[14] N. Miyamoto, T. Chikahisa, T. Murayama, R. Sawyer, Description and analysis of diesel engine rate of combustion and performance using Weibe's functions, SAE paper 850107, 1985.

[15] Hellier P, Talibi M, Eveleigh A, Ladommatos N. An overview of the effects of fuel molecular structure on the combustion and emissions characteristics of compression ignition engines. Proceedings of the Institution of Mechanical Engineers, Part D: Journal of Automobile Engineering. 2017:0954407016687453.

[16] Tamilselvan P, Nallusamy N, Rajkumar S. A comprehensive review on performance, combustion and emission characteristics of biodiesel fuelled diesel engines. Renewable and Sustainable Energy Reviews. 2017; 79: 1134-59.

[17] Coniglio L, Bennadji H, Glaude PA, Herbinet O, Billaud F. Combustion chemical kinetics of biodiesel and related compounds (methyl and ethyl esters): Experiments and modeling-advances and future refinements. Progress in Energy and Combustion Science. 2013; 39: 340-82.

[18] Visconti P, Primiceri P, Strafella L, Carlucci AP, Ficarella A. Morphological analysis of injected sprays of different bio-diesel fuels by using a common rail setup controlled by a programmable electronic system. International Journal of Automotive and Mechanical Engineering. 2017; 14: 3849-71.

[19] Nayak SK, Mishra PC. Emission from a dual fuel operated diesel engine fuelled with calophyllum inophyllum biodiesel and producer gas. International Journal of Automotive and Mechanical Engineering. 2017; 14: 3954-69.

[20] Shukri MR, Rahman MM, Ramasamy D, Kadirgama K. Artificial neural network optimization modeling on engine performance of diesel engine using biodiesel fuel. International Journal of Automotive and Mechanical Engineering. 2015; 11: 2332-47.

[21] Hasan MM, Rahman MM, Kadirgama K. A review on homogeneous charge compression ignition engine performance using biodiesel-diesel blend as a fuel. International Journal of Automotive and Mechanical Engineering. 2015; 11: 2199-211.

[22] J. B. Heywood, Internal Combustion Engine Fundamentals, McGraw-Hill, New york, 1988.

[23] G. F. Hohenberg, Advanced approaches for heat transfer calculations, SAE Paper (1979), no.790825.

[24] Cesur I, Parlak A, Ayhan A, Boru B, Gonca G. The effects of electronic controlled steam injection on spark ignition engine. Appl Therm Eng 2013; 55: 61-8.

[25] Kokkulunk G, Gonca G, Parlak A. The effects of design parameters on performance and NO emissions of steam-injected diesel engine with exhaust gas recirculation. Arab J Sci Eng 2014; 39(5): 4119-29.

[26] Kokkulunk G, Parlak A, Ayhan V, Cesur I, Gonca G, Boru B. Theoretical and experimental investigation of steam injected diesel engine with EGR. Energy 2014; 74: 331-9.

[27] Rashidi M. Calculation of equilibrium composition in combustion products. Chemical Engineering and Technology. 1997; 20: 571-5. Gonca G, Sahin B, Parlak A, Ust Y, Ayhan V, Cesur I, et al. The effects of steam injection on the performance and emission parameters of a miller cycle diesel engine. Energy 2014; 78: 266-75.

[28] Gonca G, Sahin B, Parlak A, Ust Y, Ayhan V, Cesur I, et al. Theoretical and experimental investigation of the Miller cycle diesel engine in terms of performance and emission parameters. Appl Energy 2015; 138: 11-20.