CO₂ emissions from a spark ignition engine operating on natural gas–hydrogen blends (HCNG)

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The addition of hydrogen to natural gas could be a short-term alternative to today's fossil fuels, as greenhouse gas emissions may be reduced. The aim of this study is to evaluate the emissions and performance of a spark ignition engine fuelled by pure natural gas, pure hydrogen, and different blends of hydrogen and natural gas (HCNG). Increasing the hydrogen fraction leads to variations in cylinder pressure and CO₂ emissions. In this study, a combustion model based on thermodynamic equations is used, considering separate zones for burned and unburned gases. The results show that the maximum cylinder pressure rises as the fraction of hydrogen in the blend increases. The presence of hydrogen in the blend leads to a decrease in CO₂ emissions. Due to the properties of hydrogen, leaner fuel–air mixtures can be used along with the appropriate spark timing, leading to an improvement in engine emissions with no loss of performance.

1. Introduction

Crude oil reserves are not unlimited. In the future, we will have to resort to oil fields that are much more difficult to exploit (higher depths, higher densities), and additional extraction problems will arise. These circumstances will probably require investments in more developed extraction techniques, leading to higher crude oil prices. It is also important to note that demand is increasing more than supply. This is becoming more evident with the development of new economies such as China and India, which will require huge amounts of energy.

On the other hand, growing concern for the environment in all areas of knowledge also affects the engine manufacturing industry. To make engines more environmentally friendly, studies focus on decreasing greenhouse gas emissions to the atmosphere by developing different alternatives to fossil fuels [1–3] and new engine types, such as HCCI [4,5].

Natural gas is regarded as a suitable alternative to other fossil fuels because its combustion features are cleaner and higher proven reserves are available [6,7]. Natural gas has excellent anti-knock properties due to its higher compression ratio, which provides improved efficiency and power. However, its flame propagation rate is low, and its auto-ignition temperature is high. Hydrogen is postulated as the long-term alternative. While not free, it is abundant in nature and its combustion products are almost harmless. However, most hydrogen is now obtained from fossil fuels, and therefore does not solve the problem of dependency on such fuels. Storage is also an issue because hydrogen is highly explosive and requires large, heavy tanks. Hydrogen has high flame propagation rates, making it easier to ignite, but reduces engine performance compared to fossil fuels [8,9].

An alternative solution, as a transition to hydrogen technology, is natural gas blended with hydrogen, known as HCNG. A combination of the two fuels could overcome the limitations of both pure natural gas and hydrogen.

When experimental or simulation studies on reciprocating engines are carried out, much attention is paid to pollutant CO, HC and NOₓ emissions. Nevertheless, although CO₂ is one of the most important greenhouse gases, these emissions are not usually taken into account, and measurements and calculations of CO₂ emissions are omitted from many studies. This is the case of many studies of HCNG mixtures, of which only a few analyse CO₂ emissions. For example, experimental tests are performed by Ma et al. [10] to validate the proposed model, but no other studies are conducted. Park et al. [11] use a model to study NOₓ variations with 0%, 5%, 10% and 15% of H₂ in the mixtures. Dimopoulos et al. [12] carry out a thermodynamic analysis where CO and NOₓ emissions are analysed with 0%, 10% and 15% H₂ in the mixtures. Tests with mixtures containing 0% and 29% H₂ are performed by Bysveen [13], and HC and NOₓ emissions are recorded. A quasi-dimensional model, with mixtures containing 0%, 50% and 100% H₂, is used by Perini et al. [14] to study CO and NO emissions. The tests conducted by Ma et al. [15] using a supercharged engine contain mixtures with 0%, 30% and 55% H₂, and report only CO, HC and NOₓ emissions.

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Akansu and Bayrak [22]. These works show that emissions of 
Xu et al. [19] reported CO\textsubscript{2} emissions data for mixtures with an H\textsubscript{2} content of 0%, 15%, 20% and 25%. Ceper et al. [20] and Kahraman et al. [21] determined CO\textsubscript{2} emissions with 0%, 10%, 20% and 30% H\textsubscript{2} content of 0%, 5%, 10% and 15% H\textsubscript{2}, but only determined emissions, and to perform a quantitative study on the influence of the hydrogen fraction on engine performance and CO\textsubscript{2} emissions. NO\textsubscript{x} emissions are not presented because the kinetics of the combustion have not been considered, and most NO\textsubscript{x} is produced by the oxidation of nitrogen formed in the combustion process.

2. Natural gas

With regard to emissions, natural gas is one of the cleaner fossil fuels existing today. It is therefore one of the alternatives under study for replacing oil. Nevertheless, certain properties of natural gas make spark ignition engine operation difficult. Its low flame propagation speed during combustion represents the main difficulty. This may be overcome by spark timing optimization, improvements in combustion chamber design, or by increasing turbulence [23,24].

Interest in natural gas can be evidenced by predicted increases in the number of serial vehicles manufactured using this fuel [25]. From 1991 to 2000, there was a 329% increase. From 2000 to the present, a 980% increase has been reported, and the trend continues to grow. Large increases are being recorded in Western Europe and Asia. In addition, it is interesting to consider the increase in the

\begin{align*}
\frac{\text{mean piston velocity}}{\text{m s}^{-1}} & \quad \text{Sp} \\
\text{time, s} & \quad \text{t} \\
\text{temperature, K} & \quad \text{T} \\
\text{inlet valve closing temperature} & \quad \text{T}_i \\
\text{reference temperature, 298.15 K} & \quad \text{T}_0 \\
\text{specific internal energy} & \quad \text{u} \\
\text{volume, m}^3 & \quad \text{V} \\
\text{displaced cylinder volume} & \quad \text{V}_c \\
\text{burned mass fraction} & \quad \text{x} \\
\text{instantaneous stroke, m} & \quad \text{y} \\
\text{mole fraction of species i} & \quad \text{y}_i
\end{align*}

\begin{align*}
\text{mean piston velocity, m s}^{-1} & \quad \text{Sp} \\
\text{time, s} & \quad \text{t} \\
\text{temperature, K} & \quad \text{T} \\
\text{inlet valve closing temperature} & \quad \text{T}_i \\
\text{reference temperature, 298.15 K} & \quad \text{T}_0 \\
\text{specific internal energy} & \quad \text{u} \\
\text{volume, m}^3 & \quad \text{V} \\
\text{displaced cylinder volume} & \quad \text{V}_c \\
\text{burned mass fraction} & \quad \text{x} \\
\text{instantaneous stroke, m} & \quad \text{y} \\
\text{mole fraction of species i} & \quad \text{y}_i
\end{align*}
purchase cost of a vehicle using natural gas compared to those equipped with conventional engines. This varies from 10.1% to 13.2% for a vehicle equipped with a gasoline spark ignition engine with injection in the intake manifold [26,27]. Estimates have been made assuming production-line vehicle assembly.

Fuel costs and their relationship to equivalent CO2 emissions are represented in Fig. 1 for several types of fuel [28] and data from the authors.

As observed, the global CO2 emissions associated with CNG and their costs are lower than those produced by gasoline or diesel. Hydrogen produces lower CO2 emissions than CNG, gasoline or diesel, but hydrogen always originates from renewable sources. Due to the high price of crude oil, in some cases the cost of H2 is lower than that of gasoline or diesel. In any case, this data has been prepared without taking into account the possible effects of an increase in demand or mass production.

### 3. Engine cycle simulation

A zero-dimensional model was chosen from the possible cycle simulation models indicated. It includes two regions at the combustion stage, for unburned and burned gases. The reason for this selection is based on the aim of this work: to perform parametric and optimization studies on various engines as a preliminary phase, prior to the development or modification process to make the engine operable with HCNG mixtures. Thus, it is important to avoid leaving a number of details to be changed later, such as the combustion chamber geometry.

The model used requires fewer fitting parameters than more complex models. However, this will not lead to worse results in this case. For example, those models using a turbulent combustion scheme to determine the burned mass fraction, usually based on the study performed by Blizard and Keck [29], require a large number of fitting parameters. When adopting literature values instead of performing the fitting process, the uncertainty of the results obtained increases. In addition, the combustion chamber geometry must be known in order to determine the front flame location and geometry by means of procedures such as those proposed by Bayraktar [30,31].

In the zero-dimensional model with two zones, each of these regions can be studied separately as two systems with a uniform composition and thermodynamic state. The geometry of both regions must be calculated to evaluate the heat transfer [32-35]. Models assuming similar hypotheses have been developed to study the behaviour of reciprocating engines with different pure fuels [36]. In this work, the fuel consists of a natural gas and hydrogen mixture with variable proportions.

To develop the model proposed [37], the following assumptions and approximations are considered:

1. The fluid under study behaves as an ideal mixture consisting of:
   a. Humid air, fuel and residual gases, during the intake and compression processes.
   b. Two regions, one corresponding to the unburned mixture (air, fuel and residual gases) and the other to the burned gases, during the combustion process.
   c. The combustion products, during the expansion process.
2. The fluid velocity inside the combustion chamber is negligible.
3. The blow-by effect is neglected.
4. Spherical front flame is assumed.
5. Uniform temperature is assumed in each region.
6. The determination of unburned gas properties is performed by neglecting the pre-flame reactions, assuming the gas is frozen (the gas consists of a mixture of ideal gases).
7. Local thermodynamic equilibrium is assumed, allowing the use of the ideal gas state equation with the burned and unburned gas [38].
8. The reactant gas mixture is at thermodynamic equilibrium.

#### 3.1. Mixing and intake processes

The fuel is introduced in the intake manifold and mixed with air. The chemical equation of the process is:

\[
\varepsilon \cdot \phi (v_1 \text{CH}_4(g) + v_2 \text{H}_2(g) + 0.21 \text{O}_2 + 0.79 \text{N}_2 + \text{H}_2\text{O}) + (T_p) + \varepsilon \cdot \phi (v_1 \text{CH}_4(g) + v_2 \text{H}_2(g) + 0.21 \text{O}_2 + 0.79 \text{N}_2 + \text{H}_2\text{O}) + (T_p) \quad (1)
\]

where \(\varepsilon\) is the total mole number of fuel, \(\phi\) represents the fuel/air equivalence ratio, \(\bar{\omega}\) represents the molar humidity ratio, and \(v_i\) stands for the mole amount of component \(i\) per mole of fuel mixture. If pure natural gas is used, \(v_2 = 0\), but \(v_1 \neq 0\) if pure hydrogen is used.

The thermodynamic properties of the air-fuel mixture obtained are calculated by applying the first law of thermodynamics to the mixing process. Variations of kinetic and potential energies have been neglected, and no work is assumed during the process. The resulting equation to be solved is:

\[
\sum_{i=1}^{N} \rho_i c_p^0_i \frac{dT}{dt} + 0.21 \rho_{p_{o_2}} c_p^0_{o_2} \frac{dT}{dt} + 0.79 \rho_{p_{o_2}} c_p^0_{o_2} \frac{dT}{dt} + \bar{\omega} \rho_{p_{o_2}} c_p^0_{o_2} \frac{dT}{dt} - Q = 0
\]

where \(c_p^0_i\) represents the constant-pressure specific thermal capacity of gas \(i\), considered an ideal gas [39], \(T_0\) stands for the reference temperature (298.15 K), \(T_i\) is the intake air temperature, \(T_f\) represents the fuel temperature prior to injection, and \(Q\) is the heat transfer during the process.

Once the air-fuel mixture is obtained, it is introduced into the cylinder. This phase is characterized by the mixing process of the
residual gases inside the cylinder and the air-fuel mixture entering in the cylinder.

To calculate the thermodynamic conditions during the gas exchange processes, the general equation to be solved is

\[ \frac{dp}{dt} = \gamma \cdot \frac{p}{\gamma - 1} \left( \frac{m_c}{m_e} \Delta h - \frac{m_c}{m_e} \Delta h_c \right) \]

(3)

where \( e \) stands for exhaust and \( i \) for intake. In this equation, \( \gamma \cdot \frac{m_c}{m_e} \) and \( \frac{m_c}{m_e} \) represent the thermal capacity ratio, constant-pressure specific thermal capacity and cylinder volume, respectively, \( m \) means mass flow rate, and \( Q \) stands for the heat transfer rate. In addition, the following equations must be used

\[ \frac{dm_c}{dt} = m_i - m_e \]  

(4)

and

\[ m = \begin{cases} 
C_0 A_0 \frac{p}{\gamma \cdot n_D \cdot \sqrt{p}} \sqrt{\frac{p}{\gamma - 1}} \left( 1 - \left( \frac{p}{p_0} \right)^\frac{\gamma - 1}{\gamma} \right), & \text{if } p < \left( \frac{p_0}{p_0} \right)^\frac{\gamma - 1}{\gamma} \\
C_0 A_0 \frac{p}{\gamma \cdot n_D \cdot \sqrt{p}} \sqrt{\frac{p}{\gamma - 1}} \left( \frac{p}{p_0} \right)^\frac{\gamma - 1}{\gamma}, & \text{if } p > \left( \frac{p_0}{p_0} \right)^\frac{\gamma - 1}{\gamma} 
\end{cases} \]  

(5)

where \( C_0 \) is the discharge coefficient, \( A_0 \) represents the throat area, and \( p_i \) and \( p_r \) stand for the stagnation pressure and the pressure at the throat, respectively.

Moreover, to evaluate the heat transfer rate, the convection heat transfer coefficient must be calculated. Therefore, similarly to the compression process detailed in the following section, the Woschni equation [40] is used (Eqs. (11) and (12) and Table 1).

### 3.2. Compression and expansion

For both the compression and expansion phases, the equations governing such processes are similar, except that the gas composition during the expansion process is variable due to the existence of dissociation reactions.

The thermodynamic conditions during the process are determined by applying the first law of thermodynamics to the fluid inside the cylinder. Variations of mechanical energy are neglected, and the equation of state for an ideal gas is used for the gas mixture. Then, dividing by the crank angle, the following expression can be written

\[ \frac{dp}{d\theta} = -\gamma \frac{p}{V} \frac{dV}{d\theta} - \frac{1}{V} \frac{dQ}{d\theta} \]  

(6)

The terms appearing in this equation are evaluated by means of the following expressions

\[ \frac{dQ}{d\theta} = h(\theta) A(\theta) (T(\theta) - T_w) \]  

(7)

where \( h \) and \( n \) stand for the convection heat-transfer coefficient and the crankshaft rotational speed, respectively. The wall temperature is represented by \( T_w \). Total area \( A \) is the sum of the surface areas of cylinder liner \( A_L \), cylinder head \( A_H \), and piston crown \( A_P \), respectively

\[ A = A_L + A_H + A_P = \pi D^2 \]  

(8)

which can be expressed as a function of cylinder bore \( D \) and instantaneous stroke \( y \). This magnitude can be calculated by

\[ y = h_c + a \left( \sqrt{(2\lambda + 1)^2 - e^2} - \cos \theta - \sqrt{4\lambda^2 - (\sin \theta - e)^2} \right) \]  

(9)

where \( h_c \) is the equivalent height of the combustion chamber, and \( a, \lambda, \) and \( e \) represent the crank radius, the ratio of connecting rod length to crank radius, and the relative offset (cylinder axis offset from the crankshaft axis/crank radius), respectively

\[ h_c = \frac{L}{r_c - 1} - \frac{a \left( \sqrt{(2\lambda + 1)^2 - e^2} - \sqrt{(2\lambda - 1)^2 - e^2} \right)}{r_c - 1} \]  

(10)

where \( r_c \) stands for the compression ratio and \( L \) is the piston stroke.

As stated above, the convection heat transfer coefficient is calculated using the Woschni equation

\[ h = C D^{0.8} \]  

(11)

where

\[ U = C_1 S_p + C_2 \frac{V_d T_r}{n_D} \]  

(12)

where \( S_p \) is the mean piston velocity, \( V_d \) is the displaced cylinder volume, \( T_r \), \( p \), and \( V_r \) represent the inlet valve closing temperature, pressure, and volume, respectively.

The wall temperature [41] is evaluated by means of

\[ T_w = 440 + 9 n_{tg} (nD)^{0.2} \]  

(13)

with \( n_{tg} \) being the volumetric efficiency.

Afterwards, Eqs. (6)–(13) lead to

\[ \frac{dp}{d\theta} = -\gamma \frac{p}{V} \frac{dV}{d\theta} - \frac{1}{V} \frac{dQ}{d\theta} = \left( \frac{\pi D^2}{2} \right) \left[ (\pi D^2 - \pi \frac{p}{m}) T - (440 + 9 n_{tg} (nD)^{0.2}) \right] \]  

(14)

which makes it possible to determine the fluid evolution during either the compression or expansion process.

### 3.3. Combustion

Ten chemical species [42,43] and two regions have been considered inside the chamber (unburned and burned gas regions) for the combustion process. The corresponding chemical reaction is

\[ \varepsilon \phi (v_1 CH_4 + v_2 H_2) + (0.2102 O_2 + 0.799 N_2 + \varepsilon \phi H_2O) \rightarrow \mu_1 CO_2 + \mu_2 H_2O + \mu_3 N_2 + \mu_4 O_2 + \mu_5 CO + \mu_6 H_2 + \mu_7 H + \mu_8 O + \mu_9 NO \]  

(15)

The mole amount of product \( i (i = 1, \ldots, 10) \) per mole of fuel mixture is represented by \( \mu_i \).

To solve this problem, a non-linear equation system is used, constituted by the mass balances

\[ C \rightarrow \varepsilon \phi v_1 = (y_1 + y_9) N \]  

\[ H \rightarrow \varepsilon \phi (4v_1 + 2v_2) + 2 \varepsilon = (2y_2 + 2y_6 + y_7 + y_9) N \]  

\[ O \rightarrow 0.42 + \varepsilon = (2y_1 + y_2 + 2y_4 + y_5 + y_8 + y_9 + y_{10}) N \]  

\[ N \rightarrow 0.79 - 2 = (2y_3 + y_{10}) N \]  

(16)

and the equilibrium constants \( K_p \) corresponding to the dissociation of the products in equilibrium
\[
\begin{align*}
\frac{1}{2}H_2 + H &\rightarrow K_1 = \frac{y_2 p^{1/2}}{y_1^{1/2}} \\
\frac{1}{2}O_2 + O &\rightarrow K_2 = \frac{y_9 p^{1/2}}{y_4^{1/2}} \\
\frac{1}{2}H_2 + \frac{1}{2}O_2 + OH &\rightarrow K_3 = \frac{y_9 y_4^{1/2}}{y_2^{1/2} y_6} \\
\frac{1}{2}O_2 + \frac{1}{2}N_2 + NO &\rightarrow K_4 = \frac{y_{10} y_4^{1/2}}{y_2^{1/2} y_3} \\
H_2 + \frac{1}{2}O_2 + H_2O &\rightarrow K_5 = \frac{y_7}{y_4^{1/2} y_6 p^{1/2}} \\
CO + \frac{1}{2}O_2 + CO_2 &\rightarrow K_6 = \frac{y_1}{y_2^{1/2} y_3 p^{1/2}}
\end{align*}
\]

where \( y_i \) is the mole fraction of species \( i \) in the products, and \( N \) is the total mole amount of the products. Then \( \sum_{i=1}^{10} y_i = 1 \)

\[(18)\]

It must be noted that when pure hydrogen is used, \( v_1 = 0, y_1 = 0 \), \( y_5 = 0 \) and \( K_6 \) do not apply because carbon is not present in the medium.

The equilibrium constant values are calculated by means of the expression

\[
\log K_p = A \ln \frac{T}{1000} + B + C + DT + ET^2
\]

\[(19)\]

where constants \( A, B, C, D \) and \( E \) are taken from Ferguson [43] and Olikara and Borman [44].

In addition, the first law of thermodynamics is used. Because the two regions (for unburned and burned gas) are assumed to be inside the combustion chamber, this equation can be written as

\[
Q_a + Q_b - \int_1^2 pdV = [U_a + U_b]_2 - [U_a + U_b]_1
\]

\[(20)\]

where 1 and 2 represent the initial and final states at each step in the calculation, respectively.

Taking into account Eq. (7), in this case

\[
Q_a = A_h b h(T_a - T_{w,b}) \Delta \theta
\]

\[(21)\]

\[
Q_b = A_h b h(T_b - T_{w,b}) \Delta \theta
\]

\[(22)\]

where \( \Delta \theta \) is the crank angle increment and

\[
\int_1^2 pdV = \frac{P_2 + P_1}{2} (V_2 - V_1)
\]

\[(23)\]

as well as the equations of state for unburned and burned gas, the following equation is obtained

\[
\left[ A_h b h \left( \frac{\rho_0}{\rho_a} \right) - T_{w,u} \right] + A_h b h \left( \frac{\rho_{10}}{\rho_a} - T_{w,b} \right) \Delta \theta = \frac{P_2 + P_1}{2} (V_2 - V_1)
\]

\[(24)\]

where \( u \) means specific internal energy.

Similarly to the compression process, the Woschni expression, Eqs. (11) and (12), and Table 1 are used to calculate the heat transfer coefficient, and the Muller expression [41]. Eq. (13), is used to calculate the cylinder wall temperature.

To calculate the volumes occupied by both unburned and burned gas, the mass inside the cylinder is considered constant. In addition, the Livengooz hypothesis [45] is used for the unburned gas

\[
\frac{V^W}{V^B} = \frac{\rho_a}{\rho_b}
\]

\[(25)\]

where \( \rho_a \) and \( \rho_b \) are the densities at the intake and exhaust, respectively.

\[
pV^W_a = p_{\text{initial}}V^W_{\text{initial}}
\]

\[(26)\]

Table 2

<table>
<thead>
<tr>
<th>( A )</th>
<th>( E_a )</th>
<th>( n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( H_2 )</td>
<td>( 2.82 \times 10^{-13} )</td>
<td>336</td>
</tr>
<tr>
<td>( CH_4 )</td>
<td>( 3.23 \times 10^{-2} )</td>
<td>192</td>
</tr>
</tbody>
</table>

Table 3

<table>
<thead>
<tr>
<th>Item</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement volume (cm³)</td>
<td>1039</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>10.5</td>
</tr>
<tr>
<td>Bore (mm)</td>
<td>105</td>
</tr>
<tr>
<td>Stroke (mm)</td>
<td>120</td>
</tr>
<tr>
<td>Rating power (kW)</td>
<td>154</td>
</tr>
<tr>
<td>Rating torque (Nm)</td>
<td>620</td>
</tr>
<tr>
<td>Intake valve open (°BTDC)</td>
<td>18</td>
</tr>
<tr>
<td>Intake valve close (°ABDC)</td>
<td>37</td>
</tr>
<tr>
<td>Exhaust valve open (°BBDC)</td>
<td>56</td>
</tr>
<tr>
<td>Exhaust valve close (°ATDC)</td>
<td>11</td>
</tr>
<tr>
<td>Ratio of connecting rod length to crank radius</td>
<td>1.833</td>
</tr>
<tr>
<td>Relative offset</td>
<td>0.0422</td>
</tr>
</tbody>
</table>

Table 4

<table>
<thead>
<tr>
<th>Case</th>
<th>( n ) (rpm)</th>
<th>( p_1 ) (bar)</th>
<th>( %H_2 )</th>
<th>( \phi )</th>
<th>( \theta_c (°) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1600</td>
<td>0.70</td>
<td>20</td>
<td>0.769</td>
<td>26</td>
</tr>
<tr>
<td>B</td>
<td>1600</td>
<td>1.20</td>
<td>20</td>
<td>0.769</td>
<td>26</td>
</tr>
<tr>
<td>C</td>
<td>1200</td>
<td>1.05</td>
<td>10</td>
<td>0.752</td>
<td>30</td>
</tr>
<tr>
<td>D</td>
<td>1200</td>
<td>1.05</td>
<td>30</td>
<td>0.714</td>
<td>30</td>
</tr>
<tr>
<td>E</td>
<td>1600</td>
<td>0.87</td>
<td>40</td>
<td>0.833</td>
<td>24</td>
</tr>
<tr>
<td>F</td>
<td>1600</td>
<td>0.87</td>
<td>50</td>
<td>0.800</td>
<td>22</td>
</tr>
<tr>
<td>G</td>
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<td>0.80</td>
<td>0</td>
<td>0.769</td>
<td>32</td>
</tr>
<tr>
<td>H</td>
<td>1200</td>
<td>1.05</td>
<td>0</td>
<td>0.613</td>
<td>30</td>
</tr>
</tbody>
</table>

\[
pV^W_a = p_{\text{initial}}V^W_{\text{initial}}
\]

\[(27)\]

\[
\frac{dx}{d\theta} = \frac{\theta}{\delta_c} (m + 1) y^m \exp^{-\theta^{m+1}}
\]

\[(28)\]

where \( \delta_c \) is the combustion development angle. Therefore

\[
x = \int_1^2 \frac{dx}{d\theta} d\theta = 1 - \exp^{-\theta^{m+1}}
\]

\[(29)\]

where \( m \) is the shape parameter (\( m = 2 \)) and \( \alpha \) stands for the Vibe parameter (\( \alpha = 5 \)).

The expressions used to evaluate the wet chamber surface areas for unburned gas \( A_u \) and burned gas \( A_b \) are the following

\[
A_u = (1 - x)A
\]

\[(30)\]

\[
A_b = xA
\]

\[(31)\]

3.4. Knock

Knock is an important effect to consider for poly-fuel engines. The appearance of knock has been determined by using empirical
models to calculate induction time $\tau_0$. This is calculated from pure methane and hydrogen induction times by means of the following expression [47]
\[
\tau_0 = \tau_{\text{CH}_4}^{1-\beta} \cdot \tau_{\text{H}_2}^\beta 
\]
where
\[
\tau = A \cdot \left( \frac{P}{T} \right)^n \cdot \exp \left( \frac{E_a}{RT} \right)
\]
where $p$, $T$ and $\beta$ stand for pressure, temperature, and the hydrogen molar fraction in the mixture, respectively. The values of parameters $A$, $n$ and $E_a$, depending on the fuel, are shown in Table 2.

Therefore
\[
\tau_0 = A_{\text{CH}_4}^\beta \cdot A_{\text{H}_2}^{1-\beta} \cdot \left( \frac{P}{T} \right)^{n_{\text{H}_2} \beta + n_{\text{CH}_4} (1-\beta)} \cdot \exp \left( E_{\text{H}_2} \beta + E_{\text{CH}_4} (1-\beta) \right)
\]

Knock appears when the following condition is attained
\[
\int_0^t \frac{1}{\tau_0(t)} \, dt = 1
\]

4. Validation of the model

The experimental results provided by Ma et al. [10], obtained under given operating conditions, have been used to validate the model. Therefore, the operating conditions imposed in this study [10] have been used (see Table 4 of this reference); the experimental results used for validation purposes are shown in Fig. 8 of the same reference, and the specifications of the engine used by Ma et al. [10] are detailed in Refs. [48,10]. Thus, the specifications of the engine simulated in this work are compiled in Table 3, and the different operating conditions used to validate the model are shown in Table 4, where $\phi_{ig}$ represents the spark timing crank angle and $\phi$ stands for the fuel/air equivalence ratio.
5. Results and discussion

5.1. Effect of hydrogen addition on engine performance

In order to evaluate the influence of the hydrogen fraction on engine performance, different fuels are used to run the model. The specifications of the simulated engine are shown in Table 3, and the operating conditions in Table 5.

Fig. 4 shows variations in pressure with respect to the crank angle for three mixtures (pure natural gas, HCNG with 50% hydrogen, and pure hydrogen) and different spark timing values. Fig. 5 shows the indicated work as a function of spark timing. Fig. 6 shows variations in pressure with respect to the crank angle for the three mixtures and different compression ratio values. Fig. 7 represents the power delivered by each fuel as a function of the crankshaft engine rotational speed.

As shown in Figs. 4 and 5, the maximum pressure in the cylinder and the indicated work increase as the hydrogen fraction rises. The maximum pressure is 8% higher with pure hydrogen than with pure CNG. Consequently, the indicated work and power delivered are also enhanced by increasing the amount of hydrogen. The indicated work is 15.2% higher with pure hydrogen than with pure CNG. This occurs because the specific energy of hydrogen is higher than that of natural gas. Therefore, the temperature reached in the cylinder is also higher. As observed in Fig. 4, the crank angle at which the maximum pressure occurs is different for each fuel.

Fig. 5 shows the optimum spark timing required to attain the maximum work depending on the hydrogen content of the mixture.

Similar behaviour to that described earlier is observed at two different compression ratios (see Fig. 6). The maximum pressure rises as the hydrogen content of the mixture increases. An analogous trend is observed for the power delivered as a function of the engine speed (Fig. 7). As in the case of the indicated work, the power increase is proportional to the increase in hydrogen content, exhibiting a nonlinear variation with the hydrogen content in the mixture.
As the air/fuel ratio increases, with the maximum temperature equilibrium temperature of the combustion products will decrease. Large cycle-by-cycle variations, thus decreasing the thermal efficiency. This affects the efficiency, which increases with higher air/fuel ratios. This occurs because the burned gas temperatures drop after combustion, thus decreasing the thermal capacities of the burned gas, and therefore increasing the effective value of the thermal capacity ratio in the expansion stroke. Efficiency increases due to the burned gas expand through a higher temperature increment before the exhaust. Then the expansion stroke work increases by mass fuel unit.

It must also be noted that the mean effective pressure diminishes with increasing air/fuel ratios. Although the efficiency increases, such an increase is balanced by the increase in the air/fuel ratio, and the latter has a greater influence. Fig. 8 shows that because both the power and the CO₂ emissions decrease as the air/fuel ratio increases, the latter exhibits greater drops, eventually leading to a decrease in specific CO₂ emissions. As an example, for 50% mixtures at 2000 rpm, power increases of 9.7% with respect to CNG are reached under the conditions studied, and reductions of up to 25.9% in specific CO₂ emissions are attained.

The behaviour caused by rotational speed variation can be justified based on the effect of the temperature reached inside the cylinder and its effect on CO₂ emissions. As the rotational speed increases, the engine behaves in a more adiabatic way. The temperature inside it rises, leading to lower CO₂ emissions with a more complex burned gas composition, in which species such as OH, O and H are present. In this case, power increases and CO₂ emissions decrease, leading to a clear drop in specific CO₂ emissions.

5.2. Effect of hydrogen addition and air/fuel ratio on CO₂ emissions

To analyse the effect of hydrogen addition and air/fuel ratio on CO₂ emissions, several blends of natural gas and hydrogen were studied: compressed natural gas (CNG), and HCNG with hydrogen fractions from 10% to 90%, with an air/fuel ratio within reasonable operating limits. Hydrogen has a high flame propagation speed and low ignition energy, making it possible to work with leaner mixtures than pure natural gas.

There is a limit for lean air–fuel mixtures because if this limit is reached, the combustion becomes unstable and incomplete. Operating close to this limit decreases the combustion speed and increases the ignition energy of the air–fuel mixture, leading to large cycle-by-cycle variations, thus decreasing the thermal efficiency.

Fig. 8 shows specific CO₂ emissions with respect to the air/fuel ratio for different fuel compositions at three different engine speeds, respectively. It is observed that specific CO₂ emissions decrease when fuel mixtures with increasing hydrogen content are used, when the air/fuel ratio increases, and when the crankshaft rotational speed increases.

A decrease in specific CO₂ emissions with an increasing H₂ content in the fuel mixture can be attributed to a progressive decrease in the carbon content, and also to the enhancement of the combustion process.

To explain the observed behaviour of CO₂ emissions with increasing air/fuel ratios, several aspects must be considered. The equilibrium temperature of the combustion products will decrease as the air/fuel ratio increases, with the maximum temperature value corresponding to an air/fuel ratio near the stoichiometric ratio. This affects the efficiency, which increases with higher air/fuel ratios. This occurs because the burned gas temperatures drop after combustion, thus decreasing the thermal capacities of the burned gas, and therefore increasing the effective value of the thermal capacity ratio in the expansion stroke. Efficiency increases due to the burned gas that expand through a higher temperature increment before the exhaust. Then the expansion stroke work increases by mass fuel unit.

It must also be noted that the mean effective pressure diminishes with increasing air/fuel ratios. Although the efficiency increases, such an increase is balanced by the increase in the air/fuel ratio, and the latter has a greater influence. Fig. 8 shows that because both the power and the CO₂ emissions decrease as the air/fuel ratio increases, the latter exhibits greater drops, eventually leading to a decrease in specific CO₂ emissions. As an example, for 50% mixtures at 2000 rpm, power increases of 9.7% with respect to CNG are reached under the conditions studied, and reductions of up to 25.9% in specific CO₂ emissions are attained.

The behaviour caused by rotational speed variation can be justified based on the effect of the temperature reached inside the cylinder and its effect on CO₂ emissions. As the rotational speed increases, the engine behaves in a more adiabatic way. The temperature inside it rises, leading to lower CO₂ emissions with a more complex burned gas composition, in which species such as OH, O and H are present. In this case, power increases and CO₂ emissions decrease, leading to a clear drop in specific CO₂ emissions.

It is important to note that, as observed for the power increase, the drop in CO₂ shows a nonlinear variation as the hydrogen content increases. This can be seen in Fig. 9, which shows the case of a relative air/fuel ratio equal to 1.3. This is an important feature when selecting the optimum hydrogen content in the mixture, as lower proportions of hydrogen lead to smaller drops in CO₂ and smaller increases in power. As the hydrogen content increases, these phenomena are much more significant, becoming evident from 40% H₂ onwards. In any case, other factors must be considered, such as fuel costs, the cost of modifying the required engine, engine maintenance costs, and the safety problems that arise when the H₂ content is increased. Determining the optimum proportion of H₂ in the mixture therefore becomes a complex task, depending on the generation technologies (W-t-W studies) and their cost.

6. Conclusions

Given the growing importance of alternative fuels, an indicated cycle model for a spark ignition engine operating with variable blends of hydrogen and natural gas (HCNG) has been developed. This model makes it possible to modify geometrical parameters, engine operating conditions, and fuel composition. The model was used to determine the engine’s performance and CO₂ emissions, and was experimentally validated, always producing mean indicated pressure errors under 3%. The maximum cycle pressure and indicated work obtained increase along with the proportion of hydrogen in the HCNG, and leaner mixtures can be used. As the hydrogen content in the mixture rises, CO₂ emissions drop. The decrease in CO₂ emissions and the increase in power both exhibit a nonlinear variation as the hydrogen content increases, and these phenomena are much more significant when the hydrogen content in the mixture is high. This, along with the resulting increase in power, makes HCNG advantageous compared to other fuels.

Acknowledgement

This work has been partially supported by the Universidad Politécnica de Madrid within the framework of Project Code No. AL11-PI(1+D)-03.
References


