A Numerical Simulation Determining Optimal Ignition Timing Advance of SI Engines Using 2.5-Dimethylfuran-Gasoline Blends

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Abstract—Today, humans are facing two urgent issues: energy security and environmental pollution. Finding sources to replace traditional fuels such as gasoline and diesel that are not outside their interest. Lignocellulose biomass can be obtained a variety of basic chemicals or intermediates that generate energy, such as ethanol, butanol, and dimethylfuran. 2.5-dimethylfuran (DMF) is considered a potential alternative fuel because it is a water-insoluble substance used as an additive mixed with gasoline fuel. Formerly, there have been many studies on engines’ combustion and emissions properties using the DMF-gasoline blend, especially SI engines. However, there has been no published research about the optimal ignition timing advance of SI engines when using these blends. This paper present how to determine the optimal ignition timing advance of SI engines using DMF-gasoline blends with AVL-Boost simulation software. The simulation conditions were set up at 50% load, and speed at 2500 and 3000 rpm using blends are DMF20, DMF30, and DMF40 (corresponding with the DMF ratio in DMF-gasoline blends is 20%, 30%, and 40% in volume). The simulation result shows that the optimal ignition timing advance of SI engines using DMF-gasoline blends at speed 2500 and 3500 rpm corresponding with 23 and 31 crank angle degrees (CAD) (reduce 2CAD compare to when using pure gasoline). At these optimal ignition timing advances, the engine’s power, torque, and thermal efficiency (BTE) reach its maximum value, while the fuel consumption rate is also the lowest.

Keywords—2.5-dimethylfuran (DMF); SI engine; biomass; ignition timing advance.

I. INTRODUCTION

To achieve the targets of reducing environmental pollution, diversifying fuel sources, and at the same time utilizing agricultural residues to produce renewable energy sources, the researchers concentrating on three main directions. The first direction is replacing internal combustion engines with other energy sources (such as hydrogen [1], [2]. The second direction is applying new technology on traditional engines to improve fuel consumption and reduce emissions [3]–[6]. The third direction is using biofuels (renewable fuels [7]) to partially or entirely replace traditional fossil fuels [8]–[10].

According to the third research direction, lignocellulose from biomass is a rich source of raw materials, suitable for production on an industrial scale to become an alternative energy source for traditional fuels [11]. We can obtain a range of basic chemicals or intermediates from lignocellulose, such as ethanol, butanol, lactone, or methyl furan, and dimethylfuran. Among them, 2.5-dimethylfuran (the second generation of biofuel), usually known as DMF, is considered as the potentially gasoline-alternative fuel [12-14]. Currently, DMF research works mainly in manufacturing. There are very few articles mentioning the burning process of DMF in engines, especially SI engines [15-17]. Chongming Wang et al. published a study on the comparison of combustion characteristics and emissions of some fuels using in a DISI engine: MF, DMF, ethanol and gasoline [18]. In this paper, the authors concluded that the MF's anti-knocking capabilities are like those of the DMF, and both fuels are better than gasoline in anti-knocking. On the other side, although the chemical structures of MF and DMF are quite similar, their combustion characteristics differ significantly. The comparison between dual-injection and direct-injection in the SI engine when using DMF-gasoline blends was conducted by Ritchie Daniel et al [19].
The test results show that the dual-injection has many advantages compared to traditional fuel injection methods. In DISI (Dual-injection Spark-ignition), the mixture's preparation is improved, so that the combustion duration is lower and the in-cylinder pressure is higher. On the other hand, the DISI increases the indicated thermal efficiency (up to 4%) and reduces the fuel consumption rate (up to 3.2%) compared with the same D25 mixture in DI. In addition, the DISI method results in 1.2% lower fuel consumption than when using pure gasoline in DI, even though the DMF has a lower energy density than gasoline. At another project, Ritchie Daniel et al. published a study on spark timing and load when using DMF on a DISI engine compared to gasoline and ethanol [20]. The test results showed that the combustion and emissions of DMF were better than gasoline and surpassed ethanol in some cases. The burning rate of DMF and ethanol was higher than gasoline, and the initial combustion duration was lower. The combustion efficiency of DMF and ethanol was better than gasoline, so that it led to the emissions of HC and CO were lower. The study about the combustion and emissions of DMF in a DISI engine was also presented by Shaohua Zhong et al [21]. The above research results all show that DMF is a new potential fuel and can replace gasoline in the future [22].

Among the studies mentioned above, very few works mention determining the optimal ignition timing advance of the engine [19], [20]. Ignition timing advance is defined as the ignition timing of until TDC (top dead center); it significantly affects the combustion process's timeliness. In case that the ignition timing advance is smaller than the optimal ignition timing advance. It means that the spark is too early, so the mixture is ignited before the internal combustion engine. It is causing the pressure in the cylinder to rise too early and increases the maximum pressure when burning. Thus, increasing the power consumption of combustion and reducing the area of the P-V diagram. At the same time, due to ignition too early, the mixture's temperature at the end of the fire membrane increases, thereby increasing the knock of the engine [25]. In contrast, when the ignition is too late, the mixture's combustion is prolonged to the expansion process. The highest pressure and temperature have decreased, which reduces the P-V diagram area and reduces engine power [26]. Simultaneously, by extending the burning time, it increases the heat loss passing through the cylinder wall, increasing the exhaust temperature, thereby reducing engine efficiency. When the ignition angle advance reaches the appropriate value, the highest burning pressure and temperature appear after TDC in the range of 10 CAD to 15 CAD; the combustion process is relatively timely, the heat is well utilized, so the areas of the P-V diagram is the largest, engine power and performance are highest. At that time, the pressure increasing rate and the maximum pressure when burning were not too great. The ignition timing advance corresponding to the highest power and efficiency is called the optimum ignition timing advance [27], [28].

This paper presents how to determine the optimal ignition timing advance of the engine when using DMF-gasoline blends in a four-cylinder SI engine using AVL-Boost simulation. The simulation conditions were set up at 50% load, and speed at 2500 rpm and 3500 rpm with the using blends is DMF20, DMF30, and DMF40 (corresponding with the DMF ratio in DMF-gasoline blends is 20%, 30%, and 40%). In the following sections, the process of developing the research engine model on AVL-Boost software, the installation of simulation parameters, and the results are discussed.

II. MATERIAL AND METHOD

A. Fuel Used in the Simulation

The fuel is used to mix with RON95 gasoline to become a mixture used in the simulation is DMF. The chemical formula of DMF is C₅H₇O. DMF is a yellow, viscous, oily liquid with an odor of caustic soda. DMF is flammable and may be sensitive to air (but not strong), insoluble in water. Reaction: DMF can react very strongly with oxidants, but they hardly react with strong acids and bases. Besides, the viscosity of DMF and gasoline is similar; this is more favorable for the setting of DMF injection pressure in the fuel system. At the same time, it also protects the moving parts in the engine's fuel system.

The energy density of DMF is lower than gasoline and diesel but higher than ethanol. Hence, using DMF as fuel for a gasoline or diesel engine requires a higher fuel consumption to achieve the same engine efficiency. This results in the engine's fuel system having to operate at a higher intensity. The physicochemical properties of DMF compared to gasoline RON95 are given in Table I.

### TABLE I

| Properties                  | Gasoline | DMF   |
|-----------------------------|----------|-------|
| Molecular formula           | C₅H₇O   | C₅H₇O |
| Molecular mass (kg/mol)     | 100-105  | 96.13 |
| Density @20 °C (kg/m³)      | 744.6    | 889.7 |
| Water solubility @ 25 °C (mg/ml) | Insoluble | Insoluble ³ ≤ 1.47 |
| H/C ratio                   | 1.795    | 1.33  |
| O/C ratio                   | 0.00     | 0.1667|
| Gravimetric oxygen content (%) | 0       | 16.67 |
| Stoichiometric air-fuel ratio | 14.56   | 10.72 |
| Gravimetric calorific value (MJ/kg) | 42.9 | 32.89 |
| Volumetric calorific value (MJ/l) | 31.9 | 30    |
| Octane rating               | 95       | 119   |
| Autoignition temperature (°C) | 257     | 285.85|
| Latent heat of vaporization @ 20°C (kJ/mol) | 38.51 | 31.91 |
| Boiling point (°C)          | 32.8     | 92    |
| Flash point (°C)            | -40      | 0-1   |

B. Simulation Engine

This article's simulation engine is 1NZ-FE, which is used on Toyota Vios; this is a spark-ignition engine with 4 cylinders in line. The main parameters of the engine in Table II.

### TABLE II

| Engine code | 1NZ-FE ENGINE PARAMETERS |
|-------------|--------------------------|
| Layout      | Four-stroke, Inline-4    |
| Fuel type   | Gasoline                 |
| Displacement| 1.5 L, 1,497 cm³ (91.35 cu in) |
| Fuel system | Electronic Fuel Injection (EFI) |
| Power output| 110 PS (81 KW; 109 HP) at 6,000 rpm |
| Torque output | 143 Nm (14.6 kg·m; 105.6 ft·lb) at 4,000 rpm |
|---------------|--------------------------------------------|
| Firing order  | 1-3-4-2                                    |
| Weight        | 87 kg (191.2 lbs)                           |

**C. Simulation Model**

To create the engine simulation model, these steps are the following: (1) Select the elements to use in the model corresponding to the engine's actual details. (2) Connecting elements with pipe elements. (3) Setup the specifications required for the elements. (4) Set appropriate boundary conditions for each element.

The main elements in the model include Engine (E1), Cylinder (C1-C4), Air Cleaner, Injector (J1-J11), Plenum (PL1, PL2); Restriction elements (R1-R12), Pipes, System boundary (SB, SB2) (as shown in Fig. 1). Alternatively, we can put the measuring point elements (MP1-MP11) on the pipes to measure the parameters.

For the simulation process to be accurate, the engine structure needs to be examined carefully, thereby reasonable to connect the elements in the model together. Simultaneously, the diameter and length of each connecting pipe of the rear motor must be measured exactly to put into the simulation model. There are lots of connecting points, branching points, or small-designed pipe positions to speed up the air intake or to fasten the exhaust gas on the entire pipeline. So, we need to put the appropriate resistance elements at these positions.

**D. Simulation Modes**

Simulation modes of 1 NZ-FE engine using DMF-gasoline blend with ratios varying from 20-40% in volume at 50% load, and speed at 2500 and 3500 rpm helps us to determine the optimal ignition timing advance of the 1NZ-FE engine when using this blended. After adjusting and validating the correctness of the model, we run the simulation engine mode in 50% load, and the speed at 2500 and 3500 rpm, with fuel used, are DMF20, DMF30, DMF40 corresponding to 10%, 20%, 30%, 40% of DMF volume in a blend with conventional RON95 gasoline. Because the physical and chemical properties of DMF differ from gasoline in some respects (e.g. vapor pressure, distillation, etc.), mixing DMF with gasoline can alter the mixture's overall physical and chemical properties. Blending DMF into gasoline reduces the vapor pressure and density but also increases the viscosity of the mixture. DMF is also used to increase the octane index of the mixture, but its effect on distillation temperature and the separation of water from the air may not be considered.

**III. RESULTS AND DISCUSSION**

**A. Simulation results at the Speed 2500rpm**

Simulation is conducted under controlled conditions, but it may not be appropriate when applied to an engine because of its local temperature and pressure change periodically. Therefore, it is important to analyze the combustion characteristics and engine performances in different ignition timing parameters. From the simulation results, the power diagram of the simulation engine is shown in Fig. 2.

From the diagram in Fig. 2, it is noted that the power of the engine changes when we change the ignition timing advance. The engine power when using RON95 gasoline reaches a maximum when the ignition timing advance is 25 CAD, while when using the DMF20, DMF30 and DMF40 fuel blends, the maximum power at the ignition timing advance is 23 CAD, reduce 2 CAD. With this ignition timing advance value at 23 CAD, the engine's power reaches 14.45 kW with gasoline, and when using the fuel blend, the power was reduced by 2.4%, 2.9%, and 5.1% respectively with DMF20, DMF30, and DMF40. At the other ignition angle values as far as the 23 CAD, the power and torque tend to decrease. Indeed, gasoline has the highest calorific value so its maximum power is the largest. As the A/F ratio of the alternative fuel decreases with increasing the blended DMF ratio in the mixture with RON95, the amount of fuel being fed into the combustion chamber for an increased work cycle, engine power is almost equivalent to when using RON95. As a result, this leads to an increase in specific fuel consumption. Moreover, according to Table 1, the energy density of DMF is lower than that of gasoline. The energy density of gasoline is about 31.5 MJ/L, while DMF's energy density is about 30 MJ/L. Additionally, to produce the same power, the required specific fuel consumption is inversely proportional to fuel's calorific value.

The results showed that to provide an amount of energy equivalent to 1 liter of gasoline, 1.073 liters of DMF are required. Because the air/fuel ratio of different fuels is not
the same, the throttle position's proximity must be adjusted to ensure the air excess coefficient \( \lambda = 1 \) at different loads. As the throttle increases, the amount of fuel through the intake increases and the amount of fuel needed to maintain the air excess coefficient \( \lambda = 1 \) also increases.

The amount of fuel in the mixes is not the same in the cylinder, they are calculated in detail and care to ensure the total energy generated from the cylinder is the same. This results in the indicated pressure essentially unchanged in various operating modes with different mixings. The authors find that at -20CAD ATDC, knocking can occur when using gasoline fuel. However, knocking is not found using DMF-gasoline mixtures. At the time of ignition of -20 CAD when using gasoline, the knocking becomes extremely serious for the SI engine. There is a slight knocking happening to DMF20. No special differences are found in the anti-knocking characteristics of DMF30 and DMF40.

Simulation results also show that the ignition timing advance value of 23 CAD gives the best fuel consumption and heat efficiency according to Fig. 3 and Fig. 4. However, compared to conventional gasoline, these blends' fuel consumption increased by 8.18%, 11.1%, 38.48%, and thermal efficiency also decreased by 1.99%, 2.09%, and 2.32%, corresponding with the DMF20, DMF30 and DMF40 mixtures. As the A/F ratio of the alternative fuel (DMF) decreases with increasing the ratio of DMF volume in the blends with RON95 gasoline, the amount of new fuel injected for one cycle increases, engine power is almost equivalent to that of when using RON95. So, fuel consumption rate also increases accordingly, this is reasonable. The simulation results show that the ignition timing advance's appropriate adjustment retains both technical and economic characteristics of the fuel blends compared with traditional gasoline fuel.

### B. Simulation Results at Speed 3500rpm

From the simulation results, the power diagram of the simulation engine is shown in Fig. 5.

From the diagram in Fig. 5, we see that the engine's power changes when we change the ignition timing advance. The engine power when using RON95 gasoline reaches a maximum when the ignition timing advance is 33 CAD, while when using the DMF20, DMF30 and DMF40 fuel blends, the maximum power at the ignition timing advance is 31 CAD, reduce 2 CAD. With this ignition timing advance value at 23 CAD, the engine's power reaches 19.14 kW with gasoline, and when using the fuel blend, the power was reduced by 1.88%, 3.81%, and 6%, respectively with DMF20, DMF30, and DMF40. At the other ignition angle values as far as 31 CAD, the power and torque tend to decrease. This trend is similar to the case of simulation at 2500 rpm.

Simulation results of the engine at 50% load and 3500 rpm show that the ignition timing advance value of 31 CAD gives the best fuel consumption and heat efficiency according to Fig. 6 and Fig. 7. However, compared to conventional gasoline, these blends’ fuel consumption increased by 8.06%, 10.8%, 13.9%, and thermal efficiency
also decreased by 1.44%, 1.76%, and 2.43% corresponding with the DMF20, DMF30 and DMF40 mixtures. This trend is like the case of simulation at 2500 rpm.

![Fig. 7. The BTE diagram of simulation engine at 50% load, λ=1, the speed at 3500 rpm](image)

In the sections above, we use AVL-Boost software to simulate the operating modes of the 1NZ-FE engine when using DMF-RON95 gasoline blend with different ignition timing advances. The optimal ignition timing advances are summarized in Table III. Thus, when reducing the ignition timing advance to 2 CAD compared to when using RON95 gasoline, the engine's economic and technical characteristics reach the best value. And this is also the optimal ignition timing advance of the engine.

When using DMF fuel, the average fuel consumption increase is about 2% - 5% compared to when using gasoline. In this case, the engine power increases by 20% on average (with DMF30) as mentioned above, but the fuel consumption increases and decreases by 5.7%. The reason is that the density of DMF is higher, besides the low calorific value of DMF (50 MJ/kg) is higher than gasoline RON 95 (44 MJ/kg) to 13.6%. The thermal brake efficiency of the engine when using DMF fuel is higher than RON95 gasoline. This is due to the DMF's high combustion efficiency and the oxygen content of its molecular formula (the oxygen component accounts for 16.7% of the mass in the molecular formula of DMF).

### TABLE III
**RESULTS OF OPTIMAL IGNITION TIMING ADVANCE FOR EACH WORKING MODE**

| Fuel / Blends | Modes | \( \varphi_{e} \) (CAD) | \( N_e \) (kW) | \( g_e \) (g/kWh) | BTE (%) |
|---------------|-------|-----------------------|----------------|----------------|--------|
| RON95         | 2500  | 25                    | 14.45          | 280.1          | 27.11  |
|               | 3500  | 33                    | 19.14          | 295.23         | 28.38  |
| DMF20         | 2500  | 23                    | 14.09          | 303.58         | 29.51  |
|               | 3500  | 31                    | 18.78          | 319.05         | 27.97  |
| DMF30         | 2500  | 23                    | 14.03          | 311.21         | 29.48  |
|               | 3500  | 31                    | 18.41          | 327.13         | 27.88  |
| DMF40         | 2500  | 23                    | 13.71          | 318.58         | 29.41  |
|               | 3500  | 31                    | 17.99          | 336.45         | 27.69  |

With an increase of ignition timing advance, the quality of mixture and burning temperature in the combustion chamber using DMF increases rapidly. This makes creating mixture and burning better, so the ratio of the increase in fuel consumption to the increase in engine power decreases faster than using RON 95 gasoline. On the engine, when using DMF, it is much improved compared to using RON 95 gasoline with the average improvement ratio like the external specification. Especially in the case of an increase in mixing ratio of up to 30%, the engine's fuel consumption is improved throughout the power range, an improvement compared to the case of the addition of a smaller DMF ratio.

IV. CONCLUSION

This article has developed a 1NZFE engine simulation model, performing engine simulation when using 2,5-dimethylfuran-RON95 gasoline blends (DMF ratio varies from 20%-40% physically mixed with gasoline) to determine the optimum ignition timing advance of the engine. Simulation mode is set at 50% load, engine speed at 2500 and 3500 rpm. The simulation results show that the engine's technical and economic characteristics when using DMF-gasoline RON95 blends will achieve the best value when reducing the ignition timing advance of the 2 CAD.

The simulation results also show that using a DMF-gasoline blend with a large DMF ratio reduces traditional fuel dependence and reduces environmental pollution emissions. DMF preparation also takes advantage of traditional, diverse, and abundant biomass resources in Vietnam.

ACKNOWLEDGMENT

This research is supported by Industrial University of Ho Chi Minh City (IUH) under grant number 68/H-DHCN. Additionally, the authors are grateful to Ho Chi Minh City University of Technology (HUTECH) for providing necessary facilities during the research.

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