

Thermodynamic Analysis of SI Engine Operation on Variable Composition Biogas-Hydrogen Blends Using a Quasi-Dimensional, Multi-Zone Combustion Model

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ABSTRACT

In this work, a quasi-dimensional, multi-zone combustion model is analytically presented, for the prediction of performance and nitric oxide (NO) emissions of a homogeneous charge spark ignition (SI) engine, fueled with biogas-H₂ blends of variable composition. The combustion model is incorporated into a closed cycle simulation code, which is also fully described. Combustion is modeled on the basis of turbulent entrainment theory and flame stretch concepts. In this context, the entrainment speed, by which unburned gas enters the flame region, is simulated by the turbulent burning velocity of a flamelet model. A flame stretch submodel is also included, in order to assess the flame response on the combined effects of curvature, turbulent strain and nonunity Lewis number mixture. As far as the burned gas is concerned, this is treated using a multi-zone thermodynamic formulation, to account for the spatial distribution of temperature and NO concentration inside the burned volume.

The simulation code is applied to published experimental data of a SI engine operated on variable composition biogas-H₂ mixtures. It is revealed that the model is able to capture the effect of the fuel parameter satisfactorily in terms of both engine performance and NO emissions. It is concluded that the addition of increasing amounts of H₂ in biogas results in a decrease of the flame-development period, while the increase in the combustion velocities seems to be effective almost up to the point of 10% mass fraction burned (MFB). However, the course of heat release seems to be independent of the fuel case, being univocally determined by the geometry of the combustion chamber. Additionally, due

to the very high mass diffusivity of H₂ and the positively stretched flames, it results that these always take advantage of stretch effects, enhancing their burning intensity. At the same time, the positioning of the investigated flames into the thin reaction zones regime provides insight into their phenomenology. Finally, detailed information is gained concerning the effect of H₂ enrichment of biogas on the temporal and spatial formation of NO inside the engine cylinder.

INTRODUCTION

Over the last years, the ever increasing concern over the environmental impact of the transportation sector with the resulting legislation of continuously stringent emissions regulations, along with the need to reduce dependency on petroleum-based energy sources, have stimulated a vast amount of research and development work on the use of alternative, clean-burning fuels in internal combustion engine applications [1]. As a result, the automotive and fuel industry have coordinated their efforts towards the production of the so-called alternative fueled vehicles, either dedicated or non-dedicated (bifueled, flexible, dual fuel) [2].

It has been long recognized that the gaseous mixture derived from the anaerobic decomposition of biomass waste, known as biogas and having a typical volumetric composition of 60% CH₄ and 40% CO₂, can be a favorable renewable fuel for SI engines [3,4]. Biogas can be also encountered in the literature as landfill gas, sewage gas, or digester gas, depending on the site of its production, while it can also include small traces of H₂S, H₂, N₂, CO, O₂, vapor H₂O, as well as other gases and vapors of various organic compounds [5].

Among the additional benefits stemming from the use of biogas in internal combustion engines, in relation to other renewable fuels, significant role plays the reduction of the greenhouse gas effect, which in turn can result in the alleviation of the global warming problem. Specifically, CH_4 , which is the main constituent of biogas, causes about 21 times greater global warming effect than CO_2 [6], if directly released to the atmosphere. Therefore, the transformation of the more potent CH_4 , in terms of greenhouse effects, into the milder CO_2 by means of the biogas combustion reduces the emissions of hazardous gases into the environment. Additionally, the use of biogas for energy production can be of great interest in view of economical terms, if one considers the zero-, or even negative-, value of the feedstock required to produce biogas and the relatively moderate modifications needed on existing engines to allow for biogas fueling [7,8]. Besides, the great availability of indigenous biomass wastes, especially in the developing world, directs further towards the utilization of biogas as a sustainable energy source [9].

So far, several experimental and computational works have been published investigating the effects of biogas fueling on SI engine performance and pollutants emissions [3,4,6-8,10-19]. From the respective findings, it is concluded that the presence of the inert CO_2 in biogas affects adversely the engine operation, mainly due to the induced reductions in the following: laminar burning velocity of the combustible mixture, energy input per cycle, range of flammable air-fuel ratios and adiabatic flame temperature. Therefore, special care should be taken for the optimization and fine control of the engine operating and design parameters, if biogas is to be successfully exploited in a SI engine.

Apart from measures related to engine operating and design parameters towards the optimization of the biogas fueled SI engine, the use of small traces of H_2 in biogas can be also beneficial in terms of performance and emissions [6,17,20], following similar experience with natural gas engines [21,22], as long as care is taken again for the close control over the respective engine operating parameters. Specifically, the addition of small amounts of H_2 in biogas increases the lean and rich operational limits of the engine. Furthermore, under lean conditions, it results to an increase in the power output and thermal efficiency of the engine, with a simultaneous reduction in the hydrocarbons emissions due to the enhancement of the combustion process, and a limitation of the extent of cyclic variability. Additionally, thermodynamic improvements of the combustion process from the second-law viewpoint have been reported with H_2 enrichment of biogas [23,24].

In the present work, the development of a quasi-dimensional, multi-zone combustion model is analytically presented, for the prediction of performance and NO emissions of a homogeneous charge SI engine under variable composition biogas- H_2 blends fueling. The combustion model is incorporated into a closed cycle

simulation code, which is also fully described. The quasi-dimensional modeling approach used for the simulation of combustion, constituting a compromise between the simple zero-dimensional models and the complex multi-dimensional ones [25], accounts for the effect of combustion chamber geometry details, turbulent flow characteristics and physicochemical reactive mixture properties on the mass burning rates. The Wiebe function, which was used in a previous zero-dimensional version of the simulation code [26,27], is now replaced by modeling the combustion process on the basis of turbulent entrainment theory and flame stretch concepts. An expression of the turbulent burning velocity of a flamelet model is adopted for simulating the entrainment speed into the flame region, which accounts for a number of important phenomena affecting flame growth and propagation in a turbulent flow field. A submodel of flame stretch is also used, in order to assess the flame response on the combined effects of curvature, turbulent strain and nonunity Lewis number mixture. Particularly, the latter is expected to play a significant role in the present case, due to the very high mass diffusivity of H_2 . Regarding the burned gas behind the flame, this is treated by means of a multi-zone thermodynamic formulation, dividing the burned gas into several burned zones, spherically allocated inside the combustion chamber. In this way, the temperature and NO concentration gradients, developed throughout the burned mixture, can be captured, allowing for more realistic NO emissions predictions in comparison with those of the gross single-zone burned gas models.

The simulation code is calibrated and validated using published experimental data of a SI engine fueled with variable composition biogas- H_2 blends [20]. It is revealed that the predicted cylinder pressure diagrams are in good agreement with the respective experimental ones for all fuel composition cases tested, while the measured NO emissions are qualitatively well captured by the model. Additionally, computed results are presented regarding the effect of H_2 enrichment on burn rate and flame propagation parameters, illustrating the acceleration of the burning process during the early stages of combustion achieved with H_2 addition. Special insight is also provided concerning the flame response to stretch effects, ultimately revealing the positive contribution of stretch for all investigated flames, and the phenomenology of the structure of the flames in the in-cylinder turbulent flow field in which they are embedded. Additionally, the simulation model provides information concerning the in-cylinder spatial distributions of temperature and NO concentration, as well as their temporal evolution. Therefore, understanding of the way the combustion determines, both temporally and spatially, the formation of NO inside the cylinder, by means of the developed temperature field, is gained, while the comparison of the temporal and spatial NO formation inside the engine cylinder between the various H_2 concentration cases in the fuel mixture can be made.

GENERAL DESCRIPTION OF THE CLOSED CYCLE SIMULATION CODE

The main focus of the present work lies in the investigation of the effects that are induced on the operation of a homogeneous charge SI engine by the combustion of biogas-H₂ mixtures of variable composition. Therefore, only the closed part of the engine cycle needs to be modeled. The required input data of the simulation code are the following: engine geometric characteristics, engine speed, pressure and temperature of charge at inlet valve closing (IVC) (starting point of calculations), fuel-air equivalence ratio, spark timing and cylinder walls temperature.

During compression, the cylinder charge consists of a single zone; the unburned zone. This is treated as a homogeneous mixture of air, fuel and residual gas, the latter being trapped in the cylinder from the previous engine cycle. From the start of combustion, multiple, spherically allocated burned zones are sequentially generated at specified (user-defined) crank angle intervals. Each burned zone, assumed to be a homogeneous mixture of combustion products in chemical equilibrium, follows its own history of thermodynamic states during combustion. In this way, the stratification of the temperature and species concentrations throughout the burned gas can be captured. The latest-generated burned zone, in which combustion evolves, is separated from the unburned zone by a spherically propagating premixed turbulent flame. As an example, Fig. 1 shows a schematic of a SI engine combustion chamber with four burned zones, as well as the spherically propagating premixed turbulent flame. The symbols appearing in the figure will be analytically explained later during the description of the simulation code. From the end of combustion and until exhaust valve opening (EVO), the multi-zone treatment of the cylinder charge is retained, following the typical assumption that no mixing occurs between the individual burned zones during expansion.

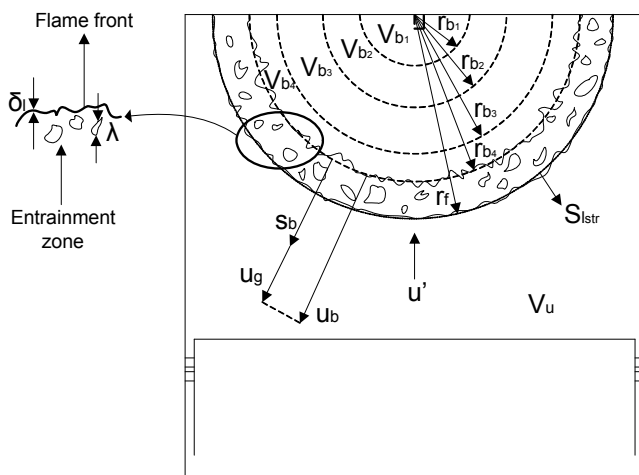


Fig. 1. Schematic of a SI engine combustion chamber with four burned zones. Also shown is a premixed turbulent flame, spherically propagating from the ignition point towards the cylinder walls.

All zones considered in the simulation are assigned uniform pressure, temperature and composition at any instant of time. Additionally, the pressure is assumed to be uniform throughout the cylinder, i.e. among all zones.

THERMODYNAMIC ANALYSIS

COMPOSITION AND THERMODYNAMIC PROPERTIES

Unburned zone composition

The unburned zone, existing in the cylinder during the compression and combustion phases, is considered to be a homogeneous mixture of air, fuel and residual gas from the previous cycle that has been trapped in the cylinder. The composition of the inducted into the cylinder air-fuel mixture is determined from the value of the fuel-air equivalence ratio. Then, the air-fuel mixture is mixed with the residual gas from the previous cycle, thus forming the unburned zone. The relative amount of residual gas in the unburned zone is defined by the value of its mass fraction at IVC, which is estimated by the model proposed by Fox *et al.* [28]. According to this model, the residual gas mass fraction is evaluated as a function of design and operating engine parameters, accounting explicitly for the effect of backflow of the exhaust gases to the cylinder during the valve overlap period, yielding

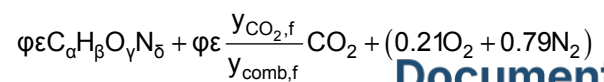
$$x_{rg} = 1.266 \frac{OF}{N} \left(\frac{p_i}{p_e} \right)^{-0.87} \sqrt{|p_e - p_i|} + 0.632 \frac{\phi}{r_c} \left(\frac{p_i}{p_e} \right)^{-0.74} \quad (1)$$

where N is given in 'rev/s', while p_i and p_e are in 'bar'. Also, OF , given in '°CA/m' in Eq. (1), characterizes the effective flow area of the gas during the valve overlap period and is estimated by the following empirical formula for typical cam profiles [28]

$$OF = \frac{1.45}{D} \left(107 + 7.8 \Delta\theta_{ol} + \Delta\theta_{ol}^2 \right) \frac{L_{v_{max}} D_v}{D^2} \quad (2)$$

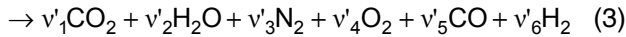
where $\Delta\theta_{ol}$ is given in '°CA', with the valve timings defined at 0.15 mm lift, while D , $L_{v_{max}}$ and D_v are in 'mm'. It is noted that the last two variables are averaged values for the intake and exhaust valves.

For the computation of the residual gas composition, the approach used by Ferguson [29] is followed, according to which the residual gas has the composition of low-temperature combustion products with carbon to oxygen atom ratios less than one. For the present case of biogas-H₂ blends used as fuel, the relevant one-step overall combustion reaction is



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In formulating this reaction, an effective combustible part of the fuel, denoted as $\text{C}_\alpha\text{H}_\beta\text{O}_\gamma\text{N}_\delta$, is assumed, where α , β , γ and δ are the numbers of carbon, hydrogen, oxygen and nitrogen atoms, respectively, in its molecule. The effective combustible part of the fuel consists of CH_4 , originated from biogas, and H_2 , while the inert CO_2 , existing also in biogas, does not actually participate in the reaction.

In the fuel mixture, the molar fractions of CH_4 and CO_2 are, respectively

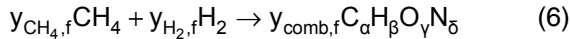
$$y_{\text{CH}_4,\text{f}} = (1 - y_{\text{H}_2,\text{f}}) y_{\text{CH}_4,\text{bg}} \quad (4a)$$

$$y_{\text{CO}_2,\text{f}} = (1 - y_{\text{H}_2,\text{f}}) y_{\text{CO}_2,\text{bg}} \quad (4b)$$

where $y_{\text{CH}_4,\text{bg}}$ and $y_{\text{CO}_2,\text{bg}}$ are the molar fractions of CH_4 and CO_2 , respectively, in biogas, and $y_{\text{H}_2,\text{f}}$ is the molar fraction of H_2 in the fuel mixture. Therefore, the molar fraction of the effective combustible part of the fuel is

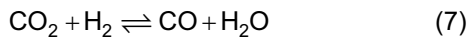
$$y_{\text{comb},\text{f}} = y_{\text{CH}_4,\text{f}} + y_{\text{H}_2,\text{f}} \quad (5)$$

and α , β , γ and δ are given from



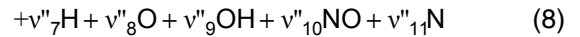
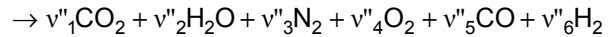
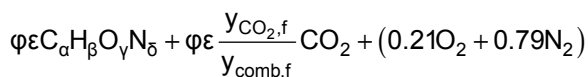
considering the four atom-balance equations (C/H/O/N).

For lean or stoichiometric conditions ($\phi \leq 1$), the four atom-balance equations (C/H/O/N) are sufficient for computing the coefficients v'_i ($i = 1 \div 6$) in Eq. (3), since there is neither CO nor H_2 in the products. However, under rich conditions ($\phi > 1$), where the combustion products do not include any O_2 , the water-gas reaction at chemical equilibrium is additionally considered

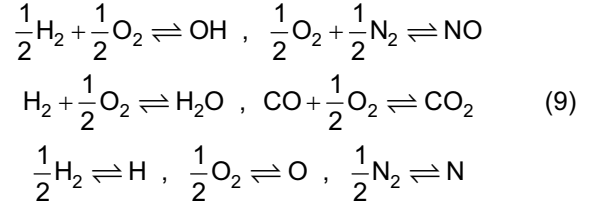


Burned zones composition

Each burned zone is considered to be a homogeneous mixture of eleven combustion products in chemical equilibrium at the zone's local temperature and the uniform cylinder pressure, following Ferguson's method [29]. The one-step overall high-temperature combustion reaction for the present case of biogas- H_2 fueling is



For the computation of v''_i ($i = 1 \div 11$) in Eq. (8), the four atom-balance equations (C/H/O/N) are considered, along with following seven reactions at chemical equilibrium



Thermodynamic properties

The thermodynamic properties of the various species are calculated by polynomial expressions, as a function of the zone's temperature in which they exist. For this reason, the well established coefficients [30] of the relevant curves that have been fitted to the species thermochemical data from JANAF Tables [31] are used. Then, the corresponding thermodynamic properties (and derivatives) of each zone, needed for first-law applications, are derived applying the gas mixture rule, according to the molar fractions of the species existing in each zone.

CONSERVATION AND STATE EQUATIONS

Throughout the closed cycle simulation code, conservation and state equations are applied to the various zones, constituting the governing equations of the multi-zone formulation. Here, the corresponding equations are presented in their most general form, as applied during combustion. For the compression and expansion phases, the same equations are valid too, though incorporating adaptations regarding the number of zones included and the value of MFB.

Specifically, the energy conservation equation is applied to the unburned zone, the $n-1$ already burned zones (where 'n' represents the number of burned zones existing currently in the cylinder) and the cylinder charge, yielding, respectively

$$\frac{dQ_u}{d\theta} = \frac{dU_u}{d\theta} + p \frac{dV_u}{d\theta} + \frac{dm_b}{d\theta} h_u \quad (10)$$

$$\frac{dQ_{b,i}}{d\theta} = \frac{dU_{b,i}}{d\theta} + p \frac{dV_{b,i}}{d\theta} \quad (i = 1 \div n-1) \quad (11)$$

$$\frac{dQ}{d\theta} = \frac{dU}{d\theta} + p \frac{dV}{d\theta} \quad (12)$$

These equations have been derived assuming that the blow-by out of the cylinder is negligible. It is noted that,

once a new burned zone is generated, the previous one is treated as a closed system. Additionally, the values of internal energy and enthalpy are actually the absolute ones, i.e. they account for the heat of formation in addition to the sensible heat.

Also, the cylinder volume balance (constraint) equation is applied, requiring that the sum of the volumes of the various zones existing in the cylinder is equal to the instantaneous cylinder volume, as calculated by the engine geometric characteristics as a function of crank angle. It, therefore, holds after differentiating with respect to crank angle

$$\frac{dV}{d\theta} = \sum_{i=1}^n \frac{dV_{b,i}}{d\theta} + \frac{dV_u}{d\theta} \quad (13)$$

Additionally, the mass conservation equation is applied to the cylinder charge, yielding

$$\begin{aligned} \frac{dm}{d\theta} &= \frac{dm_u}{d\theta} + \frac{dm_b}{d\theta} = \frac{dm_u}{d\theta} + \sum_{i=1}^n \frac{dm_{b,i}}{d\theta} \\ &= \frac{dm_u}{d\theta} + \frac{dm_{b,n}}{d\theta} = 0 \end{aligned} \quad (14)$$

since the $n-1$ already burned zones are systems of constant mass, i.e. $dm_{b,i}/d\theta = 0$ ($i = 1 \div n-1$).

Finally, each zone of the simulation code is assumed to obey the ideal gas state equation

$$pV_j = m_j R_j T_j \quad (j = u, b_1 \div b_n) \quad (15)$$

Eqs. (10)-(13) constitute the $n+2$ governing equations of the multi-zone formulation, which need to be solved for the $n+2$ unknowns, i.e. cylinder pressure p , burned zones temperatures $T_{b,i}$ ($i = 1 \div n$) and unburned zone temperature T_u . In Appendix A, the mathematical manipulation and final formulation of the $n+2$ governing equations, for the derivation of the final system of the $n+2$ differential equations of the above mentioned $n+2$ unknowns, is analytically presented.

COMBUSTION MODEL

For the prediction of mass burning rates, a quasi-dimensional combustion model is developed, based on turbulent entrainment theory and flame stretch concepts. The latter is implemented by incorporating a submodel that assesses the flame response on combined effects of curvature, turbulent strain and nonunity Lewis number mixture (i.e. mixture with inequality between thermal diffusivity and mass diffusivity of the deficient reactant). Specifically, nonunity Lewis number mixture effects are expected to play a significant role in the present case of

H₂ addition in biogas, due to the very high mass diffusivity of H₂.

The present combustion model simulates the early flame development, flame propagation and flame termination periods [30], neglecting spark ignition processes and initial plasma and flame kernel formation considerations. Instead, the assumption is made that, at the time of spark, a burned gas kernel (i.e. of the burned zone's composition) of 1 mm diameter is spontaneously created. This size of initial kernel is approximately equal to the gap of the spark plugs that are usually placed in both production and optical SI engines [32]. The temperature of the initial gas kernel is suggested to be the adiabatic flame temperature that corresponds to the cylinder pressure and unburned zone's temperature and composition at the end of the compression phase (i.e. at the time of ignition), as derived by the following equation

$$h_u(T_u, p) = h_b(T_{ad}, p), \quad \theta = \theta_{IT} \quad (16)$$

Burning law equations

Assuming that the phenomenology of the burning process is as depicted in Fig. 1, it allows for the turbulent entrainment combustion model to be used. This model was originally developed by Blizard and Keck [33] and was later extended and refined by various researchers [34-40], in order to be able to simulate SI engine premixed turbulent combustion. According to this model, combustion evolves as a two-step procedure. First, unburned gas is entrained into the flame zone with a characteristic (entrainment) speed and, then, laminar burn-up of the entrained eddies occurs at the Taylor microscale of turbulence. At this point, it is worth mentioning that the mechanism of entrainment and subsequent burning of eddies has never been adequately confirmed by experiments. However, the turbulent entrainment combustion model constitutes a proper mathematical formulation that accounts for the finite flame brush thickness.

The present formulation of the turbulent entrainment combustion model incorporates two main modifications, in comparison with its typical version [33-40]. First, the entrainment speed is simulated by a semi-empirical expression for the turbulent burning speed of a flamelet model, derived by Herweg and Maly [41], considering laminar flamelet concepts, as has been also proposed in [42]. However, the idea for relating the entrainment speed with the turbulent burning speed of a flame kernel was originally reported in [43,44], though using a slightly different expression. Secondly, a submodel that quantitatively estimates the effect of flame stretch on the laminar burning velocity of a premixed flame is also incorporated, including the influence of both the Karlovitz and Lewis numbers, as has been adopted in several relevant studies, e.g. [32,41-45]. The choice here for incorporating the effect of the Lewis number, in addition to that of the Karlovitz number, in contrast, for example, to [46-51] where only the Karlovitz number impact was

taken into account, is based on the very high mass diffusivity of H_2 , which is added in biogas, resulting therefore in the expectation that the nonunity Lewis number mixture effect cannot be negligible.

Early Flame Development and Flame Propagation Periods

During the early flame development and flame propagation periods, the rate equation of the mass entrained into the flame zone is

$$\frac{dm_e}{dt} = \rho_u F_f S_e \quad (17)$$

with the entrainment speed given as [41]

$$S_e = \underbrace{S_\ell I_0 + S_\ell I_0^{1/2}}_{\text{stretch}} \cdot \underbrace{\left(\frac{u'}{u' + S_\ell} \right)^{1/2}}_{\text{turbulence factor}} \cdot \underbrace{\left[1 - \exp\left(-\frac{r_f}{L}\right) \right]^{1/2}}_{\text{effective integral length scale}} \cdot \underbrace{\left[1 - \exp\left(-\frac{t}{\tau_{0G}}\right) \right]^{1/2}}_{\text{effective integral time scale}} \cdot \underbrace{\left(\frac{u'}{S_\ell} \right)^{5/6}}_{\text{fully-developed flame}} \quad (18)$$

while the burned mass rate equation is

$$\frac{dm_b}{dt} = \rho_u F_f S_\ell I_0 + \frac{m_e - m_b}{\tau_b} \quad (19)$$

The characteristic time τ_{0G} represents an effective turbulence integral time scale, which the flame lifetime must exceed before the flame becomes a fully-developed one, and is given as

$$\tau_{0G} = \frac{L}{u' + S_\ell} \quad (20)$$

while the characteristic burning time τ_b expresses the time an eddy of the size of the Taylor microscale needs in order to be burned with the laminar burning velocity

$$\tau_b = \frac{\lambda}{S_\ell} \quad (21)$$

At this point, it should be clarified that the term 'fully-developed flame' refers to a propagating flame, whose lifetime and size are sufficiently large, so that the turbulence length and time effects can influence it up to the maximum possible extent [41]. Additionally, it was decided here to use Eq. (18) for the modeling of the entrainment speed, instead of the typical expression [38] that suggests that the entrainment speed is composed of the sum of the laminar burning velocity plus the

turbulence intensity, the latter being corrected with an exponential term during the early flame development period. This was done because Eq. (18) accounts for a larger number of phenomena, influencing mostly the early flame development period. These comprise of (see also Eq. (18))

- unsteady flame stretch at small flame front radius, expressed via the flame stretch factor I_0 , whose mathematical expression will be given in a following subsection
- effects of laminar propagation at small values of u'/S_ℓ , taken into account by the turbulence factor
- turbulence integral length and time scales, when the flame front radius r_f and flame lifetime t are small relatively to the effective turbulence integral length and time scales, i.e. L and τ_{0G} , respectively, and
- transition of flame into a fully-developed one.

The two exponential terms in the second term on the right-hand side of Eq. (18) both tend to zero, when the flame begins to propagate as a freely expanding surface.

According to Eqs. (17) and (18), the rate at which unburned mixture is entrained into the flame is constituted from the additive contribution of two distinct phenomena. The first one is described by a diffusive term, which is the laminar burning velocity of the unburned mixture, corrected with the effect of flame stretch. It defines the local rate of propagation of the flame front into the unburned region, determined by chemistry, pressure and temperature conditions, as well as stretch contributions. The second phenomenon is characterized by the interaction between turbulence and early flame development and flame propagation. The turbulence effects are expressed via a convective term, which is the turbulence intensity that determines the turbulence level of the flow field in the cylinder, as well as the effective turbulence integral length and time scales, which only influence the initial flame growth period.

Respectively, Eq. (19) reveals that the burning rate is specified by the rate at which unburned mixture is promptly consumed at the leading edge of the turbulent flame, plus the rate at which unburned mixture behind the flame front is burned. The second burning mechanism, which is expressed by the second term on the right-hand side of Eq. (19), is related to the amount of unburned mixture already enflamed, but not yet burned.

A schematic of a premixed turbulent flame in a SI engine combustion chamber is given in Fig. 1, illustrating the physical basis of the turbulent entrainment combustion model. The turbulent flame brush is clearly depicted. The front of the turbulent flame can be approximated by a spherical surface, denoted by a dotted line, which diffuses towards the unburned mixture locally at the stretched laminar burning velocity. Additionally, unburned gas crosses this front with a characteristic speed, determined partly by the turbulence intensity. Parcels of unburned mixture, engulfed by the flame front,

are also discerned into the entrainment zone. The schematic on the left shows a detailed picture of the turbulent flame brush, where the reaction-sheet thickness is essentially the laminar flame thickness and the small-scale turbulent eddies are of the Taylor microscale size.

Flame Termination Period

When the flame front coincides with the cylinder walls, having fully engulfed the cylinder content, the end of flame propagation occurs. However, some amount of unburned mixture still exists in the cylinder (i.e. the part of the charge that has been entrained into the flame zone, but has not been consumed yet), being henceforward burned in an exponential pattern [36,37] during the flame termination period

$$\frac{dm_b}{dt} = \left(\frac{dm_b}{dt} \right)_F \exp \left(-\frac{t - t_F}{\tau_b} \right), \quad t > t_F \quad (22)$$

The terms $(dm_b/dt)_F$ and t_F represent the mass burning rate and time, respectively, at the end of flame propagation. During the flame termination period, the rate of entrainment of Eq. (17) is equal to zero, since $F_f = 0$.

Turbulence characteristics

The turbulence intensity and turbulence length scales of the flow ahead of the flame, needed by the burning law equations of the combustion model, are evaluated by application of rapid distortion theory (i.e. conservation of angular momentum for the large-scale eddies) to the unburned region just after ignition [34,35,52], yielding

$$u' = u'_{IT} (\rho_u / \rho_{u_{IT}})^{1/3} \quad (23)$$

$$L = L_{IT} (\rho_{u_{IT}} / \rho_u)^{1/3} \quad (24)$$

These relations predict an increase in the turbulence intensity and a decrease in the integral length scale with the compression of the unburned gas after the initiation of combustion. Although the rapid distortion theory constitutes a very simplified approach for the evaluation of turbulence characteristics, its predictions are qualitatively similar with those of more sophisticated turbulence models, such as the single- and two-zone energy cascade and $k-\epsilon$ ones [53].

It is additionally assumed that the turbulence intensity and integral length scale at the time of ignition are proportional to the mean piston speed and clearance height, respectively, as suggested in [34,35,52]

$$u'_{IT} = c_1 u_p \quad (25)$$

$$L_{IT} = c_2 h_{cl} \quad (26)$$

where c_1 and c_2 are experimentally calibrated constants. Also, $u_p = 2NS/60$, with S representing the piston stroke, while h_{cl} is the clearance height. It is pointed out that experimental evidence supporting the first and second assumption, leading to the formulation of Eqs. (25) and (26), respectively, has been reported in [54,55] and in [56,57], respectively.

For the calculation of the Taylor microscale during combustion, it is suggested that the small-scale structure of turbulence is isotropic [58], which yields the following relation

$$\lambda = \left(\frac{15}{A} \right)^{1/2} L \left(\frac{u' L}{\nu} \right)^{-1/2} \quad (27)$$

where A is a constant of order one, while ν refers to the unburned gas.

Laminar burning velocity correlation

For the evaluation of the laminar burning velocity of the biogas-H₂-residual gas-air mixture, a Le Chatelier's Rule-like formula is adopted, using the laminar burning velocity of biogas-residual gas-air and H₂-residual gas-air mixtures at the same conditions as the original mixture. It has been shown in [59] that the use of a Le Chatelier's Rule-like formula can provide quite reasonable estimations of the laminar burning velocity of H₂-CH₄-air blends, using the values of the laminar burning velocity of H₂-air and CH₄-air blends. Therefore, assuming that the presence of the inert CO₂ in the fuel mixture under investigation in the present work, originated from biogas, does not significantly modify the above mentioned behavior observed for H₂-CH₄-air mixtures, the following formula can be written for the estimation of the laminar burning velocity of biogas-H₂-residual gas-air mixtures

$$S_\ell (T_u, p, y_{H_2, f}, y_{CO_2, bg}, \Phi, y_{rg}) = \left[\frac{1 - y_{H_2, f}}{S_{\ell, bg} (T_u, p, y_{CO_2, bg}, \Phi, y_{rg})} + \frac{y_{H_2, f}}{S_{\ell, H_2} (T_u, p, \Phi, y_{rg})} \right]^{-1} \quad (28)$$

where y_{rg} is the molar fraction of the residual gas in the unburned mixture (biogas-H₂-residual gas-air mixture).

The laminar burning velocity of biogas-air mixtures is evaluated from the correlation reported in [60], where CH₄-diluent (CO₂ among other inert gases)-air blends have been burned in a spherical, constant volume chamber under near zero-gravity conditions and for a wide range of diluent concentrations in CH₄. The mixtures ignited in that work were always quiescent. Therefore, the stretch rates were quite low, since only curvature effects contributed to stretch (inexistence of

aerodynamic straining of flames due to turbulence in the unburned region) and only during the initial burning period, where the flame curvature is significant. This fact, combined with the almost unity Lewis numbers of the investigated mixtures, resulted in the measurement of approximately stretch-free laminar burning velocities. Additionally, the effect of presence of exhaust gases from the previous engine cycle in a biogas-air mixture on the laminar burning velocity of the resultant blend is simulated according to [61], where it was concluded that the percentage reduction in the value of the laminar burning velocity due to the presence of burned gases in an indolene-air mixture is independent of the properties of the unburned mixture, being a function only of the amount of diluent present. Under these considerations, the following correlation is used for the estimation of the laminar burning velocity of biogas-residual gas-air blends

$$S_{\ell,bg}(T_u, p, y_{CO_2,bg}, \varphi, y_{rg}) = S_{\ell,bg,ref}(y_{CO_2,bg} = 0, \varphi) \cdot \underbrace{\left(\frac{T_u}{T_{ref}}\right)^{\alpha(\varphi)} \cdot \left(\frac{p}{p_{ref}}\right)^{\beta(\varphi)} \cdot (1 - \gamma \cdot y_{CO_2,bg}^{\delta(\varphi)})}_{\text{from [60]}} \cdot \underbrace{\left(1 - 2.06 \cdot y_{rg}^{0.77}\right)}_{\text{from [61]}} \quad (29)$$

where

$$S_{\ell,bg,ref}(y_{CO_2,bg} = 0, \varphi) = 0.375 + 0.129(\varphi - 1) - 2.420(\varphi - 1)^2 - 0.271(\varphi - 1)^3 + 5.000(\varphi - 1)^4 \quad (\text{m/s})$$

$$\alpha(\varphi) = 1.570 - 1.950(\varphi - 1)$$

$$\beta(\varphi) = -0.333 + 0.493(\varphi - 1)$$

$$\gamma = 1.260$$

$$\delta(\varphi) = 1.270 - 0.336(\varphi - 1)$$

with the reference conditions being $T_{ref} = 298 \text{ K}$ and $p_{ref} = 1 \text{ bar}$, while the range of validity of the correlation is within the regions: $0.5 < p(\text{bar}) < 10.4$, $295 < T_u(\text{K}) < 454$, $0.6 < \varphi < 1.4$, $10 < S_{\ell,bg}(\text{cm/s})$ and $0 < y_{CO_2,bg} < 0.60$.

Respectively, for the estimation of the laminar burning velocity of H_2 -residual gas-air mixtures, the correlation proposed in [62] is used

$$S_{\ell,H_2}(T_u, p, \varphi, y_{rg}) = S_{\ell,H_2,ref}(\varphi) \cdot \left(\frac{T_u}{T'_{ref}}\right)^{\alpha'} \cdot \left(\frac{p}{p'_{ref}}\right)^{\beta'(\varphi)} \cdot (1 - \gamma'(\varphi) \cdot y_{rg}) \quad (30)$$

where

$$S_{\ell,H_2,ref}(\varphi) = -4.770\varphi^3 + 8.650\varphi^2 - 0.394\varphi - 0.296 \quad (\text{m/s})$$

$$\alpha' = 1.232$$

$$\beta'(\varphi) = 2.90\varphi^3 - 6.69\varphi^2 + 5.06\varphi - 1.16, \quad \varphi < 0.6$$

or

$$\beta'(\varphi) = 0.0246\varphi + 0.0781, \quad \varphi \geq 0.6$$

$$\gamma'(\varphi) = 2.715 - 0.5\varphi$$

with the reference conditions here being $T'_{ref} = 365 \text{ K}$ and $p'_{ref} = 5 \text{ bar}$. At this point, it should be noted that this correlation does not correspond to stretch-free flames, as stated in [62], since H_2 -residual gas-air flames at engine-like conditions are unstable from their inception, both from the Lewis number and the preferential diffusion point of view. However, since the related experimental conditions concerned quiescent mixtures prior to ignition, the aerodynamically induced straining of the flames (producing the so-called turbulent stretch rate), which is caused for example by the highly turbulent flow inside an engine combustion chamber, could not have been accounted for. For this reason, this correlation is regarded in this work as one that is not absolutely free of stretch effects, but already incorporating small stretch rates. Inevitably, such a consideration introduces some computational uncertainties, since, according to the flame stretch submodel described next, stretch-free laminar burning velocity data are naturally needed.

Flame stretch submodel

The modifications that are induced to the laminar burning velocity of a premixed flame to due effects of curvature, turbulent strain and nonunity Lewis number mixture are accounted for using the flame stretch factor I_0 , as originally suggested by Chung and Law [63], which, after neglecting the heat losses from the flame surface, becomes

$$I_0 = \frac{S_{\ell, str}}{S_{\ell}} = 1 - \frac{Ka}{Le} + Ka \left(\frac{1}{Le} - 1 \right) \left(\frac{T_{act}}{2T_{ad}} \right) \quad (31)$$

The term $S_{\ell, str}$ represents the stretched laminar burning velocity with which the premixed flame locally propagates into the unburned mixture. By introduction of

the Markstein number, $Ma = \left(\frac{1}{Le} - 1 \right) \left(\frac{T_{act}}{2T_{ad}} \right)$, which is a property of the unburned gas that characterizes the response of its laminar burning velocity to flame stretch and is used in order to lump into it multiple mixture parameters, the formulation of Eq. (31) can be simplified [64] to

$$I_0 = \frac{S_{\ell, str}}{S_{\ell}} = 1 - \frac{Ka}{Le} + KaMa \quad (31a)$$

It is to be noted that this correlation for flame stretch is valid under mild stretch conditions, i.e. for relatively low Karlovitz numbers.

Furthermore, the Karlovitz number is defined as the ratio of the stretch (or strain) rate to the inverse of a characteristic chemical time within the reaction region [41,43], whose thickness is assumed to be of the order of the laminar flame thickness

$$Ka = \frac{K}{S_\ell / \delta_\ell} \quad (32)$$

The stretch rate is constituted from the additive contributions of the geometric stretch rate, which is due to the surface increase of the expanding flame (considered spherical), and the turbulent stretch rate associated with the strain effects in the small-scale eddies, so yielding [41-43]

$$K = K_g + K_t = \frac{1}{F_f} \frac{dF_f}{dt} + \frac{u'}{\lambda} = \frac{2}{r_f} \frac{dr_f}{dt} + \frac{u'}{\lambda} = \frac{2}{r_f} \left(\frac{\rho_u}{\rho_b} \right) S_\ell + \frac{u'}{\lambda} \quad (33)$$

The last equality in Eq. (33), suggesting that the expression of the geometric stretch rate $\frac{2}{r_f} \frac{dr_f}{dt}$ can

become $\frac{2}{r_f} \left(\frac{\rho_u}{\rho_b} \right) S_\ell$, is valid under the assumption that

the laminar flame thickness is very small compared to the flame front radius ($\delta_\ell / r_f \ll 1$) [43]. Also, the laminar flame thickness is defined here as [43]

$$\delta_\ell = \frac{D_m}{S_\ell} \quad (34)$$

where D_m is the mass diffusivity of the deficient reactant, i.e. the reactant that limits the rate of reaction. In the present case, where only lean mixtures will be considered, the deficient reactant is the fuel. It should also be pointed out that the fuel under consideration in the present analysis is actually a multi-component mixture, i.e. a biogas- H_2 mixture, or, more analytically, a CH_4 - CO_2 - H_2 mixture. Therefore, the deficient reactant is the effective combustible part of the fuel, i.e. the CH_4 - H_2 blend.

The ratio of the thermal diffusivity of the unburned mixture to the mass diffusivity of the deficient reactant defines the Lewis number of the unburned gas

$$Le = \frac{D_T}{D_m} = \frac{k}{\rho c_p D_m} \quad (35)$$

where all symbols refer to the unburned mixture. Eq. (35) actually defines an effective Lewis number, since the deficient reactant is a two-component mixture. For

calculating, now, the effective Lewis number for a two-component fuel mixture (i.e. the CH_4 - H_2 mixture for the present case), the expression suggested in [65] is adopted, using the Lewis numbers for the two fuel components separately, as well as their respective fractions of heat release, so yielding for the present case

$$\frac{1}{Le} = \frac{q_{CH_4}}{Le_{CH_4}} + \frac{q_{H_2}}{Le_{H_2}} \quad (36)$$

where

$$q_{CH_4} = (x_{CH_4,f} LHV_{CH_4}) / (x_{CH_4,f} LHV_{CH_4} + x_{H_2,f} LHV_{H_2}) \quad (37a)$$

$$q_{H_2} = (x_{H_2,f} LHV_{H_2}) / (x_{CH_4,f} LHV_{CH_4} + x_{H_2,f} LHV_{H_2}) \quad (37b)$$

are the heat release fractions of CH_4 and H_2 , respectively. Additionally, the Lewis numbers for CH_4 and H_2 are calculated using the thermal diffusivity of the unburned mixture and their respective mass diffusivities

$$Le_{CH_4} = \frac{D_T}{D_{m_{CH_4}}} = \frac{k}{\rho c_p D_{m_{CH_4}}} \quad (38a)$$

$$Le_{H_2} = \frac{D_T}{D_{m_{H_2}}} = \frac{k}{\rho c_p D_{m_{H_2}}} \quad (38b)$$

where, again, all symbols refer to the unburned mixture. Therefore, from Eq. (36), the effective Le can be computed, using Eqs. (37a), (37b), (38a) and (38b). Then, the mass diffusivity of the effective (two-component) combustible part of the fuel D_m is calculated from Eq. (35).

Since, in the present work, only lean air-fuel mixtures ($\phi < 1$) will be examined, it is additionally assumed that the composition of the excess reactant approximates that of air, for ease of computation of the relevant mass diffusivities. In Appendix B, the calculation of the mass diffusivities of CH_4 and H_2 in the air is analytically presented.

Flame front geometry

For calculating the flame front geometric characteristics, i.e. flame front area F_f and radius r_f , during the early flame development and flame propagation periods, which are needed by the burning law equations of the combustion model (Eqs. (17)-(19)), use is made of the typical assumption of a spherically propagating flame front centered at the ignition point [30]. Experimental evidence supporting this assumption has been reported in [36-38], making use of flame motion picture records obtained from optically accessible engines.

Therefore, the geometric model developed by Annand [66] is used here, which simulates the propagation of a spherical flame front inside an engine's cylinder. The center of the spherical flame front is fixed at the point of ignition of the combustion chamber, which is placed on a flat cylinder head. During flame travel, the flame front is truncated by the surfaces of the cylinder head, liner and piston crown. In this way, for a certain crank angle θ from TDC (top dead center) (i.e. for a certain cylinder height) and flame front radius r_f , the enflamed volume V_f , flame front area F_f and surface areas of the cylinder walls (i.e. cylinder head, liner and piston crown) in contact with the enflamed volume, i.e. F_h , F_l and F_p , respectively, can be analytically determined, producing look-up tables of the following form

$$V_f = V_f(\theta, r_f) \quad (39a)$$

$$F_f = F_f(\theta, r_f) \quad (39b)$$

$$F_h = F_h(\theta, r_f) \quad (39c)$$

$$F_l = F_l(\theta, r_f) \quad (39d)$$

$$F_p = F_p(\theta, r_f) \quad (39e)$$

for later use during the cycle simulation. Specifically, the plot derived from Eq. (39b) is referred to as 'spherical flame map', according to [67]. All plots produced from Eqs. (39a)-(39e) are unique for a certain combustion chamber of specific geometry (e.g. cylinder bore and distance of ignition point from cylinder center) and, therefore, characterize it.

During the early flame development and flame propagation periods, the enflamed volume can be considered to be composed of the sum of the volumes of the multiple burned zones and the volume of the unburned gas behind the flame front that has not been burned yet (see also Fig. 1), yielding

$$V_f = \sum_{i=1}^n V_{b,i} + \frac{m_e - m_b}{\rho_u} \quad (40)$$

Therefore, from the known crank angle θ and enflamed volume V_f , the flame front radius r_f can be computed using two-dimensional interpolation of data from the relevant look-up table. Then, from the known crank angle θ and flame front radius r_f , the flame front area F_f is calculated by a similar procedure.

HEAT TRANSFER MODEL

During the closed cycle simulation, the various zones exchange heat with the surrounding cylinder walls, while local heat transfer effects between adjacent zones are not taken into account, as these can be considered negligible in comparison with the gas-wall heat losses because of the different temporal scales [68]. The unburned zone transfers heat due to convection, while

the burned zones exchange heat due to both convection and radiation.

The heat loss rate is simulated using Annand's heat transfer formula [69], which is applied separately to each zone of the simulation, yielding

$$\frac{dQ_j}{dt} = F_j \left[a \frac{k_j}{D} Re_j^b (T_j - T_w) + c (T_j - T_w)^4 \right] \quad (j=u, b_1 \div b_n) \quad (41)$$

where a , b and c are experimentally determined constants. The heat losses Q_{L_j} ($j=u, b_1 \div b_n$) of the various zones, appearing in Eq. (41), are related to the heats Q_j ($j=u, b_1 \div b_n$) in Eqs. (10) and (11) by the following relation: $Q_{L_j} = -Q_j$ ($j=u, b_1 \div b_n$). Also, a Reynolds number is defined for each zone separately, using each zone's own properties

$$Re_j = \frac{\rho_j Du_p}{\mu_j} \quad (j=u, b_1 \div b_n) \quad (42)$$

The thermal conductivity k_j and dynamic viscosity μ_j of each zone are expressed as functions of its own temperature T_j . Regarding the cylinder walls temperature T_w , it is considered constant during the whole closed cycle period as well as uniform for all surfaces, i.e. cylinder head, liner and piston crown.

Burned zones geometry

The surface areas of the multiple zones in contact with the cylinder walls F_j , for use in the heat transfer equation (Eq. (41)), are calculated by the use of a geometric model for the burned zones location inside the combustion chamber. Therefore, it is assumed that these are spherically allocated inside the cylinder, as depicted in Fig. 1, resembling the spatial distribution presented in [68]. From this figure, it can be seen that the location of a certain burned zone is delimited between two spherical surfaces, both centered at the ignition point. The closest to the ignition point spherical surface contains all burned zones that have been created before this specific one, while the more distant spherical surface includes additionally the current burned zone. For each burned zone a radius can be defined, coinciding with the radius of the more distant spherical surface.

If the term $V_{sph,i}$ represents the volume of the sphere that includes the first i ($i=1 \div n$) burned zones, then it is calculated as

$$V_{sph,i} = V_{sph,i-1} + V_{b,i} \quad (i=1 \div n) \quad (43)$$

Then, from the known values of crank angle θ and sphere's volume $V_{sph,i}$, the radius of the sphere $r_{sph,i}$, which is also the radius of the i burned zone, $r_{b,i}$ is