Modelling and Simulation of the Performance and Combustion Characteristics of a Locomotive Diesel Engine Operating on a Diesel–LNG Mixture

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Abstract: The article describes a compression-ignition engine working with a dual-fuel system installed in diesel locomotive TEP70 BS. The model of the locomotive engine has been created applying AVL BOOST and Diesel RK software and engine performance simulations. Combustion characteristics have been identified employing the mixtures of different fuels. The paper compares ecological (CO₂, NOₓ, PM) and energy (in-cylinder pressure, temperature and the rate of heat release (ROHR)) indicators of a diesel and fuel mixtures-driven locomotive. The performed simulation has shown that different fuel proportions increased methane content and decreased diesel content in the fuel mixture, as well as causing higher in-cylinder pressure and ROHR; however, in-cylinder temperature dropped. CO₂, NOₓ and PM emissions decrease in all cases thus raising methane and reducing diesel content in the fuel mixture.

Keywords: compression ignition engine; liquefied natural gas; locomotives; environmental indicators; engine simulation

1. Introduction

There is increasingly urgent attention focused on ecology, despite a continuous rise in vehicle traffic worldwide. Due to emission products such as carbon dioxide (CO₂), hydrocarbon (HC) and nitrogen oxide (NOₓ) of the internal combustion engine, the greenhouse effect is still ongoing, because the main greenhouse gas emission sectors include transport, farming and energy producing plants [1]. In order to reduce emissions from internal combustion engines, exhaust gas recirculation systems (EGR), the “AdBlue” system and diesel particulate filters (DPF) are installed and further measures are taken. As a result of the increasing ecological requirements and standards, alternative fuels such as hydrogen, natural gas [2] or bio-methane are used. However, hydrogen storage poses a number of problems for solving which various methods, including compression, refrigeration or placement in metal-hydride and adsorption storage tanks are implemented [3]. Still, none of the techniques suggested is completely suitable. Liquefied natural gas (LNG) fits well for heavy vehicles (trucks, tractors, locomotives, ships, etc.). Natural gas (NG), as a transport fuel, brings significant benefits to consumers, the environment and economy as a whole and is a quick and cost-effective way to achieve the key goals established by the EU, including decarbonisation in the road transport sector and improvements to air quality in cities. To achieve climate neutrality, the amount of consumed natural gas must gradually decrease.
However, in the field of energy, gases will continue to play an important role and their CO$_2$ emissions should be kept to a minimum (e.g., hydrogen or bio-methane) [4].

The Natural and bio Gas Vehicle Association (NGVA Europe) is actively developing the network of CNG and LNG stations in Europe. At present, more and more European countries are joining the Blue Corridor Project, demonstrating that gas can be a great alternative to diesel. Moreover, gas can also be produced from renewable sources and mixed with natural gas emitting less CO$_2$ than any other hydrocarbon fuel and acting as an additional part of bio-methane that can further reduce CO$_2$ emissions. In general, for burning natural gas, the engine emits significantly less PM and NO$_x$, and by reason of its low sulphur content and high energy density, LNG is becoming the choice of shipping industry [5].

The data published by organisation “Cowy” shows that the transport sector is ranked third in terms of energy production and consumption in the European Union in 2015 [6]. The largest share of the fuel consumed in the transport sector covered diesel (49.8%), gasoline (20.7%), kerosene (12.3%), other petroleum products (10%), biofuel (3.7%), liquefied petroleum gas (2%) and liquefied natural gas (1.4%).

In 2015, the Association of American Railroads found that rail freight reduced greenhouse gas emissions by 75% [7]. James A. Pritchard from the University of Southampton shows that rail freight should not be ignored as it has the potential to offer huge savings in emissions over transporting goods by road [8]. Studies by the European Environment Agency show a clear dependence of GHG emissions on the mode of transport: rail transport has the lowest emissions per kilometre while aviation and road transport have the highest [9]. A report by researchers from Brazil stated that more than 490 million tons of cargo had been transported by railroads in 2013 and had increased to 550 million tons in 2016 [10]. As reported by the Lithuania Statistics department, 52,638.2 tons of cargo were transported by railroads in Lithuania in 2017 and 56,775.8 tons of cargo in 2018 [11]. There is an upward trend in the volume of freight transportation, which has led to an increase in emissions from diesel locomotives. It is therefore important to increase rail freight transport, but simultaneously, should make rail transport as efficient and environmentally friendly as possible.

As a result, dual-fuel systems are increasingly being used, which gives an opportunity for the engine to work on two different fuels (in this case, on diesel and LNG at the same time) [12]. Exhaust emissions are reduced using LNG compared to the engine working on pure diesel fuel [13]. The compression ignition (CI) engine works with one part (about 10%) diesel fuel and a larger part (about 90%) consists of gas fuel. Pilot diesel injection acts similarly a spark plug during the ignition process. Then, the control unit sends signals to gas injectors spraying gas into the taken air and create an air/gas mixture sucked into engine cylinders [14,15].

Daria Gritsenko examined the development of LNG infrastructure in the Baltic Sea region and noted that the main reason for developing infrastructure was political decisions. She argued that LNG was expanding as the key energy technology for three main reasons: energy security, the need to bunker low-sulphur fuels and the balance of renewable energy sources [16].

There are not many LNG locomotives in the world. Some of them run on pure natural gas, whereas others use dual-fuel systems [14,17]. The first LNG switcher locomotive (1200 HP) leased from the BNSF Railway entered service at the West Basin Container Terminal (Los Angeles) in 2008 for a period of 36 weeks [2]. Later, the Canadian National Railway converted two diesel–electric locomotives into dual-fuel locomotives where the combustible mixture of engines consisted of 90% of natural gas and 10% of diesel fuel [12]. Natural gas-powered locomotives are still rare because of various reasons, such as lack of infrastructure, suitable engines and regulation [10,18]. However, it is believed that their wider use fundamentally changes the ecological situation [19].
A review of literature has shown there is a sufficient number of experimental studies on dual-fuel systems running on diesel–NG mixtures that have shown good engine efficiency results.

The results of the research carried out by the scientists at Jilin University have demonstrated that ignition quality of the pilot diesel portion plays an important role in determining the combustion process of the diesel–NG mixture. By advancing pilot diesel injection, NG combustion duration is shortened from 35.5 °CA to 16.5 °CA. The shortest combustion duration corresponds to lower brake specific energy consumption and emissions [20].

Millo et al. [21] experimentally investigated and performed Wartsila 31DF engine simulation. The experimental research disclosed that diesel injection timing had a minimal effect on ignition timing: in the case diesel was injected into the cylinder later, diesel vapour ignited faster due to high pressure in the cylinder compared to the early injection of diesel, which was characterised by a longer ignition delay. Changes in the pilot-injected quantity of diesel shortens a decrease in ignition timing, and therefore heat increases in both cases; working on pure and dual-fuel. Based on experimental findings, numerical analysis was performed with the aim of developing a suitable simulation tool providing reliable predictions of the ignition process of dual fuel engines.

Shu et al. [22] conducted research on a six-cylinder, direct injection, turbocharged diesel engine with a common rail system. The aim of the study was to investigate thermodynamics, the combustion process and the emissions of a dual-fuel engine with a different pilot injection degree at low speed and load operation. Based on the conducted experimental research, one- and three-dimensional CFD models were developed and used for analysing the combustion process and emission characteristics of the dual-fuel engine. The carried out research has shown that advancements in the pilot injection degree increase the start of combustion and raise the maximum in-cylinder pressure. There is also a rise in effective expansion efficiency and the percentage of heat transfer loss. The analysis of pollutant emissions demonstrated that improvements in diesel injection significantly increased brake specific NO\textsubscript{x}, although brake specific THC hardly changed.

Abagnale et al. [23] performed a CFD-based study of a dual-fuel NG/diesel engine using numerical simulation and involving gas exchange periods. The aim of the study was to analyse in detail the progress of combustion and the formation of pollutants under different conditions thus changing operating parameters and the fuel ratio. The findings of the calculations were compared with the experimental data obtained using a light duty 2.0-L direct injection diesel engine at a steady state test bench. The performed analysis showed that under an increase in the amount of natural gas, the combustion mode shifted from the lean premixed-diffusive process to that similar to spark ignition premixed charge engines.

The literature review also confirmed that no locomotive engine simulation studies had been conducted. Thus, the main goal of this paper is to select locomotive engine TEP70BS that is still used in some Eastern European countries, to create a simulation model for the combustion of this engine and compare ecological (CO\textsubscript{2}, NO\textsubscript{x}, PM) and energy indicators for diesel and diesel–LNG mixtures used in the locomotive.

2. Methodology for Simulating Locomotive Engine Indicators

Two software packages, AVL Boost [24] and DieselRK, were used for the analysis and synthesis of the combustion process of the environmental and energy performance of the internal combustion engine. The amount of heat released during combustion employing AVL Boost software is calculated from the angle of crankshaft rotation. The Vibe heat release function is applied [25]:

\[
\frac{dx}{d\phi} = \frac{a}{\Delta\phi_c} (m_v + 1) \cdot y^{m_v} \cdot y^{-a \cdot y^{m_v + 1}} \quad (1)
\]
where \( dx = \frac{dQ}{Q} \); \( Q \) is the heat amount released from fuel used during the work cycle of the engine; \( \varphi \) is the crank angle; \( m_v \) is the combustion intensity shape parameter; \( a \) is the Vibe constant (under 99.9% of burned fuel, \( a = 6.905 \)); and \( y \) is the relative combustion duration:

\[
y = \frac{\varphi - \varphi_0}{\Delta \varphi_c}
\]

where \( \varphi_0 \) is the start of combustion; and \( \Delta \varphi_c \) is the combustion duration.

The integration of the Vibe function calculates the proportion of fuel mass burnt from the start of the combustion process:

\[
x = \int dx = \frac{1 - e^{-a y (m_v+1)}}{d\phi}
\]

The 2A–5D49 model of the TEP70BS locomotive engine (Figure 1) was created in line to the main characteristics indicated in Table 1. Simulation was performed under the assumption that the locomotive engine was powered by the dual-fuel system (diesel and LNG). Other parameters used in the model are presented in Tables 2–4.

![Figure 1. TEP70 BS engine model employing “AVL Boost” software: I1—connection; SB1, SB2—system boundaries; PL1, PL3—exhaust manifold; PL2—inlet manifold; PL4—exhaust silencer; CL1—air cleaner; TC1—turbocharger; 1 . . . 49—connection tubes; C1 . . . C16—engine cylinders; CO1—intercooler; MP1—measuring point.](image)

Fuel mixtures are created applying the “Gas Properties Tool” of the AVL Boost software. Additionally, using this function from the Chemkin thermodynamic database, fourteen coefficients of entropy are calculated, which indicates the stability of the completely thermodynamic system. Table 3 shows the values of the parameters for the main fuel mixtures.

After creating fuel mixtures, the main simulation of engine performance was organized. The fuel mixtures were made following the principle that the relevant part of diesel was replaced by methane (CH\(_4\)) gas. For example, designation D90 + LNG10 represents a fuel mixture composed of 90% of diesel and 10% of methane.

An additional simulation of the engine of the TEP70 BS locomotive was performed using DieselRK software. First, the simulation of the engine running on diesel fuel was performed, and engine characteristics and ecological values were obtained (Table 5).
Table 1. Technical parameters for the engine [26,27].

| Parameter                          | Value                                      |
|------------------------------------|--------------------------------------------|
| Model of locomotive                | TEP70 BS                                   |
| Year of production                 | 2004                                       |
| Manufacturer                       | Kolomna Locomotive Works, Russia           |
| Weight, t                          | 131                                        |
| Engine power, kW                   | 2940                                       |
| Nominal engine speed, rpm          | 1000                                       |
| Engine code                        | 2A-SD49                                    |
| Piston diameter, mm                | 260                                        |
| Stroke, mm                         | 260                                        |
| Number of cylinders                | 16                                         |
| Engine volume, liter               | 220.8                                      |
| Specific fuel consumption, g/(kW·h)| 211                                        |
| Compression ratio                  | 1:13.4                                     |
| Max. in-cylinder pressure, MPa     | 13                                         |
| Turbocharger pressure, kPa         | 180                                        |
| Exhaust temperature, °C            | 600                                        |

Table 2. The main indicators for the combustion process.

| Parameter                               | Value  |
|-----------------------------------------|--------|
| Fuel injection angle, °                 | –10    |
| Duration of fuel injection, °            | 44.01  |
| Combustion intensity shape parameter    | 1.5    |

Table 3. Data on fuel mixture formation.

| Parameter                                | Diesel Fuel | Methane    |
|------------------------------------------|-------------|------------|
| Molar mass, kg/mol                       | 0.100206    | 0.016043   |
| Lower heating value, MJ/kg               | 42.83       | 50.04      |
| Air/fuel ratio                           | 15.17       | 17.23      |
| Total carbon content of the fuel         | 0.839       | 0.748      |
| Heat of vaporisation, J/kg               | 2.75·10⁵    | 5.13·10⁵   |

Table 4. Fuel mixtures used in the simulation process.

| Fuel Mixture   | Lower Heating Value, MJ/kg | Air/Fuel Ratio |
|----------------|-----------------------------|----------------|
| D              | 42.80                       | 15.18          |
| D90 + LNG10    | 43.55                       | 15.38          |
| D70 + LNG30    | 44.99                       | 15.79          |
| D40 + LNG60    | 47.16                       | 16.40          |
| D10 + LNG90    | 49.32                       | 17.02          |

Table 5. The initial results obtained during simulation using Diesel RK.

| Parameter                        | Value       |
|----------------------------------|-------------|
| Engine power, kW                 | 2940.5      |
| Engine torque, Nm                 | 27.951      |
| PM emission, g/(kW·h)            | 0.17018     |
| CO₂ emission, g/(kW·h)           | 673.87      |
| NOₓ emission, ppm                | 1448.7      |

The obtained parameter values were compared with real engine parameters proving the validity of the simulation model. Comparing the results obtained during the modeling
and the parameters declared by the manufacturer, the following difference is found: engine power—0.02%; in-cylinder pressure—11.8%; exhaust temperature—13.7%.

3. The Analysis of Research Results

The performed simulations show that in-cylinder pressure does not change significantly when the engine is running on diesel and fuel mixtures (Figure 2). All pressure graphs almost overlap with each other. The maximum developed pressure values are attained between 11° and 12° above the upper top dead centre (TDC).

![Figure 2. In-cylinder pressure of different fuel mixtures: (a) pressure of the whole cycle; (b) maximum pressure.](image)

The maximum in-cylinder pressure was achieved using the engine running on diesel only, which made 11.47 MPa. The lowest pressure applying the D10 + LNG90 fuel mixture was 10.84 MPa (Figure 2b). A pressure drop in cylinders during combustion occurs because the speed of the flame front of natural gas is slower than that of diesel. Likewise, the period of natural gas flammability itself is longer, thus resulting in less intensive combustion in the cylinder rather than in pure diesel [28–30].

An increase in the amount of gaseous fuel (methane gas) in the fuel mixture shows that in-cylinder temperature decreases during combustion (Figure 3). The highest temperature was recorded when the engine worked on pure diesel 2394 K, and the lowest temperature was established when the engine used the D10 + LNG90 fuel mixture—2267 K.

![Figure 3. In-cylinder temperature of the engine working with different fuel mixtures: (a) temperature of the whole cycle; (b) maximum temperature.](image)
The maximum in-cylinder temperature during combustion is influenced by the specific heat capacity of natural gas [31].

The specific heat capacity of natural gas is higher than air capacity, which affects a lower temperature at the end of the compression stroke and the entire mixture during combustion [32]. The temperature in the cylinder also decreases due to the subsequent burning of gaseous fuel [33]. As the amount of natural gas decreases, higher amounts of diesel promote deeper penetration of diesel droplets into gas, which results in fire sources for ignition gas. Simultaneously, it raises the speed of combustion and in-cylinder temperature [34].

With an increasing proportion of the gas–air mixture in combination with diesel, the mixture itself is better mixed in the cylinder and therefore burns better. During such combustion, a higher amount of the rate of heat release (ROHR) is observed, which is confirmed by the performed simulations (Figure 4). The peak of ROHR is reached at 6–7° for TDC. Additionally, with the engine running on a dual fuel supply system, at the second stage of combustion, ROHR is slightly higher than that of pure diesel only, which influences the overall increase in ROHR [35].

![Figure 3. In-cylinder temperature of the engine working with different fuel mixtures: (a) temperature of the whole cycle; (b) maximum temperature.](image1)

![Figure 4. The rate of heat release ROHR for different fuel mixtures: (a) ROHR of the whole cycle; (b) maximum ROHR.](image2)

CO₂ concentration was the lowest using the engine running on the D10 + LNG90 fuel mixture, and the highest amount was released when the engine used diesel only (Figure 5a). An increase in the proportion of gaseous fuels in the mixture shows that CO₂ emissions are decreasing. A reduction in CO₂ concentration is noticed because methane alone has the lowest carbon content of all hydrocarbons, which makes the engine more efficient [36]. Partial combustion is more likely when the engine runs on a mixture of diesel and gas. Thus, a part of fuel burns to carbon monoxide (CO) and is released into the environment, which further reduces CO₂ production. There were also some changes in turbocharger pressure (Figure 5b). The findings show that an increase in turbocharger pressure leads to a decrease in CO₂. This is because a lean mixture of fuel is formed in engine cylinders.

The formation of NOₓ during the combustion process mainly depends on the temperature of the combustible mixture zone itself and the amount of oxygen occupied during combustion [37,38]. The use of the fuel mixtures with an increasing proportion of the gas part decreases NOₓ quantities (Figure 6a). A lowering temperature during in-cylinder combustion reduces NOₓ emissions, respectively [14,39]. NO emissions are higher under a growth in engine loading [40].

An increase in turbocharger pressure (Figure 6b) causes a rise in NOₓ concentration, which is due to the higher concentration of the air in the cylinders during intake required for the formation of NOₓ [41]. The highest NOₓ emissions are recorded when the engine
works on diesel only, whereas the lowest emissions are observed when the D10 + LNG90 fuel mixture is used.

![Figure 5](image1.png)

**Figure 5.** CO$_2$ concentration of different fuel mixtures: (a) dependence on engine speed; (b) dependence on turbocharger pressure.

![Figure 6](image2.png)

**Figure 6.** NO$_x$ concentration of different fuel mixtures: (a) dependence on engine speed; (b) dependence on turbocharger pressure.

Particulate matter (PM) consists of carbon, various hydrocarbons, sulphur compounds and other elements. The maximum amount of PM is for the engine working on diesel fuel, while the lowest amount is noticed employing the D10 + LNG90 mixture (Figure 7a). An increase in turbocharger pressure (Figure 7b) leads to a drop in the quantities of PM, which is because PM itself is formed under lack of oxygen in the cylinder during combustion.

When using natural gas, PM emissions decrease because the engine works applying the dual-fuel system where a part of diesel is replaced by natural gas. As a result, less diesel is burned during diffuse combustion and the total amount of diesel burns together with the gas–air mixture. This results in lower soot formation during combustion. Additionally, due to an increase in the length of the period of natural gas ignition, pilot fuel injection takes place at a later stage, which makes it possible to better mix diesel–gas mixtures in the cylinders. Therefore, during combustion, no rich burning zone is formed in the cylinder, which allows the initial formation of soot to be avoided [26,32,42,43].
4. Conclusions

The simulation models for the compression ignition engine used in locomotives have been prepared applying software packages AVL Boost and DieselRK, and the comparative analysis of emissions working on pure diesel and on the diesel–LNG mixture has been carried out. Thus, the following conclusions in line to the achieved results are formed:

1. The emissions of the diesel engine running on the D10 + LNG90 fuel mixture are lower than those running on pure diesel, which makes CO₂ by 18.67%, NOₓ by 72.7% and PM by 18.6%.

2. The performed simulation of the engine burning process using the D10 + LNG90 fuel mixture has shown a reduction in the following parameters: in-cylinder pressure decreased by 5.8%, in-cylinder pressure rise dropped by 6%, in-cylinder temperature decreased by 5.6% and in-cylinder temperature rise reduced by 4.8% compared to the engine working on pure diesel.

3. D10 + LNG90 fuel mixture ROHR is higher by 15.2% compared to the engine working on pure diesel.

4. For a constant engine speed (1000 min⁻¹), a significant reduction in CO₂ and PM starts at the turbocharger pressure of 1.3 bars.

5. An increase in turbocharger pressure leads to a rise in NOₓ emissions due to higher airflow into engine cylinders.

6. The use of diesel–gas mixtures reduces fuel cost as a part of diesel fuel is replaced by gas in the fuel mixture.

5. Future Work

The paper has developed a numerical model for a locomotive engine and has simulated engine performance. In the case the LNG locomotive project is implemented in the Lithuanian Railway Company LTG Tech in the future, experimental research on a real locomotive is planned for the further implementation of the diesel–LNG mixture in the diesel engine of the locomotive.

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