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Original Research

Developing a reduced chemical kinetic mechanism for natural gas/biodiesel mixture combustion

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ABSTRACT

The use of natural gas-biodiesel in LTC engines, according to their characteristics, Recently, it has attracted the attention of combustion scientific circles. Natural gas abundance, clean combustion characteristics relatively low cost among various fuels, and the renewability of biodiesel make them attractive fuel in combustion engines. In this line, various experimental tests using natural gas-biodiesel fuels have been performed until now. So for further development, the use of numerical simulations can be effective. The main problem in this way is the lack of a precise combustion mechanism for biodiesel-natural gas. In this regard, an accurate mechanism which consists of 153 species and 727 reactions is developed from two up-to-date mechanisms. For natural gas, the Drost mechanism, which consists of 49 species and 332 reactions and is considered as 90% CH4, 9% C2H6, and 1% C3H8, and for biodiesel, the Zhang mechanism with 156 species and 589 reactions has been employed, which is considered as 25% MD, 25% MD9D and 50% n-Heptane. In the development process, DRG, DRGEP, sensitivity analysis, path flux analysis, and QSSA methods are used. Comparing ignition delay times of based and developed mechanisms revealed that arithmetical mean error (AME) is 10.77% for 0%-NG and 11.2% for 0%-biodiesel, respectively. In the 1-D simulation, flame speed is calculated and the AME for 0%-biodiesel and 0%-NG is 7% and 8.3%, respectively. In the end, the RCCI engine CFD simulation is verified again to the develop mechanism appropriately.

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1- Introduction

Nowadays, the use of natural gas (NG) as the main fuel in power plant sectors has led to research in the field of gas fuel combustion in all types of combustion engines [1]. As NG is abundant, low production cost and emissions, it has been adverted as an alternative fuel for gasoline in recent years [2]. NG can reduce NOx emission, make soot zero, and produce less hydrocarbon (HC) due to its lower C/H ratio than other fuels. But a thing that is more important in the usage of this fuel is its high octane number and heating value in comparison with other fuels. As NG's octane number is higher than other similar fuels, it is permitted to employ it in a higher compression ratio engine [3]. Also, this feature of NG makes it suitable fuel as a low reactive fuel in reactivity-controlled compression ignition (RCCI) engines or major fuel in the dual-fuel engine in low-temperature combustion (LTC) categories [3, 4]. Due to these special specifications, usually NG is used as a mixture with another high-reactive fuel like diesel or biodiesel [5].

Another alternative fuel that has received much attention in usage in Internal combustion (IC) Engines in recent years is biodiesels [6]. Biodiesels have many features of conventional diesel and can be employed in engines individually or as a blend with diesel [7]. Compared to diesel fuel, it can shorten the ignition delay time because it has a higher cetane number [8]. Also, biodiesel can be effective in reducing pollution as it is an oxygenated fuel [9]. According to research, Biodiesels can reduce carbon monoxide (CO), particle matter (PM), and Unburned Hydrocarbons (HC) emissions [10-12]; but its effect on NOx is uncertain; some researchers have reported biofuels increase nitrogen oxides [13] and in some other reported decrease it; which is depend on kind of biodiesel [14]. In general, biodiesels are produced by transesterification of rapeseed and soybean oils with methanol [15], which is the most economical process for commercial biodiesel production [16]. The main structure of biodiesels is large fatty acid methyl esters (FAME), such as methyl palmitate (MP), methyl stearate (MS) as a saturated methyl ester (ME), and methyl oleate (MO), methyl linoleate (ML) and methyl linoleate (MLE) as unsaturated methyl ester [17, 18]. This large molecule structure size has a complex chemical kinetic mechanism, which contains more than 3000 species and 10000 reactions [19]. Since Computational fluid dynamic (CFD) simulations are an adequate approach for developing internal combustion engines, in biodiesel engines, the main challenge is employing biodiesel's kinetic mechanism in CFD simulations, as it is extremely time-consuming and computationally expensive [14].

As a result, to overcome this challenge, nowadays, mechanism reduction methods are used to optimize the detailed chemical mechanism to a reduced one while maintaining physical and chemical properties [20].

According to the discussions, it can be concluded that natural gas and biodiesel fuels can have a special place in the future fuel portfolio. Although, their combined use in internal combustion engines, especially in RCCI and dual-fuel engines, has been investigated in numerous articles and they have been referred to as a proportional fuel pair [21-23]. But the important point in all this research is that due to the lack of an optimized combustion mechanism for the biodiesel-natural gas combination, research has been conducted experimentally; and numerical research has not been conducted. The development of this engine is dependent on the numerical simulations and the resulting optimizations.

Therefore, in this research, an attempt has been made to develop a biodiesel-natural gas chemical mechanism by using regular and optimized mechanisms for natural gas and biodiesel fuels and their integration. Also, the reduced mechanism has been used to develop the final combustion mechanism for use in RCCI engines.

1-1- Natural gas mechanism selection

According to previous studies, various research has been done on the chemical kinetic

mechanism of natural gas fuel. Since methane is the main component of natural gas, which includes more than 90% of the structure of this gas, most of the mechanism development has been done considering methane as a representative of natural gas [2]. On the other hand, ethane and propane, which together make up approximately 10% of this gas, have been used in some other chemical kinetic mechanisms of natural gas to increase accuracy. As a result of this research, a chemical kinetic mechanism for natural gas was developed as summarized in [24].

GRI-mech 3 is one of the most famous chemical kinetics mechanisms for predicting natural gas combustion; which has been extensively used until now [24]. Since GRI-Mech can predict ignition delay (ID) time in the temperature range of (1350-1800 K), Its low-temperature prediction will be accompanied by large errors [2]. To solve such problems, various chemical kinetic mechanisms for natural gas were developed in the last decade. Mechanisms that can cover more temperature range, pressure range as well as more appropriate balance ratio for engines. USC 2.0 [25], Aramco-Mech [26], SanDiego [27], and CRECK Mech [28] were an example of these mechanisms. Also, other chemical kinetics have been developed through the reduction of the mentioned basic mechanisms. Wang et al [29] in 2013 could reduce USC 2.0 (111 species and 784 reactions) to 56 species and 428 reactions, which could satisfy ignition delay time, flame speed propagation, and species profile within a 10% error.

Drost et al [1] in 2020, also developed a mechanism with 49 species and 332 reactions from Aramco mech 3.0 reductions; which was validated against ignition delay time and flame speed. As its accurate estimation of ignition delay concerning reviewed research and especially GRI-Mech and SanDiego in low temperature, in this study, Drost [1] mechanism is employed as a natural gas chemical kinetic mechanism.

1-2- Biodiesel mechanism selection

In the last decade, a lot of research has been done on the chemical kinetic mechanism of different biodiesels, to create the ability to simulate biodiesels and their mixture combustion. Considering that the structure of biodiesel is a combination of saturated and unsaturated methyl esters, in some research only saturated esters have been investigated such as methyl butanoate (MB, $C5H10O2$) and n-heptane chemical kinetic mechanism which was developed by Brakora et al [30]. The achieved mechanism consisted of 53 species and 156 reactions and was validated against ignition delay time and flame speed. Another mechanism containing MB and n-heptane was developed by Liu et al. [31]; which contained 869 reactions and 145 species. The developed mechanism was validated against in-cylinder pressure, heat release rate (HRR), and NOx. Lee et al. [32] also developed this composition of mechanism for biodiesel surrogates and achieved 76 species and 243 reactions which were validated against in-cylinder pressure, HRR, carbon monoxide (CO), NOx, and particulate matter (PM) emission.

But for the first time, Ismail Harun et al. [14] developed a mechanism by considering unsaturated methyl ester. This mechanism consisted of MB/MB2D/n-heptane which contains 113 species and 399 reactions and could predict NOx and soot appropriately. Also, Hoon Kiat NG et al. [33] developed a contained unsaturated methyl ester mechanism for a diesel-biodiesel blend which consists of 80 species and 209 reactions. They assumed MB and MC as saturated and unsaturated methyl ester (ME), respectively. Finally, their developed mechanism was obtained by reducing the blend of MB/MC/n-heptane, which could predict NOx and soot profile appropriately.

To achieve greater accuracy, a detailed chemical kinetic mechanism for biodiesel based on methyl decanoate (MD, $C12H22O2$) was investigated by Herbinet et al. [9], [34]. Detail mechanism for MD5D and MD9D (as an unsaturated methyl ester) was derived from MD and by merging it with n-heptane, a detailed kinetic of the biodiesel combustion

mechanism was attained. Teng Liu et al. [35] developed a biodiesel mechanism by adding reduced methyl linoleate (ML) into Chang's [36] mechanism which led to the mechanism with 102 species and 263 reactions. They announced that single-double bond unsaturated methyl esters (like MD5D and MD9D) cannot predict biodiesel specification individually, so they added a two-double bond unsaturated methyl ester (ML) into the surrogate mechanism.

Han Li [37] investigated a new chemical kinetic mechanism for heavy-saturated methyl esters. They achieved to methyl palmitate (MHD) and methyl stearate (MOD) mechanism with 140 species and 890 reactions and validated it against ignition delay and CO emission. Gang Wu et al. [38] proposed a reduced chemical kinetic mechanism for biodiesel surrogates which consisted of long carbon chains and polyunsaturated compounds. Their five-component skeletal mechanism consisted of MHD/MOD/MOD9D12D/MD5D/n-decane, which has 187 species and 982 reactions. The mechanism was validated against in-cylinder pressure and ignition delay time. Yuanqi Bai et al. [17] also proposed a new biodiesel surrogate that contained MD, methyl trans-3-hexanoate (MH3D), n-hexadecane (HXN), and 1, 4-hexadiene (HXD14) as saturated and unsaturated methyl esters in biodiesel surrogate. The four-component developed mechanism consisted of 98 species and 314 reactions which calculated ignition delay, laminar flame speed, soot, and in-cylinder pressure of the engine appropriately.

In this study Zhang et al [39] mechanism is selected as a primary biodiesel surrogate mechanism; due to its accuracy in NOx, soot, and ignition delay time prediction. So Drost natural gas mechanism and Zhang biodiesel surrogate mechanism are selected as low as high reactivity fuel respectively; and they are mixed and reduced by special methods to achieve a compact mechanism that can predict ignition delay, flame speed propagation, and combustion pressure in dual fuel or RCCI engine appropriately. In a closed homogenous reactor zero dimensional simulation, 54 conditions are adopted which consist of 6 conditions of temperature (800-1100 temperature), 3 conditions of pressure (30, 45, and 60 bar), and 3 conditions of equivalence ratio (0.25, 0.5 and 0.75). Also, simulation in 1-D Flame Simulator is carried out in 300 and 400 K temperature, 1, 10, and 20 bar pressure, and 0.5-1.5 equivalence ratio. For evaluation of the final mechanism results, which consist of 153 species and 727 reactions, in ignition delay and flame speed propagation, the developed mechanism with 0%-biodiesel content is compared with the Drost natural gas mechanism, on the other hand developed mechanism with 0%-NG content is comparing with Zhang biodiesel mechanism. The final comparison shows that the arithmetical mean error (AME) of results is in criteria and the use of a developed mechanism in CFD simulation has brought relatively accurate results.

2- Reduction methods

2-1- Elements of a Paper

The directed relation graph (DRG) method, by solving the connection of coupling of components, detects unimportant species in a reaction mechanism. Direct coupling of species is defined by an instantaneous error in the production rate of species A, which is introduced by eliminating another species, B, from the mechanism. An immediate error is shown as r_{AB} as follows:

$$r_{AB} = \sum_{i=1,I} \left|v_{A,i}\omega_i\delta_{Bi}\right| \Big/ \sum_{i=1,I} \left|v_{A,i}\omega_i\right| \qquad (1)$$

$$\delta_i = \begin{cases} 1 & ,if\ the\ ith\ reaction\ involves\ species\ B \\ 0 & ,otherwise \end{cases}$$

where, $v_{A,i}$ shows the stoichiometric coefficient of species A in the ith reaction and ω_i is ith reaction's rate.

In DRGEP, once species A is kept in the mechanism, all other species that are reachable

from species A through direct and indirect coupling are examined using their "R-value", which is defined as:

$$R_A(B) = max_S\{r_{ij}\} \quad (2)$$

If A is connected to B within a reaction and B is related to C through another reaction, there is a path which connect A to C via B and the relation value (R) of this path is rAB× rBC. Based on this definition, if there is at least one connecting path between A and B in the mechanism which it's R-value is larger than a defined threshold, species B must be kept in mechanism [39, 40].

2-2- Path Flux Analysis (PFA)

In DRG and DRGEP, just the first-hand products of the selected species are examined, but in the PFA method, both the first-hand products and the second-hand products or higher generations are important, and instead of using the absolute reaction rate, it is produced to be and consumption fluxes are used to identify important reaction pathways [41].

Consumption and Production fluxes of species A are calculated by equation 3:

$$P_A = \sum_{i=1,I} max(v_{A,i}\omega_i, 0)\,, C_A = \sum_{i=1,I} max(-v_{A,i}\omega_i, 0) \quad (3)$$

And the flux of species A which is related to species B can be shown as equation 4:

$$P_{AB} = \sum_{i=1,I} max(v_{A,i}\omega_i\delta_{Bi}, 0)\,, C_{AB} = \sum_{i=1,I} max(-v_{A,i}\omega_i\delta_{Bi}, 0) \quad (4)$$

Here, P_{AB} and C_{AB} indicates the amount of production and consumption of species A due to the presence of species B, respectively. The interaction coefficients for the production and consumption of species A through B from the first-hand products are:

$$r_{AB}^{pro-1st} = \frac{P_{AB}}{max(P_A, C_A)}, r_{AB}^{con-1st} = \frac{C_{AB}}{max(P_A, C_A)} \quad (5)$$

Using the production and consumption fluxes of first-hand products, the interaction coefficients, which are measures of the flux ratio between A and B through a third reactant (M_i) for second-hand products, are defined:

$$r_{AB}^{pro-2nd} = \sum_{M_i \neq A,B} \left(r_{AM_i}^{pro-1st} r_{M_iB}^{pro-1st}\right), r_{AB}^{con-2nd} = \sum_{M_i \neq A,B} \left(r_{AM_i}^{con-1st} r_{M_iB}^{con-1st}\right) \quad (6)$$

So the final total errors are shown as:

$$r_{AB} = r_{AB}^{pro-1st} + r_{AB}^{con-1st} + r_{AB}^{pro-2nd} + r_{AB}^{con-2nd} \quad (7)$$

2-3- Linear quasi-steady state approximation (LQSSA)

The LQSSA method is used when the reduced mechanism is used in a simulation. The system of equations used to solve for the concentrations of semi-stable species is usually coupled in a non-linear manner due to the presence of reactions that include more than one semi-stable reactant in their detailed/skeletal mechanism. Become A semi-stable species typically has a low concentration because its rate of creation is always balanced by the rate of self-destruction. This means that the collision frequency of two semi-stable species is completely insignificant, and the effects of semi-stable species in the concentration of the third body and other velocity correction terms are insignificant. Therefore, the reaction with more than one semi-stable reactant can control only non-important reaction pathways, and the species for which these pathways are the dominant formation pathway are probably not important for the production rate of the major species. Since these species are typically eliminated in a skeletal mechanism produced by the DRG method, the contribution of nonlinear terms related to semi-stable species for all remaining semi-stable species is small. As a result, the method (LQSSA) can be used to remove all non-linear terms including semi-steady species in the system of equations. This step makes solving the system of equations very easy. The quasi-steady state

approximation (QSSA) of a mechanism with the number of irreversible initial reactions I and species K (steady state species M among them) can be expressed in algebraic equations as equation 8 [41]:

$$w_{C,i} = w_{D,i}\ i = 1,2,\dots,M, w_{C,i} = \sum_{j=1,I}\left(v''_{i,j}Q_j\right), w_{D,i} = \sum_{j=1,I}\left(v'_{i,j}Q_j\right) \quad (8)$$

where the subscripts i and j represent semi-stable species and reaction j respectively. By using the LQSSA method, it is possible to remove all nonlinear terms related to semi-stable species in the system of equations and obtain a set of linear equations for semi-stable species [41].

$$\sum_{k\neq i} C_{ik}x_k + C_{i0} = D_i x_i \qquad i = 1,2,\dots,M \quad (9)$$

where x_i is the concentration of the ith semi-stable species:

$$D_i = \frac{w_{D,i}}{x_i}C_{ik} = \sum_{j=1,I}\frac{v''_{i,j}Q_j sign\left(v'_{k,j}\right)}{x_k},$$
$$sign(v'_{k,j}) = \begin{cases} 1 & v'_{k,j} > 0 \\ 0 & v'_{k,j} = 0 \end{cases} C_{i0} = \sum_{j=1,I} v''_{i,j}Q_j\delta_j, \delta_j \quad (10)$$
$$= \begin{cases} 1 & if\ reaction\ j\ has\ no\ QSS\ reactant \\ 0 & otherwise \end{cases}$$

where D_i, $C_{ik}$and C_{i0} are independent of the concentration of semi-stable species.

3- Mechanism development strategy

As it was mentioned, to develop a biodiesel-natural gas blend mechanism, the first step is coupling the mechanisms which leads to eliminating some similar species and reactions. In the coupling procedure, the main and donor mechanism selection is Zhang and Drost respectively. In the development procedure, two reactors are used, 0-D closed homogenous and 1-D flame simulator reactors. The conditions which are adopted in reactors are achieved from the real condition of dual or RCCI engines. As an experimental work which is performed in this study, 54 conditions is adopted into the 0-D reactor; which is consisted of 6 conditions of temperature (800-1100 temperature), 3 conditions of pressure (30, 45, and 60 bar), and 3 conditions of equivalence ratio (0.25, 0.5 and 0.75). Also, simulation in 1-D Flame Simulator is carried out in 300 and 400 K temperature, 1, 10, and 20 bar pressure, and 0.5-1.5 equivalence ratio.

The first step after merging NG and biodiesel mechanisms is the determination of the ignition delay time of the merged mechanism in 0%-NG and 0%-biodiesel situations as same as pure one's temperature, pressure, and equivalence conditions. As it was announced in previous research [42], the AME of ignition delay time results is not allowed to exceed 20% in comparison with pure one. So to reduce the AME of ignition delay result, first, the important and effective reactions should be recognized. This demand is made through sensitivity analysis in the merged mechanism. The sensitivity analysis is performed by considering MD, MD9D, n-heptane, CH4, C2H6, and C3H8 as output variables. Table 1 shows the effectiveness of reactions in ignition delay calculation which is obtained by sensitivity analysis.

In the following, Figure 1 also shows the effect of each reaction on ignition delay parameter. According to Figure 1, at different temperatures and under the same conditions of pressure and equivalence ratio, the normalized sensitivity of each reaction to the ignition delay is observed. It should be mentioned that the normalized sensitivity of reaction is defined as equation 11, in which, nS_i is defined as normalized sensitivity, $|S_i|$ and $\bar{S}_i$ is represented size of vector of sensitivity and sensitivity of ith reaction respectively.

$$nS_i = \frac{\bar{S}_i}{|S_i|} \tag{11}$$

Table 1 Key sensitive reactions in biodiesel/NG mechanism

Reaction	Reactions	Arrhenius factors		
		A	b	E_a
G9	$H_2O_2(+M) \leftrightarrow 2OH(+M)$	2.00E12	0.90	4.87E04
G13	$H_2O_2 + OH \leftrightarrow H_2O + HO_2$	1.74E12	0.00	318.0
G30	$\text{left} - \text{right}CH_4 + OH \leftrightarrow CH_3 + H_3O$	5.83E04	2.60	2190.0
G33	$CH_3 + HO_2 \leftrightarrow CH_4 + O_2$	1.16E05	2.23	-3022.0
G162	$C_2H_4 + OH \leftrightarrow C_2H_3 + H_3O$	2.23E04	2.74	-2215.5
G443	$MD + OH \leftrightarrow MD2J + H_3O$	1.14E11	0.51	63.00
G630	$MD9D \leftrightarrow Ms7J + C_3H_5 - a$	2.50E16	0.00	3.10E04
G709	$nC_7H_{16} + HO_2 \leftrightarrow nC_7H_{15} + H_2O_2$	1.68E13	0.00	2.04E04

At low and high temperatures, the G9 equation has a huge effect on ignition delay time due to OH radicals. Although the reactions which hhavehigher activation energy (E_a), such as: (G9, G30, G33 and G443), have higher resistance against ignition in the mechanism. In fact, the highest sensitivity of this reaction is due to the forward and backward reaction rate coefficient which is calculated against the Arrhenius equation as expressed in equation 12.

$$k = A\,exp\left[-\left(\frac{E_a}{RT}\right)^b\right] \tag{12}$$

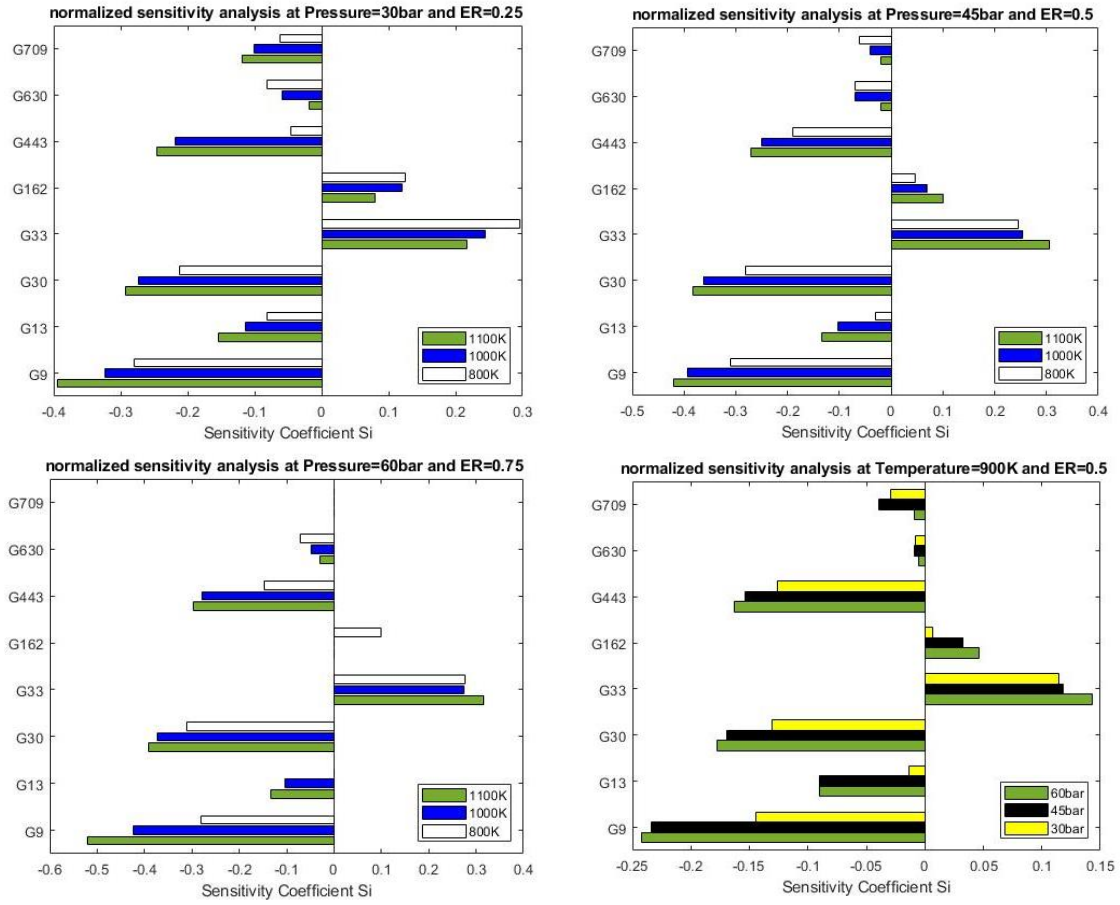

Figure 1 Normalized sensitivity analysis in merged mechanism at different conditions

As it was mentioned before, after recognizing the effectiveness of reactions in ignition delay time prediction of mechanism, this reaction should be tuned correctly. To achieve to lowest AME in the ignition delay time parameter as it is possible, the ID of 0%NG and 0% biodiesel of merged mechanism in 0-D homogeneous reactor should be verified by pure ones in Zhang and Drost mechanism respectively. For this purpose, the most sensitive reactions are tuned in the Pre-Exponential Factor as in Table 2.

Table 2 Tuning of the Pre-Exponential Factor of the most sensitive reactions in ignition delay time prediction

Reaction	Reactions	Pre-Exponential Factor	
		Previous	Tuned
G9	$H_2O_2(+M) \leftrightarrow 2OH(+M)$	2.00E12	2.00E11
G30	$CH_4 + OH \leftrightarrow CH_3 + H_3O$	5.83E04	6.00E05
G33	$CH_3 + HO_2 \leftrightarrow CH_4 + O_2$	1.16E05	5.00E04
G443	$MD + OH \leftrightarrow MD2J + H_3O$	1.14E11	5.00E10

In this step, the AME of ignition delay time of 0%NG and 0% Biodiesel is calculated at 10.21% and 10. 54% respectively. Also, the merged tuned mechanism consists of 193 species and 871 reactions, which size seems a bit large for CFD calculations. So continuous reduction methods are employed to reduce the size of the tuned merged mechanism.

The reduction process is performed in Chemkin Pro with the same conditions as sensitive analysis. So in 54 conditions, the percentages of NG/Biodiesel mixture are defined as 12.5% MD, 12.5% MD9D, 25% n-Heptane, 45% CH4, 4.5% C2H6, and 0.5% C3H8.

In the first step of reduction, the DRGEP method is employed and reduces the merged mechanism into 176 species and 802 reactions. The species and parameters which are chosen as a target in this reduction is CH4, C2H6, C3H8, MD, MD9D, n-C7H16, CO, NO and ignition time; whose tolerance is Defined as 10%. In continuation, the Path Flux Analysis (PFA) and LQSSA methods are used with the same targets and tolerances, so the final mechanism has been reduced to 153 species and 727 reactions. The achieved mechanism parameters should be verified to ensure the reduction process were done well. Figure 2 shows the development process in a flowchart.

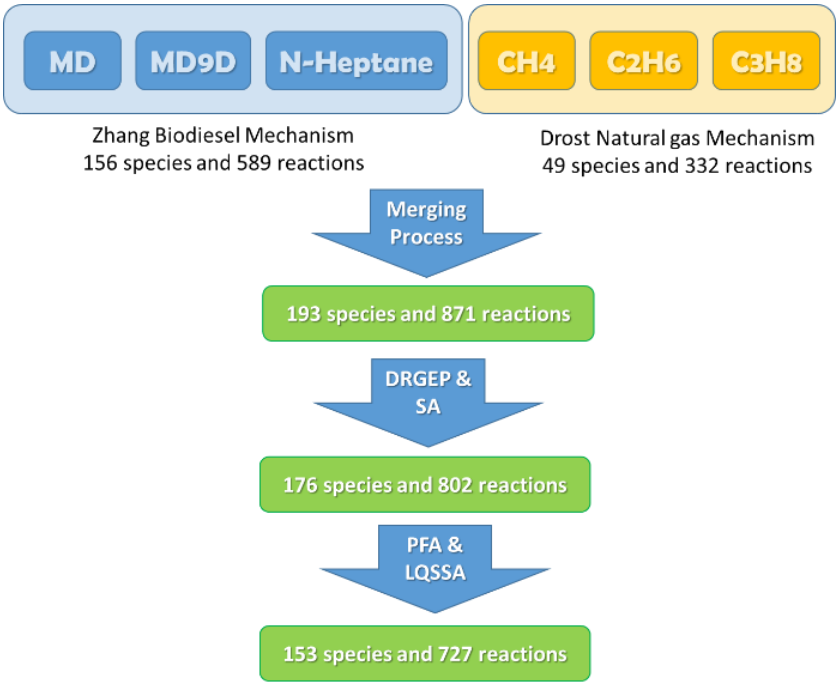

Figure 2 Reduction and development process flowchart

4- Mechanism Results and validation

To ensure that the reduced mechanism is reliable and suitable for use in CFD simulations, various parameters such as ignition delay time, flame propagation speed, and internal combustion engine cylinder pressure have been investigated; In such a way that the ignition delay time and flame propagation speed for the fuel mixture in the state of 0% natural gas and 0% biodiesel is compared with pure biodiesel fuel and natural gas, respectively.

4-1- Ignition delay time

The 0-Dimension reactor is used to calculate ignition delay (ID) time of mixture and pure fuels which is chosen as a closed homogenous batch reactor in Chemkin Pro. Figure 3 illustrates ID for natural gas and biodiesel in mixture situations and pure ones. As can be seen in Figure 3 on the right, the mechanism developed for the equivalence ratio of 0.25 is not able to predict the ignition delay time due to a very low equivalence ratio. Of course, it is important to mention that in this research, since the goal of developing the mechanism for temperatures of 800-1100 in equivalence ratios below 1, the reaction coefficients have been adjusted according to the stated conditions. As can be seen in Figure 3-4, there is an appropriate agreement between the developed mechanism and base mechanisms in the same condition in ignition delay time. The whole AME of ignition delay time of 0%NG and 0% Biodiesel is calculated at 10.77% and 11. 2% concerning Zhang and Drost mechanisms respectively.

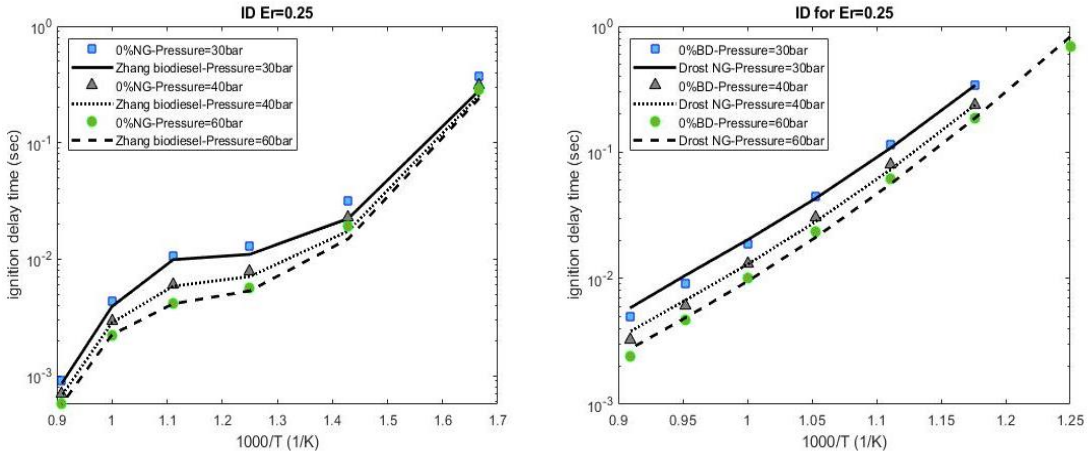

Figure 3 ignition delay (ID) time for 0%NG & pure biodiesel (BD) (left) and 0%BD & pure NG (right) @ Pressure = (30-60), Temperature= (800-1100) and Equivalence ratio= 0.25

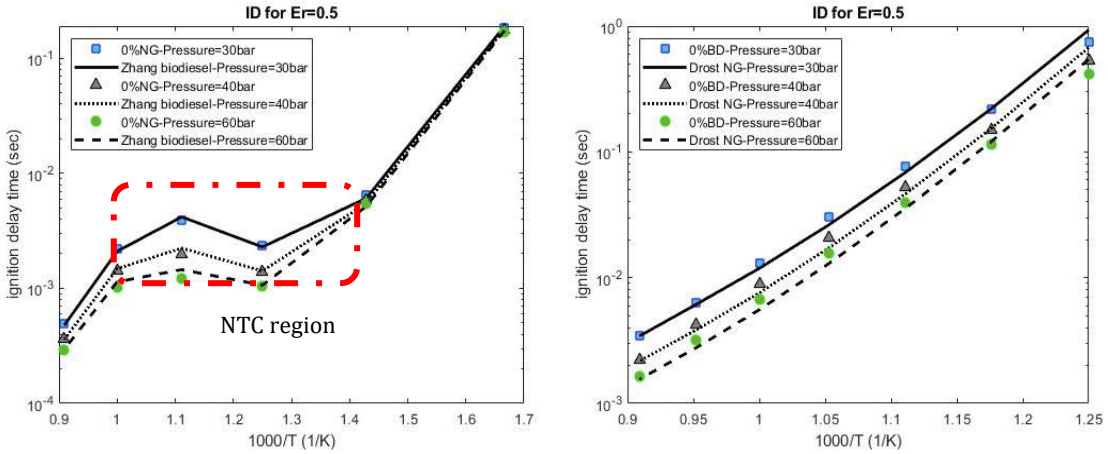

Figure 4 ignition delay (ID) time for 0%NG & pure biodiesel (BD) (left) and 0%BD & pure NG (right) @ Pressure = (30-60), Temperature= (800-1100) and Equivalence ratio= 0.5

According to Figure 3-5, it can be seen that in constant equivalence ratio and temperature, an increase in pressure will lead to a decrease in the ignition delay time. Also in the same pressure and temperature, increasing in equivalence ratio will lead to a decrease in ignition delay time.

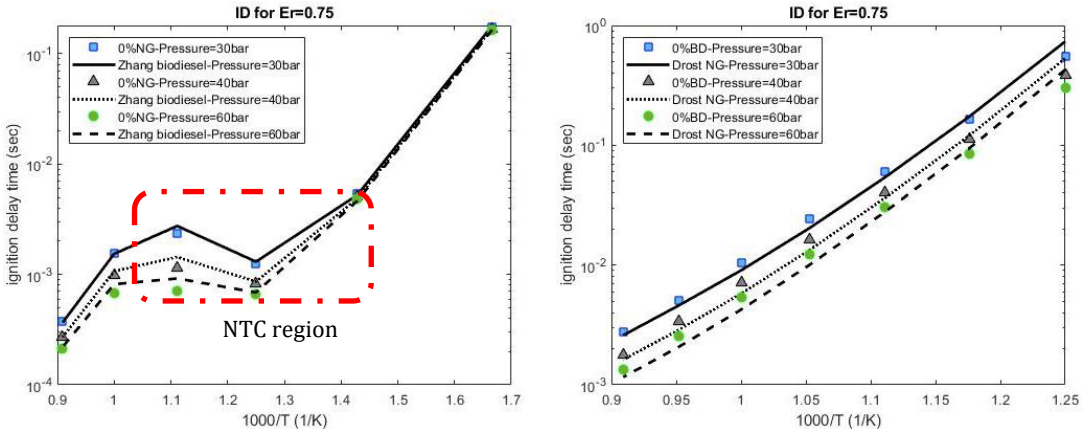

Figure 5 ignition delay (ID) time for 0%NG & pure biodiesel (BD) (left) and 0%BD & pure NG (right) @ Pressure = (30-60), Temperature = (800-1100) and Equivalence ratio = 0.75

Equation 13 shows ignition delay correlation which can confirm the mentioned behavior [43, 44] :

$$\tau = Ap^{-n}\phi^{-m}\, exp\left(\frac{B}{T}\right) \tag{13}$$

As can be seen, pressure and equivalence ratio have an inverse relationship with ignition delay time. However, there is a region in the biodiesel fuel ignition delay graph (Figure 4-5 left side), which shows that the increasing trend of the ignition delay with the decrease in temperature has experienced ups and downs. The negative Temperature Coefficient (NTC) region shows this behavior by itself. The reason for this phenomenon can be found in large hydrocarbons oxidation. Where carbon chains react in 3 temperature stages: low-, intermediate- and high-temperature reactions.

At low temperatures, the main branch's path is controlled by the addition of O_2 to the main chain of hydrocarbon to oxygenated compounds production, which decompose into branched products, finally. The low-temperature branching path is less significant at the intermediate stage, as the temperature is not yet high enough to promote the high-temperature branching reactions. So a decrease in the reactivity of the mixture will occur, which is known as the NTC range. In last, the high-temperature branch dominates and auto-ignition occurs [45].

4-2- Flame propagation speed

The flame propagation speed is another parameter that is used for the validation and accuracy of the developed mechanisms. This item should be calculated in the 1-dimension reactor which in Chemkin Pro is set as Premixed Laminar Flame Speed Propagation. In this reactor, initial pressure is set as 1, 10, and 20 bar, and the equivalence ratio is assumed as 0.25, 0.5, and 0.75; also the initial temperature is set as 300 and 400 K. inlet velocity and reactor length is set as 40 cm/s and 30 cm, respectively. Again, the simulation is defined for both NG and BD in the base mechanism and 0%BD and 0%NG in the developed mechanism.

According to Figure 6, it can be seen with a little precision that at a constant temperature, in the same equivalence ratio, with an increase in pressure, the flame speed increases. Also, at constant temperature and pressure, with the increase of the equivalence ratio, the flame speed first increases and then decreases so that the maximum speed occurs in the range of the

equivalence ratio of 1 to 1.2. In this condition, with increasing pressure, the maximum speed tends to the equivalence ratio of 1. Also, at constant equilibrium pressure and ratio, increasing the temperature will increase the flame growth rate.

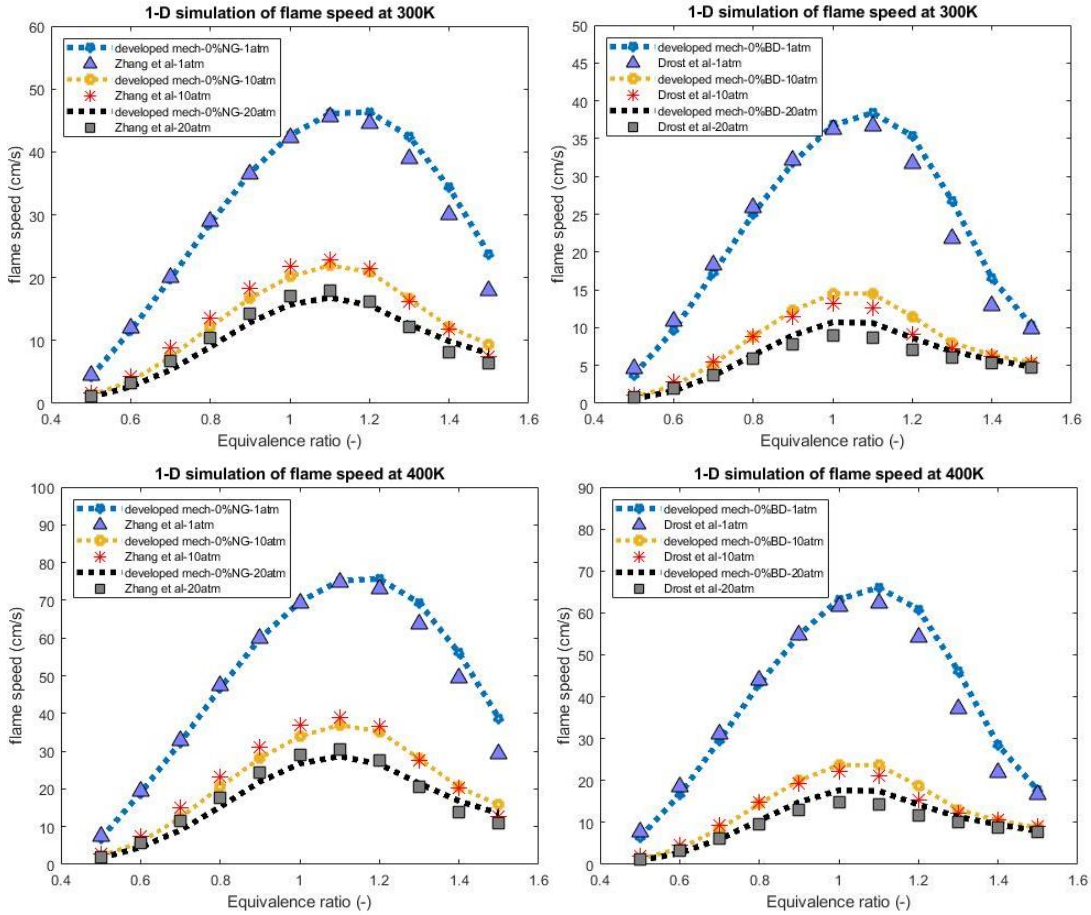

Figure 6 Laminar flame speed comparison between developed Biodiesel/NG mechanism and Drost NG (right) and Zhang biodiesel (left) mechanisms at 300-400 K initial condition.

Also, by referring to equation 14, the effect of each of the mentioned conditions can be found in the laminar flame speed [46]:

$$S_L = \frac{1}{\rho}\left(\frac{\lambda}{c_p}\omega\right)^{\frac{1}{2}} \tag{14}$$

It is obvious that temperature affects the reaction rate; as the temperature increases, the reaction rate increases [47]. So the increases in temperature cause flame speed growth. Also, ρ and omega are pressure depended on the parameter, so expected that the laminar flame speed varies with changes in pressure [46].

The whole AME of flame speed calculation in this simulation is about 7% for 0% biodiesel and 8.3% or 0% natural gas, which is an appropriate error for a developed mechanism to estimate flame speed.

4-3- Validation with real engine condition

To emphasize on accuracy of the developed mechanism, reactivity-controlled compression ignition (RCCI) simulation has been done on a Ricard single-cylinder engine with pre-chamber with the specifications of Table 3 using natural gas/biodiesel fuel and its results have been validated with similar experimental results. The experimental data

was cached with a developed test setup by Ghareghani et al [21, 48]. The main purpose of using the experimental test data is to validate CFD simulated in-cylinder pressure by using a developed mechanism at the same condition. Because of the existence of the pre-chamber with a special geometry, half of the combustion chamber has been considered for simulation and it has been properly meshed in the TDC Position in Figure 7.

Table 3 Ricardo Engine specifications

Parameter	Specification	Parameter	Specification
Engine type	Single cylinder	IVC (CA)	36 ABDC
Bore (mm)	76.2	IVO (CA)	7 BTDC
Stroke (mm)	110	EVC (CA)	7 ATDC
Displacement (CC)	507	EVO (CA)	36 BBDC
Compression ratio	17:1	Engine Speed	3000 rpm

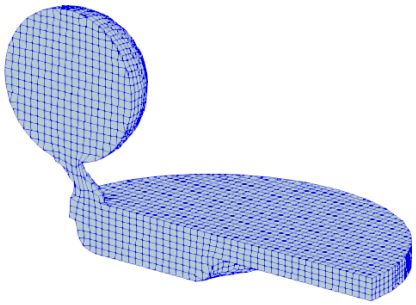

Figure 7 Computational grid for CFD simulation

According to experimental data, in 50% load of Ricardo engine, initial temperature, and pressure are considered as 355 K and 2.3 bar at 60 BTDC. Simulation is started from 60 BTDC to 40 ATDC. In this situation, the Mole fraction of species in the initial condition is calculated and is described in Table 4. Figure 8 shows the temperature contour and streamline of the combustion chamber in mid-plane. As can be seen, the combustion seed is formed in the pre-chamber and then starts growing from this area to other areas. Figure 9 also shows the values of the pressure inside the cylinder and the heat release rate in the combustion interval. According to Figure 9-10, the developed mechanism can predict the ignition process accurately.

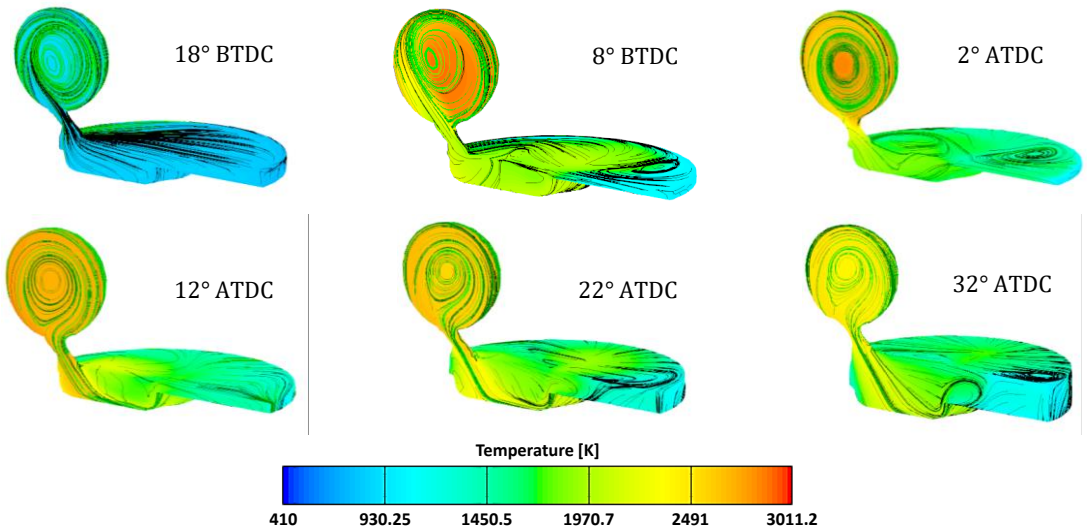

Figure 8 Temperature contour and streamline of half of the combustion chamber at 50% load in RCCI mode of Ricardo engine with NG/BD.

Table 4 Mole fraction of species in CFD simulation

Species	Mole fraction	Species	Mole fraction
O_2	0.15084	C_3H_8	0.00160
N_2	0.56722	C_7H_{16}	0.05988
CH_4	0.14613	MD9D	0.02994
C_2H_6	0.01445	MD	0.02994

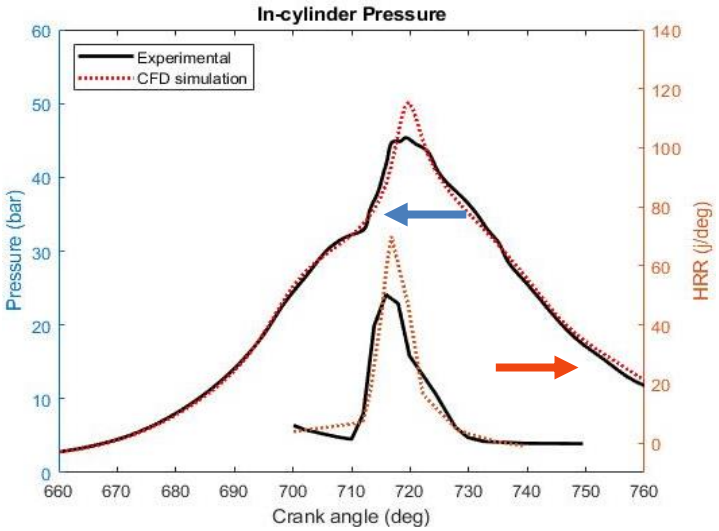

Figure 9 in-cylinder pressure and heat release rate per crank angle at 50% load in RCCI NG/BD Ricardo engine [21]

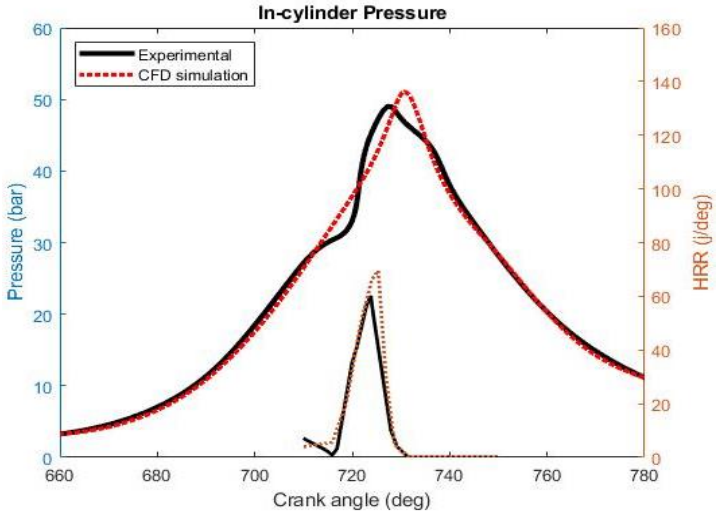

Figure 10 in-cylinder pressure and heat release rate per crank angle at 100% load in RCCI NG/BD Ricardo engine [21]

5- Conclusion

Considering the advantages of fuels such as natural gas and biodiesel, their use in developed engines can cause increasing growth in the environmental, economic, and technical fields. Therefore, according to the experimental activities carried out in the use of biodiesel/natural gas mixture, the continued growth in this field depends on the use of numerical simulations that provide researchers with more information about the combustion parameters. In this regard, in this research, an attempt has been made to provide an accurate mechanism of the natural gas/biodiesel blend using the most up-to-date chemical mechanisms for biodiesel and natural gas and using it in CFD simulations.

For this purpose, Drost's mechanism with 49 species and 332 reactions has been used for natural gas which is considered as 90% CH4, 9% C2H6, and 1% C3H8. The mechanism used for biodiesel is Zhang's mechanism with 156 components and 586 reactions which is considered as 25% MD, 25% MD9D and 50% n-Heptane. Finally, the developed mechanism with 153 components and 727 reactions has been obtained. The process of mechanism development consists of different sections such as merging master and donor mechanisms, sensitivity analysis, reaction rate adjustment, and reduction by special methods (DRG, DRGEP, path flux analysis, QSSA). Comparing ignition delay times of based and developed mechanisms revealed that arithmetical mean error (AME) is 10.77% for 0%-NG and 11.2% for 0%-biodiesel, respectively. In the 1-D simulation, flame speed is calculated and the AME for 0%-biodiesel and 0%-NG is 7% and 8.3%, respectively. To ensure the applicability and accuracy of the developed mechanism, this mechanism was used in the CFD of an RCCI engine and the obtained results such as in-cylinder pressure and the heat release rate, were in appropriate agreement with the experimental results.

It is worth mentioning once again the valuable results obtained from this research as follows:

- Developed mechanism can accurately predict NTC region in ignition delay Biodiesel, which occurs in mid-temperature.
- According to natural gas ignition delay, the developed mechanism can predict non-linear logarithmic data as well as the Drost mechanism in temperatures 800-1100
- According to laminar flame speed propagation, the maximum flame speed occurs in an equivalence ratio of 1-1.2 and as the temperature increases, the maximum speed point moves away from the equivalence ratio of 1.
- According to laminar flame speed propagation, by increasing pressure the maximum speed point tends to equivalence ratio 1.

List of Symbols

ith reaction's rate	ω_i
amount of production of species	P
amount of consumption of species	C
third reactant	M_i
Rate of Destruction	w_D
rate of creation	w_C
stoichiometric coefficients of the reactants	v', v''
Concentration	x
Activation energy	E_a
defined as the mass fuel/air ratio concerning the stoichiometric ratio	φ
temperature	T
Pressure	P
Adjustment coefficient	$A, n, m \; and \; B$
Laminar flame speed	S_L
Density	ρ
Thermal conductivity	λ

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مقاله پژوهشی

توسعهٔ سازوکار سینتیک شیمیایی جدید برای احتراق مخلوط سوخت زیست‌دیزل و گاز طبیعی

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اطلاعات مقاله

کلیدواژه‌ها:
سازوکار جنبشی شیمیایی
زیست‌دیزل
گاز طبیعی
تأخیر در اشتعال
سرعت شعله

چکیده

استفاده از گاز طبیعی-زیست‌دیزل در موتورهای احتراق سرد، با توجه به ویژگی‌های این دو سوخت، اخیراً مورد توجه محافل علمی احتراقی قرار گرفته است. فراوانی، قیمت کم و احتراق پاک گاز طبیعی و همچنین تجدیدپذیر بودن زیست‌دیزل از عوامل گرایش به این دو نوع سوخت در دنیاست. در این راستا آزمایش‌های تجربی مختلفی صورت پذیرفته است و در برای توسعه هرچه بیشتر نیازمند استفاده از شبیه‌سازی‌های عددی خواهد بود. مشکل اصلی در این مسیر، فقدان سازوکار احتراق زیست‌دیزل-گاز طبیعی است. در این راستا، یک سازوکار دقیق شامل ۱۵۳ گونه و ۷۲۷ واکنش، ارائه شده است. برای گاز طبیعی، سازوکار Drost با ۴۹ گونه و ۳۳۲ واکنش، با ترکیب گاز طبیعی با ۹۰٪ CH4، ۹٪ C2H6 و ۱٪ C3H8 در نظر گرفته شده است. برای زیست‌دیزل از سازوکار Zhang با ۱۵۶ گونه و ۵۸۹ واکنش استفاده شده است که ترکیبات آن شامل ۲۵٪ MD، ۲۵٪ MD9D و ۵۰٪ n-هپتان است. فرآیند توسعهٔ سازوکار با روش های DRG، DRGEP، تحلیل شار مسیر، تحلیل حساسیت و QSSA صورت پذیرفته است. در بحث صحه‌سنجی نیز، مقایسه زمان‌های تأخیر احتراق سازوکارهای اصلی و توسعه‌یافته نشان می دهد که خطای میانگین محاسباتی (AME) بترتیب ۱۰,۷۷٪ برای ۰٪ – NG و ۱۱,۲٪ برای ۰٪ زیست‌دیزل است. همچنین AME سرعت شعله برای ۰٪ زیست‌دیزل و ۰٪ NG به ترتیب ۷٪ و ۸,۳٪ محاسبه شده است. برای اطمینان بیشتر، از سازوکار توسعه یافته در شبیه‌سازی CFD یک موتور RCCI استفاده شده و نتایج قابل قبولی بدست آمده است.

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