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Definition and Validation of a Zero-Dimensional IC Engine Model for Assessing the Performance of Different Methane-Hydrogen Mixtures

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Abstract. To decarbonize the maritime transport sector, a solution inspired by the automotive industry involves using a solid oxide fuel cell (SOFC) in conjunction with an internal combustion engine. For optimal emission efficiency, the internal combustion engine is fueled with a primary fuel, typically methane already on board for feeding the SOFC, plus anode off-gases from SOFC, which are a mixture of variable composition of hydrogen, carbon dioxide, and carbon monoxide. To assess the performance of the integrated system (SOFC+ICE) and subsequently search for an optimal set-up, it is useful to use a zero-dimensional model of each component of the system. Particularly, the internal combustion engine model must balance speed of execution with flexibility in terms of fuel composition, engine dimensions, and other relevant parameters. In this study, an engine model originally developed for gasoline-fueled ICE, is adapted for variable methane-hydrogen mixtures. The model is validated against experimental data measured on an engine operating with similar mixture compositions and available in the literature.

1. Introduction

For the future, the decarbonization of all transport sectors is necessary. The transport sub-sectors, i.e. road, aviation, rail, and ship, accounts for 16.2% of global emissions [1]. Ship sub-sector accounts for 1.8% of global emissions [2], despite this, ship emissions are particularly felt in harbors for maneuvering and hoteling operations. Therefore, in the world of shipping the issue of limiting pollutant emissions is very topical, as highlighted by the increasing restrictions adopted by the International Maritime Organization (IMO) in the theme of the emissions [3]. Also, the issue of decreasing CO2 emissions is being considered with increasing attention. In the field of maritime propulsion, the reduction of the emissions could be pursued by increasing the overall efficiency of the propulsion system and using fuels with low or zero carbon content.

The main targets are, thus, on one hand, to maximize efficiency and to minimize emissions of the energy system identified as the prime mover of the maritime propulsion, on the other hand to feed the prime mover with a low-carbon content fuel. To this end, the Solid Oxide Fuel Cells (SOFC), already largely investigated for terrestrial applications, and the Internal Combustion Engines (ICEs), powered by methane or Natural Gas (NG), could be integrated. The authors participate to the SOFFHICE national project which aims to investigate the propulsive system composed of a SOFC and an ICE, which was identified as the prime mover for a short-distance ferry trip, where the power of the SOFC would not be enough to navigate even with high waves. The hybrid SOFC + ICE system was revealed to be able to respond to sudden and significant load variations through hybridization with the engine, thereby

enhancing the dynamic characteristics of the SOFC [4-7]. In the SOFFHICE project, the SOFC+ICE system should enable the two energy systems to operate jointly in offshore navigation: i) maximizing ICE efficiency and thus reducing emissions/fuel consumptions; ii) making the SOFC mostly work in port/coastal areas (hotelling/maneuvering fully driven by SOFC), allowing the reduction of local pollutants emissions (e.g., NOx, SOx, PM).

One of the main objectives of SOFFHICE project is to model the thermodynamic interaction of the two technologies: in this context, the authors of the present work have to develop a 0D engine model capable of reproducing the performances and the emissions of the chosen maritime engine equipping the reference vessel under the assessed energy demand for a typical vessel journey profile.

In this context of alternative fuels, the main aims are the depletion of petroleum-derived conventional fuels (such as gasoline and diesel) with high-carbon content. In the mid-term scenario, the use of methane (or NG) instead of conventional petroleum-derived fuels is an interesting and ready-to-use solution. Nowadays, methane is the only competitive alternative to diesel fuel due to highest production capacity, expanding infrastructure, highest gravimetric energy density, non-toxicity, high technical feasibility in ICEs and FCs, reduction in CO2, and large reductions in SOx and particulate matter emissions while maintaining comparable NOx emission [8]. The importance of methane as a hydrocarbon-based fuel for maritime engines is well assessed due to the high thermal efficiency of burning methane in lean-burn natural gas engines. Methane has a low-carbon content, but its intrinsic properties (low flame speed and combustion stability) compromise the combustion process, leading to an increase of carbon dioxide, mainly due to stability problems under ultra-lean conditions. To overcome this issue, the hydrogen enrichment strategy represents an attractive and advantageous solution because it boosts flame propagation, increasing the stable operating range of the combustion process at high-diluted conditions [9-11]. Hydrogen can be supplied in the vehicle following multiple approaches: one possibility is to make the most of the Anode Off-Gases (AOG) which are discarded by the SOFC, increasing the efficiency of the overall system SOFC+ICE. Thus, in the SOFFHICE project, to increase engine performances, the idea is to use very-lean mixtures, in which the main propellant is methane (or natural gas), combined with AOG (whose composition is load-dependent, but the main components are hydrogen, carbon monoxide and carbon dioxide because the mixture is anhydrous) from SOFC, which should boost the combustion process, increasing the combustion efficiency. To model the overall reactant mixture, where hydrogen and carbon monoxide are expected to speed up the flame propagation speed, while carbon dioxide is expected to slow it down, a methodology based on the modeling of the chemical kinetic reactions in the open-source library Cantera is adopted. Thus, in this methodology, both methane and AOG components will be treated as reagents. The performance comparison will be conducted using an in-house developed 0D ICE-code. The code uses Wiebe's law to model the heat release in combustion in which the laminar flame speed (LFS) is used to evaluate the length of the combustion period. The LFS, and the self-ignition time, are obtained by chemical-kinetic simulation for different pressure, temperature and mixture index conditions, then organized in tabular form, so that they can be read by the code.

The performance evaluation will be conducted in some stationary load points for different fuel composition and mixture index, defined, as in [12], by imposing that the overall energy released by the fuel or the fuel mixture, i.e. the product of the lower heating value LHV (calculated according the actual composition of the mixture), is conserved and the combustion efficiency is assumed constant (equal to 0.98).

In the present scientific work, an engine not having the characteristics of a marine engine but for which experimental indicating and heat release data are available for a mixture composed of natural gas (NG) and hydrogen in variable proportions, from 0% up to maximum 3% in mass, with the same energy released by the fuel [12], is used for comparison. It is worth mentioning that in the maritime case the hydrogen comes from AOGs, thus a maximum percentage of 3% is absolutely acceptable. The main focus of the work is to obtain a validated model capable of simulating the performance of an actual engine fed by multiple fuels (in the present case, methane and hydrogen only) in some stable load conditions. Once the validation of both the model and the methodology has been obtained, it will be possible to use the model for simulating the maritime engine. In particular, the maritime engine will be fed by a multi-

component fuel, whose main composition will be Natural Gas (mainly composed by methane), already available on the ship because is the feeding fuel of the SOFC, and AOGs coming from the SOFC exhaust, whose percentage composition depends on the specific load conditions but it will be constituted by hydrogen, carbon-monoxide and carbon-dioxide (it's a anhydrous mixture due to the overall condensation of the water vapor before the admission of the mixture in the engine).

The present paper is structured as follow:

1. Description of the zero-dimensional (ZD) model of the engine developed by the authors;
2. Use of the Cantera library for computing the laminar flame speed of a bi-fuel mixture (methane plus addition of hydrogen);
3. Validation of the implemented integrated methodology against in-cylinder pressure data to capture the effect of hydrogen addition to methane fuel;
4. Validation of the implemented integrated methodology against overall performance maritime engine data;
5. Some brief conclusions.

3. Zero-dimensional engine model description

Engine simulations were performed using an in-house developed zero-dimensional thermodynamic model. Due to the zero-dimensional approach, it is assumed that each point inside the engine cylinder shares the same set of state variables. This approximation is not critical for premixed charge ICEs. The model is based on the in-cylinder energy balance at closed valves (high cycle) to determine the mean temperature (Eq. 1), and on the perfect gas law to determine the mean pressure (Eq. 2). In Eq. 1, m_{mix} is the trapped mixture mass (air and fuel), C_v is the specific heat of the mixture at constant volume, T is the mean temperature, p is the mean pressure, V_c is the engine instantaneous displacement, Q_W is the heat exchanged between the gas mixture and the engine walls (piston, dome, cylinder liner), Q_C is the heat released by the combustion, R_{mix} is the gas constant of the mixture, t is time.

$$m_{mix}\, C_v\, \frac{dT}{dt} = -p\, \frac{dV_c}{dt} - \frac{dQ_W}{dt} + \frac{dQ_C}{dt} \tag{1}$$

$$p\, V_c = m_{mix}\, R_{mix}\, T \tag{2}$$

The energy balance is solved by discretizing Eq.1 according to a first order forward difference scheme in an explicit manner by using the pressure values of the previous step.

The volume variation term is given by the classical crankshaft equation once the engine geometry is given.

The heat losses at the engine walls have been modeled by means of the Woschni's approach [13], thus, by assuming a convective-like heat exchange coefficient estimated according to the Woschni's correlation (Eq. 3). In Eq. 3, C_0 is a tuning constant, B is the engine bore, v is the characteristic gas velocity given by Eq. 4, where $C_{1/2}$ are constants, u_p is the mean piston speed, p_{mot} is the mean pressure at non-firing conditions, *ref* refers to quantities calculated at a reference state (the Bottom Dead Center in this work). C_1 is 2.28, C_2 is non-zero (3.24×10^{-3}) only during the combustion phase, being representative of the radiative heat transfer in a convective shape. As a result, the power exchanged with walls is that in Eq.5, in which A is the surface of the exchange wall (piston and dome are assumed as circle areas), and T_W its temperature.

$$H = C_0\, 0.0195\, p^{0.8}\, B^{-0.2}\, T^{-0.53}\, v^{0.8} \tag{3}$$

$$v = C_1\, u_p + C_2\, V_c \left(\frac{V\, T}{p}\right)_{ref} (p - p_{mot}) \tag{4}$$

$$\frac{dQ_W}{dt} = H \sum_i A_i\, (T - T_{W,i}) \tag{5}$$

The heat release from combustion has been modeled by means of the classical Wiebe correlation, thus, assuming an exponential fuel consumption during the combustion duration. The power produced by combustion is given by Eq. 6, in which LHV is the lower heating value of the fuel, m_f is the total injected fuel mass, χ is the Wiebe function described in Eq. 7. In Eq. 7, α and β are tuning constants, θ is the simulation crank angle, θ_0 is the combustion start, $\Delta\theta$ is the combustion duration.

$$\frac{dQ_C}{dt} = LHV\ m_f\ \frac{d\chi}{dt} \tag{6}$$

$$\chi = 1 - exp\left[\alpha\ \left(\frac{\theta - \theta_0}{\Delta\theta}\right)^{\beta}\right] \tag{7}$$

The combustion start is set at the spark timing; thus, the electric delay and the kernel growth phase have been neglected. The combustion duration is estimated by means of the turbulence promoted into the combustion chamber (which is a tuning parameter) and of the laminar flame speed of the fuel mixture, which has been determined through chemical kinetics simulations of the behaviour of a premixed laminar flame.

The properties of the mixture needed by the model (specific heat, gas constant, lower heating value) are calculated with the simple weighted average as a mixing rule. In particular, the specific heat of each specie is calculated at each time-step as a function of the mean in-cylinder temperature according to the correlations available in the chemical engineers' handbook [14].

The main data required by the model comprises the geometrical features of the engine, the fuel mixture composition, and the operation features (e.g., lambda, i.e. the air-to-fuel ratio divided by the stoichiometric ratio; engine speed; valve timing; spark timing).

The main setting parameters required by the model are: i) the cylinder filling coefficient, which is the relative volumetric efficiency of the intake system; ii) the non-dimensional in-cylinder turbulence at the spark timing (defined as the ratio between the charge velocity fluctuation and the mean piston speed); iii) the time-step for the simulation. The first parameter is needed to calculate the trapped mass and then, by using the operation lambda, the fuel mass. The second one is needed to enhance the laminar flame speed returned by Cantera to provide a realistic estimation of the combustion duration. The third parameter has been set at 0.1 crank angle degree regardless of the engine speed. Furthermore, the tuning of the constants C_0, α, β must be performed based on the engine under investigation.

4. Chemical kinetic simulations and integration

The 0D model requires the value of the laminar flame speed at start of ignition (SOI) thermophysical condition. The LFS depends on the chemical composition of the fuel, the quality of the fuel/oxidant mixture (i.e. the lambda value), the pressure and temperature of the unburned mixture.

To define the LFS for the fresh mixture under different engine thermophysical conditions, a methodology based on the 1D adiabatic flame solver provided by Cantera [15], an open-source library for problems involving chemically reacting flows, proposed and validated by the authors in previous works [16], has been used. The chemical kinetic mechanism chosen is the GRI-Mech [17], which is a detailed kinetic mechanism (53 species and 325 reactions) designed to model the combustion of natural gas, defined as a mixture of hydrogen, methane, ethane and propane, in air. The mechanism is well validated, commonly used, and sufficiently lightweight to keep computational costs low.

For validating the 0D model and for assuring its capability of predicting the performance of an engine fed by more than one fuel, the work by Molina et al. [12] has been taken as reference. The authors believe that, although the experimental data for validation refer to an engine that operates with natural gas (NG) as primary fuel with the addition of hydrogen (up to 3% and with the same energy released in combustion), the working methodology, therefore the results, can be extrapolated for a multi-component fuel, such as that envisaged in the SOFFHICE project. In the SOFFHICE project, in fact, the fuel is

represented by a multi-fuel system, constituted by methane or NG as primary fuel plus H2, CO and CO2, which all come from AOG in different percentages depending on the applied load level.

In [12] the composition of NG has not been reported, only a generic information about its provenience from the natural gas network is cited. It is well known that the natural gas is a mixture between hydrocarbons of the C1-C5 family and other impurities. Albeit its chemical composition is extremely variable, the most present compound is methane, the second most present compound is ethane, with a molar fraction of an order of magnitude lower, the other components are present only in traces. For example, the CNG introduced into the Italian national network in 2022 has a molar fraction of methane varying between 86% and 99% and an ethane molar fraction between 0% and 8% [18].

To assess the difference in LFS value of a fuel composed by pure methane and a NG-like mixture composed by methane, ethane and propane with molar fraction composition of 96.9%, 2.7% and 0.4% respectively, some simulations have been carried out (not reported in the paper for seeking of brevity). The global results show, as expected, a very small difference, so the chemical kinetic modelling results obtained with pure methane (plus subsequent hydrogen additions) were implemented in the 0D model.

For each of the considered mixture between methane and hydrogen, the LFS has been calculated according to a full factorial design by varying the equivalence ratio (from 0.5 to 1.1), the pressure (from 5 bar to 30 bar) and the temperature (from 600 K to 800 K) over a range of values representative of the engine thermophysical condition around the SOI. Next the exact value of LFS for the specific equivalence ratio, pressure and temperature have been obtained via multidimensional spline interpolation. To assess the accuracy of the interpolation method, some points inside the table definition range are chosen, their LFS computed, and compared with the values predicted by interpolation. The difference between the computed and interpolated LFS values, as depicted in the box chart of Figure 1, is sufficiently small to use the interpolator as inline calculator of the LFS.

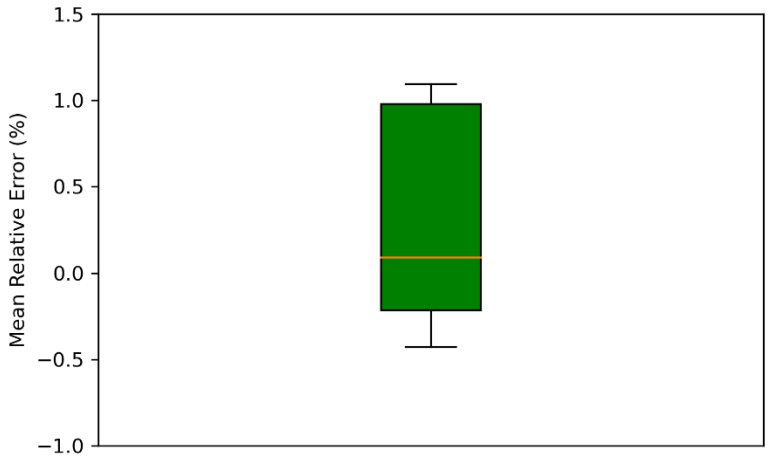

Figure 1: Boxchart of the mean relative error due to the cubic interpolation of the lookup tables of laminar flame speed. Interpolation has been performed for cross combination of air-fuel ratio, pressure, temperature inside the table definition range.

5. Application of the integrated methodology for hydrogen addition

To assess the reliability of the model from the standpoint of gas engines including hydrogen at low speed, the code has been validated against a reference engine [12] from the literature. The reference engine is a single-cylinder port-fuel injection spark ignition (SI) engine operating with CNG-hydrogen fuel mixtures. Hydrogen and CNG are separately injected in a plenum upstream of the intake manifold for composition control purposes. The main features of the engine are summarized in Table 1 together with the tested operation points.

The first test fuel from [12] has been chosen as benchmark case (CNG fuel), whilst the second test fuel has been chosen as the one with the largest presence of hydrogen among the three available (i.e. 3%wt). These two test fuels have been simulated at three different operation points, namely 1500 rpm x IMEP 7 bar, 1500 rpm x IMEP 10 bar, 3000 rpm x IMEP 10 bar. It is highlighted that methane (CH_4) has been used during simulations in place of CNG, once the Authors checked out the weak difference between those two fuels in chemical kinetics simulations, as previously reported.

Table 1. Engine architecture [12] and test fuels.

Data	Values
Number of cylinders	1
Number of strokes	4
Displaced volume (cm^3)	454.2
Stroke / Bore (mm)	86.0 / 82.0
Injection system	PFI (up to 8 bar)
Compression ratio (-)	10.7
Connecting rod length (mm)	144.0
Fuel (Case 1 / Case 2)	100%CNG / 97%CNG-3%H_2

Regarding the tuning of the model, the following routine has been applied:

- the filling coefficient is responsible for the amount of air trapped inside the cylinder, which determines the pressure curve during compression stroke before combustion. Thus, the value of the filling coefficient was set to match the experimental pressure curve before the spark timing;
- the tuning constant C_0 is a gain on the magnitude of the heat losses, which significantly affects the pressure curve during expansion and discharge strokes due to the high temperature of the combustion gases compared to those of the engine walls. Therefore, the value of C_0 has been set in order to adjust the simulated pressure curve steepness after the top dead center. In this work, C_0 has been changed (doubled) when hydrogen-methane simulations have been performed. This is likely due to the weak quenching effect on hydrogen flames which enhances the heat exchange between the gas and the walls;
- the tuning constant α of the Wiebe correlation is defined by the expression $-\log(1-\eta_{combustion})$, thus, it has been set at 4.6 corresponding to an almost perfect combustion ($\eta_{combustion}$ around 99%) which is a reasonable approximation for a premixed gas combustion;

- the tuning of constant β of the Wiebe correlation and of the non-dimensional turbulence has been performed in order to match the combustion shape (peak pressure and peak position). It is underlined that the tuned values of these two coefficients have not been changed between the two tested points. The simulated pressure curve of two different cases (no hydrogen, 3% hydrogen) is reshaped by the model according to a different combustion duration promoted by the different fuel supplied as input to the model. As a result, the Wiebe correlation does not require tailored tuning thanks to the combustion duration adjustment implemented by the different laminar flame speed.

The validations of the test cases are shown in Figure 2, Figure 3 and Figure 4. It is visible that regardless of the fuel mixture tested, the shape and the phasing of the curve pressure is nice, and the pressure peak is captured with deviations between 1.1 and 1.5 bar.

For all the six simulations, the laminar flame speed returned by the interpolator lies between 50 and 65 cm/s. This can be expected by observing the small amount of hydrogen added to the mixture (max 3%wt) as well as the slight variation of spark timing between the test points (from 22 to 19 deg BTDC) which leads to small variations of pressure and temperature at the ignition time.

As a result, one can say that the model has the ability to capture the combustion behavior of internal combustion engines fueled with methane and methane-hydrogen mix (considering a small presence of hydrogen) with nice accuracy. Therefore, it has been proven that the code can be used to accomplish engine simulations with methane plus a small percentage of hydrogen, which is consistent with typical fuel mixture input of SOFC-ICE coupled operations.

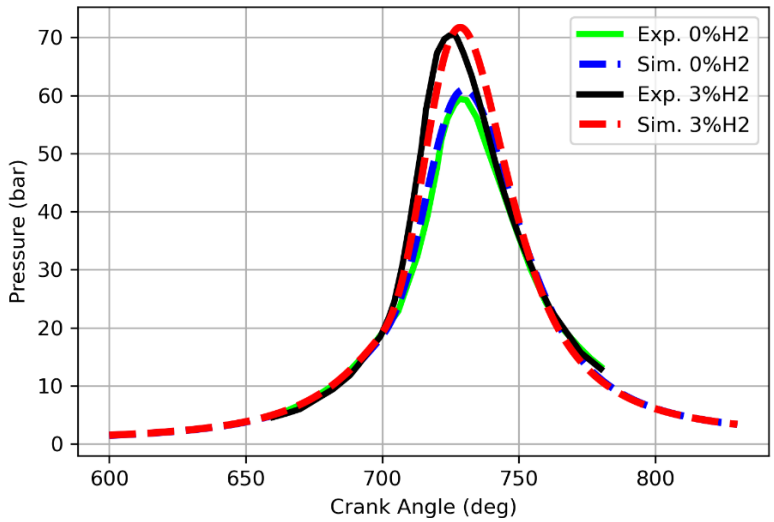

Figure 2: Validation of the engine code (dashed lines) against experimental data (solid lines) at 1500 rpm x IMEP 7 bar for two different fuel mixtures.

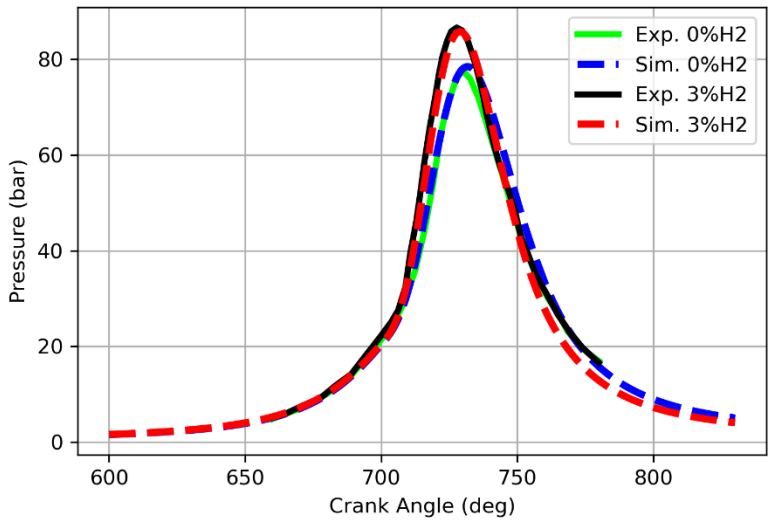

Figure 3: Validation of the engine code (dashed lines) against experimental data (solid lines) at 1500 rpm x IMEP 10 bar for two different fuel mixtures.

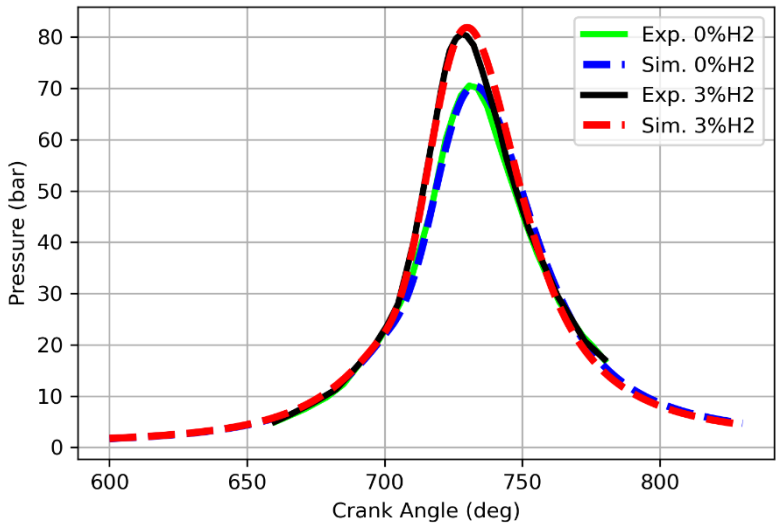

Figure 4: Validation of the engine code (dashed lines) against experimental data (solid lines) at 3000 rpm x IMEP 10 bar for two different fuel mixtures.

6. Application of the integrated methodology for gas maritime engine

Once the effectiveness of the integrate methodology (coupled engine thermodynamic 0D model and chemical kinetics tables) for methane-hydrogen gas engine has been checked, the same code has been applied to reproduce the overall performance of a real maritime gas engine. The overall performance analysis includes total efficiency, fuel consumption, and power supplied for a literature maritime engine [19] for different loads. The main features of the 3.9 MW engine are reported in Table 2. This second test case has been considered in order to ensure the correct performance of the code if applied on a large-scale gas engine consistent with maritime applications. Unfortunately, the literature lacks work that provides data on the overall performance as well as on the engine indicating analysis for those large-scale engines. Therefore, two different simulation cases on two different reference engines have been necessary to have an overview of the integrated methodology.

Table 2. Engine architecture [19].

Data	Values
Number of cylinders	9
Number of strokes	4
Displaced volume (L)	346.0
Stroke / Bore (mm)	350.0 / 400.0
Injection system	PFI
Compression ratio (-)	14.0
Connecting rod length (mm)	810.0
Fuel	CNG
Operation λ	1.8
Max boost pressure	2.7 bar

The experimental overall performance indicators have been extracted from the trip raw data in [19] by considering only the most stable trip time intervals. As a result, six different load points have been extracted: four low load points (from 9% to 23% of the maximum torque with corresponding engine speed between 500 and 520 rpm); one mid load point (45% with corresponding speed 650 rpm); one full load point (99% with corresponding speed of 750 rpm). A load span from 10% of the maximum torque to 100% of the maximum torque has been simulated by means of load steps of 5%. Each test load has been approached as a steady state point.

In the simulation of this reference engine, pure methane has been adopted as fuel in place of CNG for the sake of simplicity. However, as discussed in section 4, the differences between those fuels in terms of chemical kinetics simulation results are negligible. The chemical kinetics lookup tables for pure methane are interpolated in a cubic manner in order to calculate the laminar flame speed of the fuel at λ = 1.8 and pressure and temperature values, which depend on the engine stroke and the chosen engine load.

The simulation of each load point has been based on the same tuning routine listed in section 5. However, since the fuel is methane for all the simulations points, the Woschni gain coefficient C_0 has been set once, thus, only the filling coefficient needed the tuning for each load point. The Wiebe coefficients α and β and the non-dimensional turbulence have been set once as for C_0.

The validation of the code is shown in Figures 5-7 in terms of engine efficiency, fuel consumption, power supply, respectively. In Figure 5 it is visible that the gas engine efficiency increases in a steep linear manner from the very low to the mid loads between values 20% up to 37%. From the mid loads up to the full load, the efficiency flattens approaching values between 40% and 43%, which are consistent with the high compression ratio and the high bore that can be applied due to the very low likelihood of knock when methane is used (RON = 120 – 130). The model curve is in strong agreement with the experimental data except for a couple of points (loads 9% and 23%) that are likely affected by the non-perfectly steady operation regime.

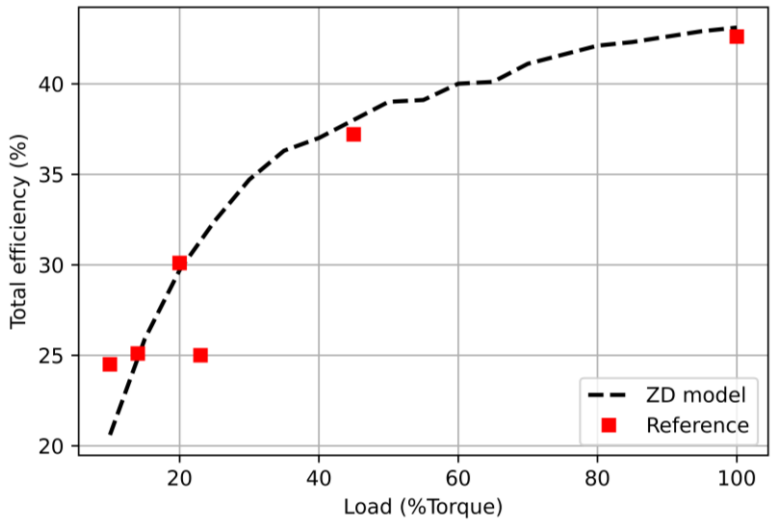

Figure 5: Comparison between simulation (dashed line) and experimental (markers) calculated engine total efficiency at different loads.

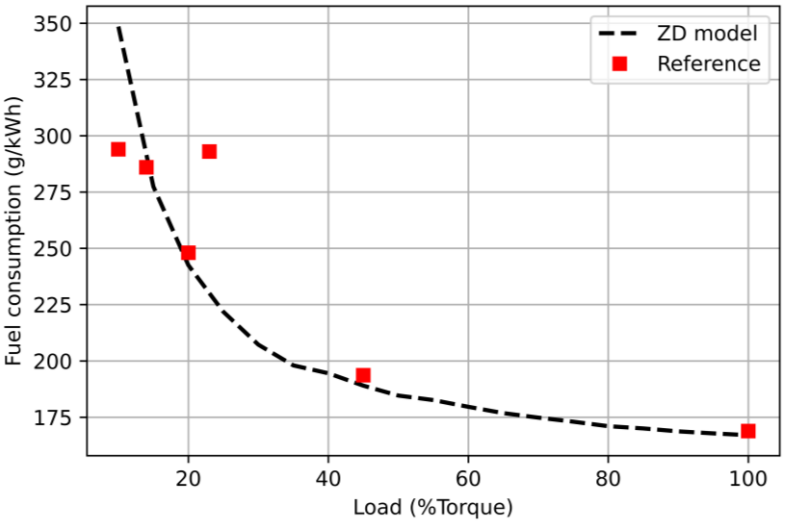

Figure 6: Comparison between simulation (dashed line) and experimental (markers) calculated engine fuel consumption at different loads.

In Figure 6 it is visible that the behavior of fuel specific consumption is mirrored by that of engine efficiency. Again, the model well reproduces the methane needed to ensure the required torque except for the two outliers. The mid-high loads feature a low methane-specific consumption in line with the engine's high efficiency at boosted conditions.

Figure 7 shows the perfect match between the power supplied by the maritime engine and that returned by the 0D code (ZD) at both naturally aspirated (low loads) and boosted conditions (mid-high loads).

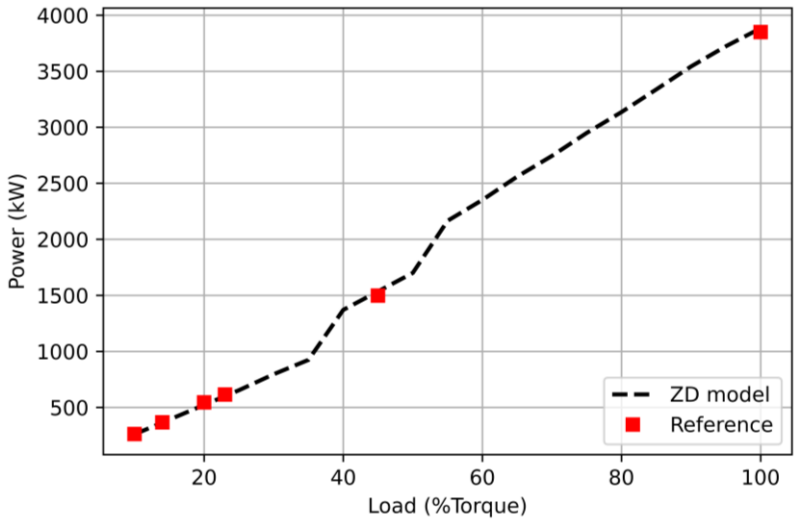

Figure 7: Comparison between simulation (dashed line) and experimental (markers) calculated engine power supplied at different loads.

7. Conclusions

In this study a 0D ICE-model, originally developed for gasoline-fuelled ICE, has been adapted for gaseous-fuelled operation with a variable methane-hydrogen mixtures.

A methodology based on the modeling of the chemical kinetic reactions in the open-source library Cantera is adopted: both methane and AOG components will be treated as reagents. The code uses Wiebe's law to model the heat release in combustion in which the laminar flame speed (LFS) is used to evaluate the length of the combustion period. The LFS, and the self-ignition time, are obtained by chemical-kinetic simulation for different pressure, temperature and mixture index conditions, then organized in tabular form, so that they can be read by the code. The main advantage of this methodology is that it is no more needed to tune the coefficients of the Wiebe curve.

The model pressure-crank resolution capability has been validated against experimental data available in the literature for a single cylinder engine of automotive origin. Then the overall prediction capability of the model in terms of efficiency and power produced are validated against the overall trip performance of a ship engine.

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