0D Laminar Flame Speed Model for Methane Lean Mixture in Dual Fuel Combustion Engine

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1 Introduction

For decades, the compression ignition (CI) engines are widespread in the market because of their reliability and efficiency. But, they have high exhaust emissions of particulate matter (PM) and nitric oxides (NO_x) which can be problematic for environment. It is necessary to emphasize on reducing emissions in order to keep up with the latest stringent regulations on emissions [1, 2]. This can be achieved with the implementation of alternative solutions like the usage of after treatment systems, usage of gaseous fuels along with diesel fuel etc. The solution to use after treatment systems is not cost efficient and decreases global efficiency because of the higher pumping work required. Dual fuel operation, where gaseous fuels are used with pilot diesel injection, is considered as one efficient solutions used in diesel engines to improve exhaust emissions. Indeed, part of the diesel liquid fuel is substituted with alternative gaseous fuels [3, 4] that is introduced into the intake manifold to form a premixed charge with air, in this way both PM and NO_x can be significantly reduced. Methane is mostly used gaseous fuel for the dual fuel compression ignition engine. It is an economical fuel with a wide availability across the globe. Methane is well-suited with the high compression ratios of CI engine. It has high auto-ignition temperature, low carbon content and high knock resistivity [5-8]. Nevertheless, dual fuel combustion results extremely complex to model, since it is characterized by the oxidation of two fuels presenting different physical and chemical features. As a matter of fact, a small amount of diesel, burning in a diffusive flame, starts via a multipoint ignition the propagation of a flame in the air-methane premixed charge.

In the present work, a dual-fuel combustion model was built in a commercial software with the aim of simulating the experimental results and investigating the characteristics of methane-diesel combustion. The software used to build and simulate the engine model is GT-Power. Modelling a dual fuel engine with methane is an important challenge as the built model must respond to the inputs in accordance with experimental results. The main emphasis will be on combustion, which includes a laminar flame speed model. For methane, the combustion model available in GT power does not have pre-defined constants for laminar flame speed model. This work aims to build a laminar flame speed model and incorporate it

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in the combustion model of the GT power. It uses approaches from Heywood [9] and Gülder [10, 11] and it was validated with experimental results.

2 Model setup

The research was carried out in a single cylinder diesel engine. It is a 522 cm^3 four-stroke diesel engine. The specifications of the engine can be seen in Table 1. The engine was modelled in the engine simulation software, according to the specifications from engine test bench, as shown in the Figure 1.

Table 1: Engine specifications.

Engine type	4-stroke, single cylinder
Stroke [mm]	92
Bore [mm]	85
Cylinder volume displacement [cm^3]	522
Combustion bowl volume [cm^3]	19.7
Compression ratio	16.5:1
Number of Valves	4

As it can be seen, the model has two injectors, one at the intake port, where methane will be injected and second one in the engine head, where diesel will be injected within the cylinder to initiate combustion. The stationary tests for calibration were performed at 4 different operating points. The engine model was updated with all the intake and exhaust conditions, initial pressures and temperatures at various locations, fuel mass flow rate for methane, start of injection (SOI) and injected fuel mass for diesel, according to the experimental results of dual fuel methane/diesel engine, for various operating points as shown in Table 2. Pilot and main injections have the same duration, and then the same amount of fuel is injected.

Once the model is built, the simulated air mass flow was checked to be coherent with the experimental values. The diameter of the orifice connection "VL-out" was modified accordingly, in order to reach the experimental air mass flow. After initial calibration, the interest was shifted to the combustion model, where a new laminar flow model was built and incorporated in set-up for methane-diesel dual fuel model.

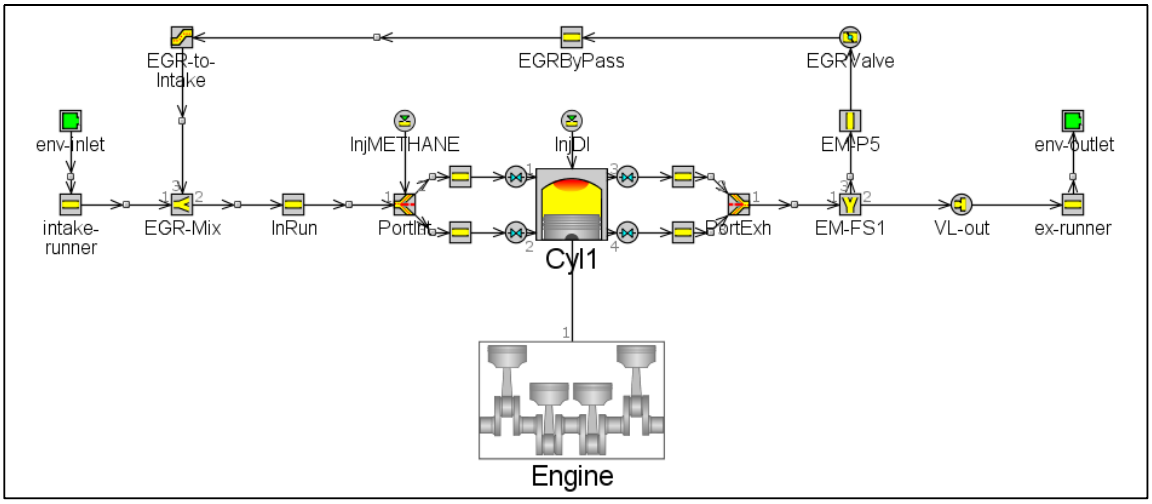

Figure 1: GT-Power model of the compression ignition single cylinder diesel engine in dual fuel mode.

Table 2: Engine operating conditions.

Case	**#1**	**#2**	**#3**	**#4**
Engine Speed [rpm]	1500	1500	2000	2000
Brake Mean Effective Pressure [bar]	2	5	2	5
Start of pilot injection [deg]	-16	-11.6	-21.2	-18.6
Start of main injection [deg]	-6	0.3	-8	-2.4
Dwell interval [deg]	10	11.9	13.2	16.2
Duration of pilot and main injections [deg]	2.6	2.4	3.4	3.1
Diesel mass of pilot and main injections [mg/cycle]	0.711	0.822	0.717	0.833
Methane mass [mg/cycle]	7.58	11.19	7.55	10.15
Rail pressure [bar]	615	867	700	891
Inlet pressure [bar]	1.5	1.7	1.5	1.7
Inlet temperature [°C]	44	46	50	51
Air mass [mg/cycle]	750.9	802.4	679.3	741.2
Methane/air equivalence ratio [-]	0.174	0.240	0.192	0.236
Premixed Ratio [%]	86.10	88.78	85.97	87.62

3 Combustion model

In the software, a specific model is provided for dual fuel combustion. Actually, it consists of two models usually used for conventional diesel combustion and flame propagation in spark ignition engines, respectively. Without considering in this phase, the effects of turbulence, it uses the well-established power law formula [12] to relate the dependency of the laminar flame speed on temperature and pressure:

$$S_L = S_{L,0}\left(\frac{T_u}{T_{ref}}\right)^{\alpha}\left(\frac{p}{p_{ref}}\right)^{\beta} \tag{1}$$

$$\alpha = 2.18 - 0.8(\phi - 1) \tag{2}$$

$$\beta = -0.16 + 0.22(\phi - 1) \tag{3}$$

The main focus of this work is the defining of the $S_{L,0}$ term. It represents the speed of the laminar flame in standard conditions (T_{ref} = 298 K and p_{ref} = 1.03 kPa) that is an intrinsic property of the mixture. The software offers only the standard correlation for its expression [12]:

$$S_{L,0} = B_m + B_{\phi}(\phi - \phi_m)^2 \tag{4}$$

However, it suggests the use of a "proprietary" model for combustion in methane mixtures. Indeed, this model is acceptable for simulations of mixtures near the stoichiometric value, while below equivalence ratios of 0.6, the flame speed assumes a negative value (Figure 2). Gaseous fuels usually burn in lean conditions, such as the test cases under investigation (Table 2), therefore, the flame propagation model requires to be adapted.

In order to avoid the negative flame speeds, the second order polynomial correlation was corrected according to Gülder [10] proposal:

$$S_{L,0}(\phi) = \omega \phi^{\eta} e^{-\xi(\phi-\sigma)^2} \tag{5}$$

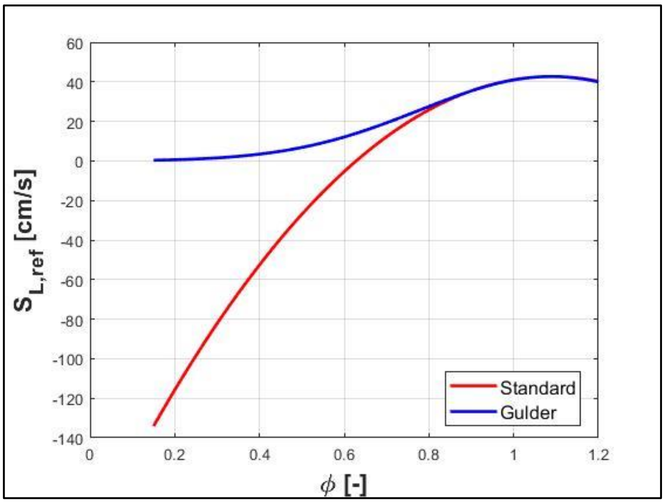

Figure 2: Reference laminar flame speed trends for different equivalence ratios for standard [12] and Gülder [10] correlations.

Table 3: Coefficients of methane [10].

ω [cm/s]	η	ξ	σ
42.2	0.15	5.18	1.075

In order to implement this correlation in the software, it is possible to adapt the standard one by providing to the term B_m (eq. 4) a matrix of values, created in Matlab, that reproduces the Gülder laminar flame speed in function of the equivalence ratio, while the quadratic part of the standard correlation is deleted by setting the term B_ϕ equal to 0.

4 Results

Initially, the engine was calibrated with motoring conditions to estimate the correct mass flow rate entering the system. Moreover, the engine is affected by mass loss (blow by) of the premixed charge of air and methane in the crevices region of the cylinder, starting from the results obtained in [13] a calibration of the parameter that regulates this phenomenon for the different cases is necessary. Once the simulated results agreed with the experimental ones, the interest was shifted to the calibration of the combustion model. Since the blow by model foresees only the loss of air, to take into account the methane loss as well, the quantity of methane injected in the intake manifold was reduced still taking into account the results in [13]. Regarding the turbulence and combustion setting, the constants were calibrated with reference to the 1500x2 case. In Figure 3, the results in terms of in-cylinder pressure are displayed.

As it is observed in Figure 2, the model is capable to provide a correct estimation of peak pressure levels. In addition, in the numerical simulations the rise to maximum is characterized by two peaks, probably due to the two injections of diesel fuel; while, the expansion phase is likely driven by the oxidation of the sole methane, that, except for the 1500x2 case, seems to be underestimated. This can be explained, as already highlighted, by the fact that turbulence and combustion conditions were not specifically modelled and the same constants were used for all the cases. On the contrary, they can be significantly affected by the engine speed and load level, considering, also, the mass loss [14].

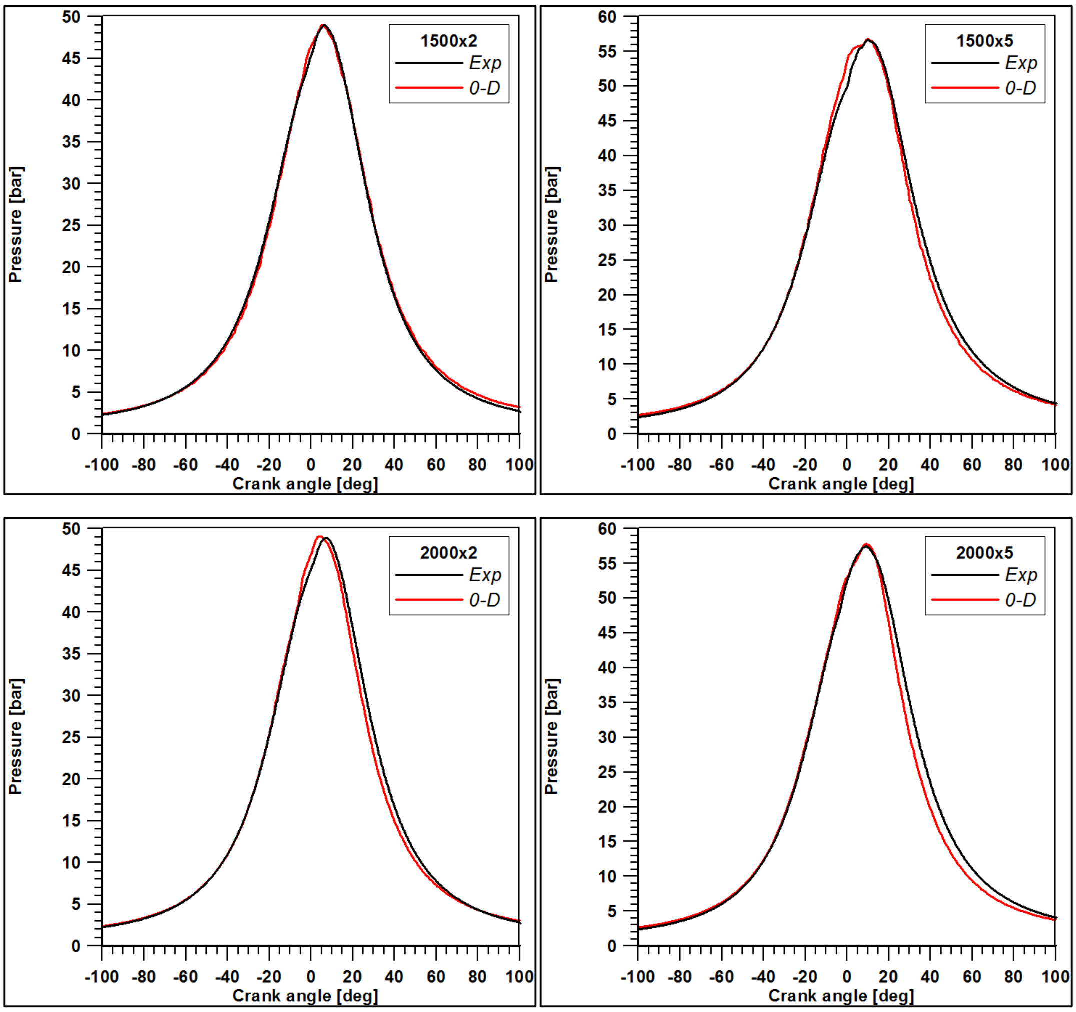

Figure 3: Pressure trends comparison for the different test cases.

In addition, the analysis of the burn rate and heat release, can be helpful to estimate the contribution of each fuel to the different phases of combustion development and to assess the differences with conventional ones.

Finally, the study of methane-diesel dual fuel combustion aims at the correct prediction of combustion process for various operating points with different speed and load conditions, especially for the applications that are difficult to investigate experimentally. As a matter of fact, it represents a feasible solution for the reduction of emissions with accessible costs in heavy-duty engines that require performances levels that only a well-established technology, such as the diesel engine can provide.

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REBUTTAL

We appreciate the reviewer's work in revising this extended abstract we submitted. We found useful observations and suggestions that we hope we were able to follow for the improvement of the abstract.

The authors present a modification of GT Power and application of the same to the analysis of dual fuel combustion in a compression ignition engine. Interest in this capability is informed by the suitability of methane for low pollutant formation and the need for an easily ignitable fuel that can initiate the combustion of the less reactive methane.

By means of a series of calibrated input-output correlations, the complex engine processes during a power cycle can be simulated in a simplified manner. But for this, the models have to be properly tuned. The merit of the paper is to overcome a situation that arises in lean combustion typical of CI and absent in near stoichiometric SI combustion. The Gülder laminar flame model is implemented to avoid negative burning velocity predictions at low equivalence ratios. What is missing is a verification that such a modified description of the lean flame speeds matches experimental data in the literature.

The model presented by Gülder in [10, 11] was validated by himself in the cited papers; actually other researchers acknowledged the reliability of this correlation:

1. Dirrenberger P, Gall L, Bounaceur R, Herbinet O, Glaude P, Konnov A, et al. Measurements of laminar flame velocity for components of natural gas. Energ Fuel 2011; 25: 3875–3884.
2. Coppens FHV, De Ruyck J and Konnov AA. The effects of composition on burning velocity and nitric oxide formation in laminar premixed flames of $CH4 + H2 + O2 + N2$. Combust Flame 2007; 149: 409–417.
3. Amirante, R., Distaso, E., Tamburano, P., and Reitz, R.D., "Laminar Flame Speed Correlations for Methane, Ethane, Propane and Their Mixtures, and Natural Gas and Gasoline for Spark-Ignition Engine Simulations," International Journal of Engine Research 18, no. 9 (2017): 951-970, doi:10.1177/1468087417720018.

We used the same correlation in [13] to describe the flame propagation in the air-methane mixture, but using a 3-dimensional approach where the results showed good agreement with experimental data. The novelty of the abstract is the implementation of this correlation in GT-Power for the description of dual fuel combustion.

The combustion model for the igniting diesel is not described nor the interaction of the two combustion models. It would be good to give more mathematical information on how the input-output relations are modified by the dual process.

We avoided to put any mathematical equation but those related to the laminar flame speed model because we want to focus on this latter model that represents the novelty of this work. Moreover, in the abstract it is stated:
"*Actually, it consists of two models usually used for conventional diesel combustion and flame propagation in spark ignition engines, respectively.*"
Therefore, the dual fuel combustion is described by two models coupled together. In particular, all the processes that lead to diesel combustion are the same as a conventional CI engine. Moreover, due to the intrinsic pragmatism of the 0D approach, the two models act in separate phases, the DI Pulse (for diesel) is used as spark for the air-methane mixture that burns with a flame propagation model (SI Turb). However, major details can be found in:

1. Heywood, J. B. (1988). Internal Combustion Engine Fundamentals.
2. Teodosio, L., Bozza, F., Tufano, D., Giannattasio P., Distaso, E., Amirante, R., "Impact of the laminar flame speed correlation on the results of a quasi-dimensional combustion model for Spark-Ignition engine", Energy Procedia 148 (2018) 631-638, doi: 10.1016/j.egypro.2018.08.151
3. Millo, F., A., F., Piano, A., Caputo, G., Cafari, A., Hyvonen, J., "Experimental and numerical investigation of the ignition process in a large bore dual fuel engine", 2021, https://doi.org/10.1016/j.fuel.2020.120073.

Methane injection is reduced to account for the enrichment caused by correcting for blow by losses. How is this reduction determined?

We are sorry for not being clear on this passage. We reformulated the sentence in order to illustrate that the methane reduction is based on the previous calculations performed with a 3D code [13].

The usefulness of this type of analysis is diminished by opacity of the input-output relations and the determination of the physical coefficients on which they depend. One is looking for a demonstration by the author that the physical phenomena are reasonably accounted for.

We are sorry if the analysis does not seem adequately deepened but, we preferred to focus on the problem regarding the correct laminar flame speed determination in lean air-methane mixtures. Nevertheless, the fair agreement of the numerical and experimental pressure curves evidences that the numerical model is capable to detect the main features of combustion (i.e. start, peak and expansion phase). As a matter of fact, the main target of a 0D approach is the ability to replicate the performances of the actual engine, the physical phenomena can be observed only with a CFD approach.