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Study Simulating Emission Efficiency of Engines When Using CNG Fuels to Replace Gasoline Fuel

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Abstract *— This paper uses AVL-Boost software to simulate the effects of converting an engine that is using gasoline to using CNG gas. Specifically, the article studies the economy process of the engine when using CNG gas fuel for gasoline engines by direct injection into the intake manifold and the method of using a mixer and then supplying it to the road. load. Experimental simulation model on Toyota - 5A engine, all structural parameters of the engine are kept original. The results of simulation study show that, when using CNG gas fuel, indicators such as: Emissions of harmful components CO, HC and NOx of engines using CNG are significantly reduced compared to using gasoline; CO decreased by 34% on average, HC decreased by 79% on average and NOx decreased by 29%. From the above simulation study, recommendations for manufacturers as well as users can be made to change when using CNG gas fuel for gasoline engines.*

Keywords *— CNG gas, Emission, Wattage, Simulation*

I. INTRODUCTION

Nowadays, along with the strong development of the economy and society, there is a rapid increase in transportation vehicles and internal combustion engine (ICE) powered equipment. Therefore, fuel consumption is increasing, especially for traditional fossil fuels such as gasoline and diesel. This is posing a rapid depletion risk of traditional fuel sources [1] and causing serious environmental pollution due to harmful emissions from engines [2,3].

Vietnam is a developing country and therefore not exempt from the general laws of global development. The situation of fuel shortage and environmental pollution caused by engine emissions is at an alarming level [4,5]. Therefore, the issue at hand is the need to research and use alternative fuels with low levels of toxic emissions in order to reduce environmental pollution on the one hand, and on the other hand, to partially offset the demand for traditional fuels. The preferred types of alternative fuels to use are those with low harmful emissions, large reserves, low cost, and can be easily used on traditional engines without much structural change. Among these fuels, compressed natural gas (CNG) is a fuel that meets these requirements and has great potential to be used as a substitute fuel for internal combustion engines. CNG is a gas fuel with many different characteristics from traditional liquid fuels, so if new engines are designed with optimal structural features for the use of this fuel, high technical and economic performance can be achieved. However, manufacturing or purchasing new CNG engines can be very costly, and not all customers can afford them, while there are many existing gasoline engines that can easily use CNG. Therefore, researching the scientific basis of alternative fuels [6,7,8,9] and natural gas fuels [10,11,12,13] is an urgent issue worldwide. CNG [14,15] has many advantages, especially in terms of emissions. Researching the use of CNG on existing gasoline engines, considering factors that affect the economic, technical, and emissions performance of the engine, such as the method of supplying CNG and using fuel additives for CNG, is necessary to improve conversion technology and increase the efficiency of using CNG fuel on current gasoline engines.

II. THE THEORETICAL FOUNDATION OF SOFTWARE AVL BOOST

2.1 The formation of CO emissions

Many experimental results have shown that the amount of CO in gasoline engine exhaust must be carefully controlled because this CO level is lower than the highest value measured in the combustion chamber but higher than the corresponding equilibrium value. In fact, the CO level increases rapidly in the flame zone, mainly generated by the incomplete oxidation of hydrocarbons due to thermal cracking, and continues to be completely oxidized to CO_2 through the kinetic control mechanism.

Therefore, the value of CO can be calculated by solving a differential equation based on the following reactions:

$$CO + OH = CO_2 + H$$
$$CO_2 + O = CO + O_2$$

CO concentration is calculated by the formula:

$$\frac{d[CO]}{dt} = \left(R_1 + R_2\right)\left(1 - \frac{[CO]}{[CO]_e}\right)$$

In which [CO]e is the equilibrium concentration of CO and the values of rate constants R1 and R2 are given by the formula:

$$R_1 = k_1^{+}[CO]_e[OH]_e$$
$$R_2 = k_2^{-}[CO]_e[OH]_e$$

2.2 The formation of HC emissions

In spark-ignition engines, non-combusted hydrocarbons come from various sources, making it difficult to provide a complete description of their formation process. However, the explanatory method model for the primary formation mechanism can be applied to study the formation of hydrocarbons as a function of engine operating parameters. The main sources of non-combusted hydrocarbons in spark-ignition engines include:

- The ratio of unburned air flow through the clearance and non-combustion when the flame is extinguished;
- Fuel vapor is absorbed into the oil film layer and deposits on the cylinder wall during both the intake and compression stroke;

- Wall quenching effect;
- Incomplete combustion or flame-out phenomenon occurs when the combustion quality is poor;
- Direct flow of fuel vapor into the engine exhaust system;

The two primary mechanisms and specifically the formation due to gaps are considered the most important and need to be noted in thermodynamic models. The wall-effect and incomplete combustion phenomena cannot be described by scalar methods but can be inferred from semi-empirical correlations.

The general equation for the rate of formation of a compound HC:

$$\frac{d[HC]}{dt} = -c_{HC} A_{HC} e^{-E_{HC}/RT_{gw}} [HC]^a [O_2]^b$$

In which: A_{HC} = 7,7 x 10^9 ((m^3/mol)$^{a+b-1}$/s); E_{HC} = 156222 (J/mol); R = 8314 (J/mol.K); $T_{gw} = (T_{gas} + T_{cyl.wall})/2$; [HC] and [$O_2$] are the densities of HC and O2 (mol/m3); cHC is the rate adjustment constant that depends on each mode and type of engine; a and b are constants, with a = b = 1.

The mass of the gas mixture in the fissure at any time is calculated according to the formula:

$$m_{kh} = \frac{p.V_{kh}.M}{R.T_{piston}}$$

In which: m_{kh} is the mass of unburned gas in the clearance volume, [kg]; p is the cylinder pressure, [Pa]; Vkh is the clearance volume, [m^3]; M is the molar mass of the unburned gas, [kg/kmol]; R is the gas constant, [J/(kmol K)]; Tpiston is the piston temperature, [K].

The distribution of mass in the oil layer is calculated in the following diffusion equation:

$$\frac{\partial w_F}{\partial t} - D\frac{\partial^2 w_F}{\partial r^2} = 0$$

In which, w_F is the mass fraction of fuel in the oil layer, [-]; t is time, [s]; r is the center position of the oil layer (measured from the cylinder wall), [m]; D is the corresponding diffusion coefficient (fuel-oil), [m/s], determined by the following formula: $D = 7,4.10^{-8}.M^{0,5}.T.v_f^{-0,6}.\mu^{-1}$

In which, M is the molar mass of the oil molecule, [g/mol]; T is the temperature of the oil, [0K]; v_f is the molar volume of the fuel at normal boiling condition, [cm^3/mol]; μ is the viscosity of the oil, [cps-centiPoise].

The phenomena of knock and wall-impingement cannot be described using the scalar approach. Lavoie and his colleagues proposed a semi-empirical correlation hypothesis, in which the unburned gas charge remaining in the Fprop cylinder is calculated by applying the following equation:

$$F_{prop} = F.C_1.\exp\left\{\frac{\vartheta_{EVO} - \vartheta_{90}}{C2\left(\vartheta_{90} - \vartheta_0\right)}\right\}$$

$$C_1 = 0,0032 + \frac{(\phi - 1)}{22} \text{ khi } \phi < 1$$

$$C_1 = 0,003 + \left((\phi - 1).1,1\right)^4 \text{khi } \phi > 1$$

$$C_2 = 0,35$$

In which: F is the correction factor, [-]; ϕ is the equilibrium ratio, [-]; ϑ_0 the 0% unburned fuel timing, [^{0}TK]; ϑ_{90} the 90% unburned fuel timing, [^{0}TK]; ϑ_{EVO} the exhaust valve opening timing, [^{0}TK].

2.3 The formation of NO_x emissions

The mechanism of NOx formation in the Boost simulation based on Pattas and Hafner is calculated based on input parameters such as engine speed, fuel, pressure, temperature, air excess ratio λ, volume and mass, time, and number of combustion chambers. The calculation process starts at the beginning of combustion. Although NO accounts for the majority (90-98%) of NOx emissions from gasoline engines, the calculation of N_2O cannot be ignored. The amount of N_2O generated is related as follows:

$$\frac{N_2O}{N_2\sqrt{O_2}} = 1.1802.10^{-6} T_1^{0.6125} exp\left[\frac{-18.71}{RT}\right]$$

The rate of formation of NOx is calculated as follows:

$$\frac{d[NO]}{dt} = 2(1 - \alpha^2)\left[\frac{R_{1e}}{1 + \alpha K_2} + \frac{R_{4e}}{1 + K_4}\right]\frac{p}{RT}$$

The NO decay rate [mol/cm^3] is calculated as follows:

$$r_{NO} = C_{Post\,ProcMult}.C_{kineticMult}.2,0.(1 - \alpha_2)\frac{r_1}{1 + \alpha.AK_2}\frac{r_4}{1 + AK_4} \text{ Với}$$

$$\alpha = \frac{C_{NO,act}}{C_{NO,equ}}.\frac{1}{C_{Post\,ProMult}} \qquad AK_2 = \frac{r_1}{r_2 + r_3};$$

$$AK_4 = \frac{r_4}{r_5 + r_6}$$

III. BUILDING A SIMULATION MODEL OF TOYOTA-5A ENGINE

3.1 The interface of AVL Boost

The new version of the software [16, 17] has been improved. Users can input data on input conditions, select appropriate data from the software's data library, run the program command, view the calculation results, and adjust the model through user-friendly interface windows and software guidance.

3.2 The elements of a program

- Cylinder element:
+ Emission boundary conditions (Aftertreatment Boundary)
+ The boundary conditions on the interior (Internal Boundary)
- The voltage stabilizing component (Plenum)
- Loading elements (Charging Elements)
- Tube element (Pipes)

Applying the laws of conservation of mass, momentum, and energy, we describe the flow in a pipe through the following equations:

- Continuous equation:

$$\frac{\partial p}{\partial t} = -\frac{\partial(\rho v)}{\partial x} - \rho v\frac{1}{A}\frac{dA}{dx}$$

- Conservation of momentum equation:

$$\frac{\partial(\rho.v)}{\partial t} = -\frac{\partial\left(\rho v^2 + p\right)}{\partial x} - \rho v^2 \frac{1}{A}\frac{\partial A}{\partial x} - \frac{F_{fr}}{V}$$

- The law of conservation of energy:

$$\frac{\partial E}{\partial t} = -\frac{\partial\left[v\left(E+p\right)\right]}{\partial x} - v\left(E+p\right)\frac{1}{A}\frac{dA}{dx} + \frac{q_W}{V}$$

In which: ρ is the gas density; u - flow velocity; x - longitudinal direction along the tube; t - time; p - static pressure; F_{fr} - friction force on the tube wall; c_V - specific heat capacity at constant volume; q_W - wall heat flux; V - volume (= A. dx);

E – The internal energy of a gas flow $E = \rho.c_V.T + \frac{1}{2}.\rho.u^2$

Frictional loss: $\frac{F_{fr}}{V} = \frac{\lambda_{fr}}{2D}\rho v|v|$ (λ_{fr} - coefficient of friction)

Heat loss: $\frac{q_W}{W} = \frac{\lambda_{fr}}{2D}\rho|v|c_p\left(T_W - T\right)$ (T_W – temperature inside the tube).

- Attached elements (Assembled Elements)

3.3 Setting up the Toyota-5A engine model on AVL Boost

Steps to set up a simulation model:

- Define the elements and then connect them together.
- Select the algorithm and input the boundary and initial condition data relevant to the model.
- Run the model and output the results.

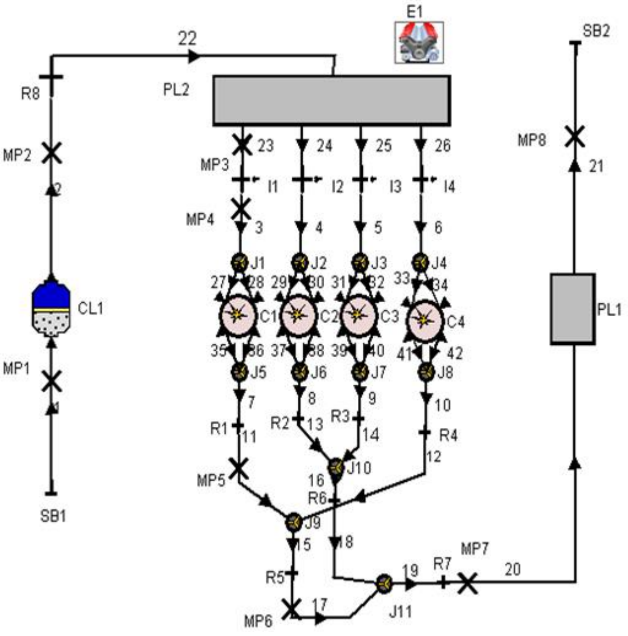

Figure 1: Simulation model of CNG gas supply using injection method

After setting up the model on the software, we evaluate the model's reliability by comparing the results of simulation and experimentation. Adjusting the parameters of the combustion model and heat transfer model ensures that the simulated calculation results are consistent with the experimental results.

The graph shows that the maximum deviation between the calculated power and actual measurement is 7.3% at a speed of 4000 rpm, with an average deviation of 4.4% across the entire speed range of the engine. The simulated fuel consumption has a maximum deviation of 5.2% compared to the actual value, with an average deviation of 3.16% across the entire speed range. With the simulation results deviating less than 5% from the actual measurements, the constructed engine model is considered reliable and can be used to simulate the working parameters of the engine when using gasoline.

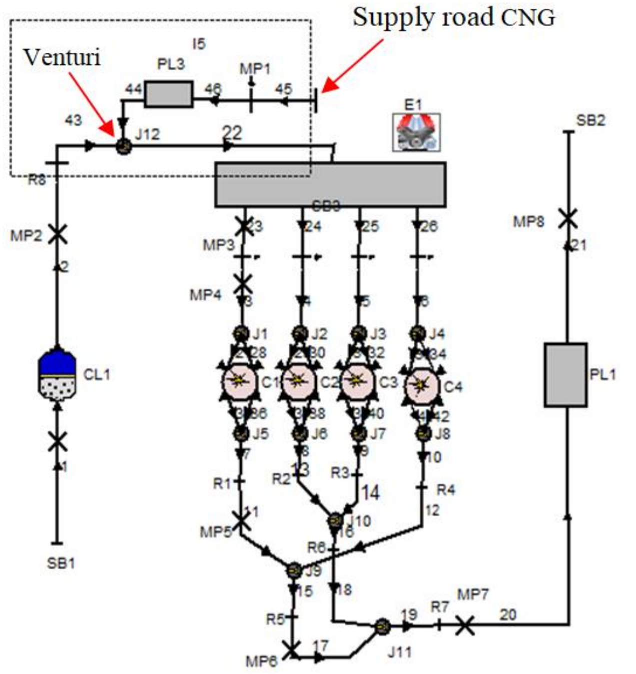

Figure 2: Model simulation provides CNG fuel through mixing method

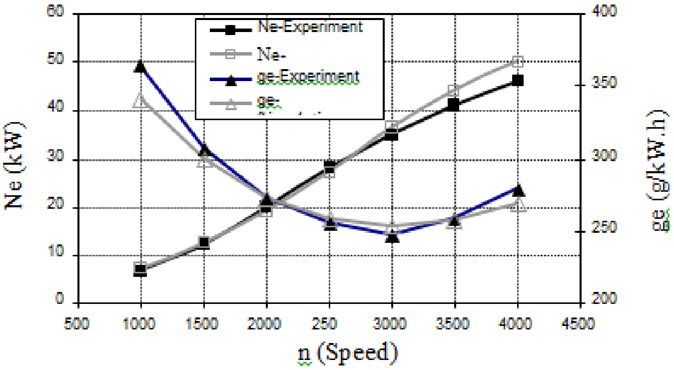

Figure 3: Compare simulation results and experimental results

3.4 Engine Emissions

The results of simulating the emission rates of HC, CO, CO_2, and NOx components of the engine using two types of fuels, gasoline and CNG, are shown in graphs 4 to 7. The graphs indicate a significant improvement in emissions when the engine is fueled with CNG compared to gasoline. The CNG injection engine emits slightly lower amounts of CO, HC, and NOx compared to the CNG mixer engine, while emitting slightly higher amounts of CO_2.

Figure 4 illustrates that the engine emits significantly lower levels of HC when using CNG across the entire engine speed range compared to using gasoline, with an average reduction of about 79%. The reason for such a significant reduction in HC emissions when using CNG is that the CNG-air mixture is more homogeneous than the gasoline-air mixture, leading to a more complete combustion. Additionally, the CNG fuel has a lower C/H ratio than gasoline fuel, while the HC emissions are calculated based on the amount of C_3H_8 produced, resulting in much lower HC emissions from the engine when using CNG compared to gasoline.

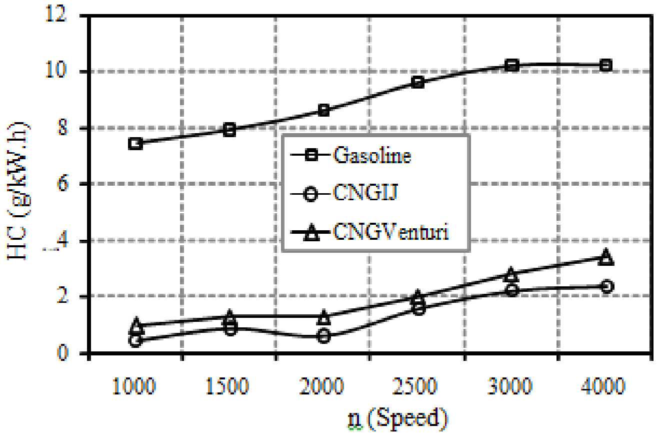

Figure 4: Compare the emissions of hydrocarbons when using gasoline and CNG at different speeds

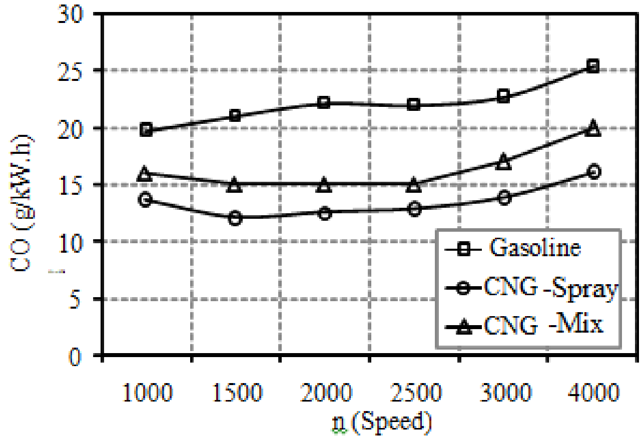

Figure 5: Compare CO emissions when using gasoline and CNG at different speeds

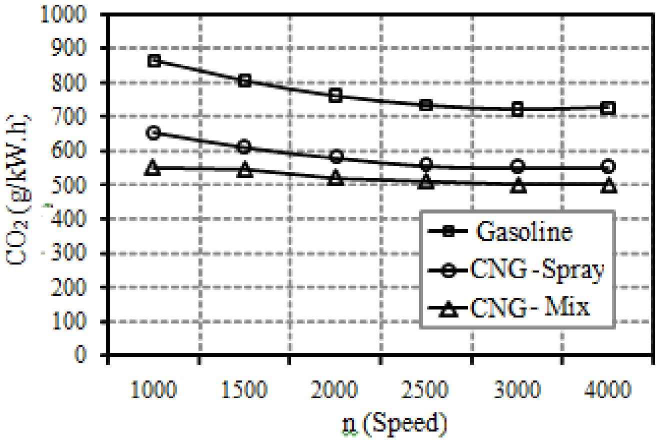

Figure 6: Compare CO_2 emissions when using gasoline and CNG at different speeds

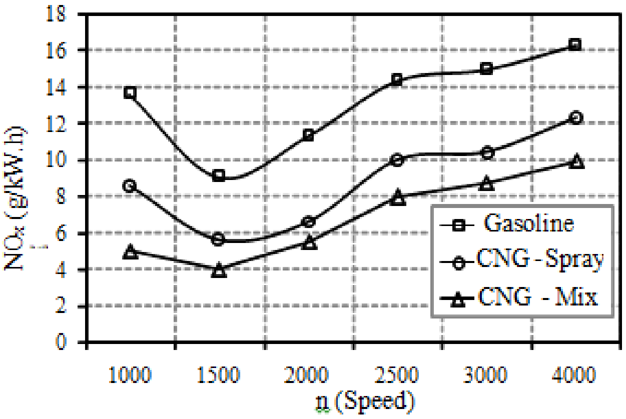

Figure 7: Compare NOx emissions when using gasoline and CNG at various speeds

The comparison of CO emissions from engines when using two types of fuels is shown in figure 5. The graph demonstrates that CO emissions from the engine when using CNG decreased by 29 to 43% across the entire speed range and decreased on average by 34%. This is because CNG (mainly composed of CH_4) has a lower C/H ratio than gasoline (mainly composed of C_8H_{18}) with a simpler structure and more homogeneous combustion, leading to significantly lower CO emissions when using CNG compared to gasoline. These characteristics of CNG also reduce the CO_2 emissions from the engine, with an average reduction of 19% across the entire speed range compared to gasoline, as shown in figure 6.

NOx emissions are significantly reduced when using CNG fuel, with a reduction rate ranging from 19% to 39%, and averaging at 29%. This can be explained by the lower combustion temperature of CNG compared to gasoline, which leads to a lower temperature during the combustion process and thus a reduction in NOx emissions, as shown in figure 7.

IV. CONCLUSION

- The research on simulating the Toyota gasoline engine - 5A using CNG fuel on AVL-Boost software has been conducted with 2 methods of CNG supply: CNG injection into the intake tract and using the venturi tube type CNG mixer.

- Emission of harmful components CO, HC, and NOx from CNG engines is significantly reduced compared to using gasoline; CO is reduced by an average of 34%, HC is reduced by an average of 79%, and NOx is reduced by 29%.

- The CNG engine using the method of injecting CNG into the intake manifold has better emissions than the method of supplying CNG through a venturi tube mixer. The emissions of CO, HC, and CO_2 are lower, but NOx is slightly higher.

From the above results, the following recommendations can be drawn:

- Using CNG on gasoline engines is a good method to reduce harmful emissions

- When converting from using gasoline to using CNG, it may not be necessary to change the structure of the engine.

- When converting from gasoline engine to using CNG, the CNG injection method and the CNG supply method through mixing system can be applied. However, it is necessary to conduct experimental research to equip these systems and evaluate the engine performance under real conditions to propose a reasonable CNG supply method for each type of engine, ensuring a balance between the convenience of application and the economic and technical targets of the conversion engine.

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