

VALIDATION OF A ZERO-DIMENSIONAL AND TWO-PHASE COMBUSTION MODEL FOR DUAL-FUEL COMPRESSION IGNITION ENGINE SIMULATION

by

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Increasing demands for the reduction of exhaust emissions and the pursuit to reduce the use of fossil fuels require the search for new fuelling technologies in combustion engines. One of the most promising technologies is the multi-fuel compression ignition engine concept, in which a small dose of liquid fuel injected directly into the cylinder acts as the ignition inhibitor of the gaseous fuel. Achieving the optimum combustion process in such an engine requires the application of advanced control algorithms which require mathematical modelling support. In response to the growing demand for new simulation tools, a 0-D model of a dual-fuel engine was proposed and validated. The validation was performed in a broad range of engine operating points, including various speeds and load condition, as well as different natural gas/diesel blend ratios. It was demonstrated that the average model calculation error within the entire cycle did not exceed 6.2%, and was comparable to the measurement results cycle to cycle variations. The maximum model calculation error in a single point of a cycle was 15% for one of the complex (multipoint injection) cases. In other cases, it did not exceed 11%.

Key words: dual-fuel, natural gas, 0-D model, reaction kinetics

Introduction

In a number of research works on dual-fuel engines it was demonstrated that the operating parameters of a dual-fuel compression ignition engine depend significantly on the pilot dose size [1-3], pilot dose injection timing [1, 4], amount and quality of gas supplied to the engine [5-7], and on the quantity and temperature of air aspired by the engine [8, 9]. To ensure optimum use of the engine capabilities all those parameters have to be adjusted relative to the rotational speed and load.

A significant improvement in dual-fuel engine performance can be achieved using advanced injection equipment for the liquid fuel. Electronic injection in a high pressure common rail system enables the application of small doses of properly sprayed fuel, which affects the combustion efficiency of the gaseous fraction [10, 11].

Still main issues for dual-fuel operation are commonly reported. High unburned HC and CO emissions resulted from the fact that some parts of the cylinder volume are not igniting or combust partially [12, 13] is one of the main issues. Low combustion efficiency was

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observed especially during low load operation. At higher loads cycle to cycle (and cylinder to cylinder in multi-cylinder engines) variations remain constant problems [14-16]. Addressing those issues requires sophisticated control algorithm which employ multiple regulation parameters like: gas/diesel blend ratio (BR), liquid fuel injection timing (including divided injection), and injection pressure, gaseous fuel injection timing, exhaust gas re-circulation, turbocharging/throttling, or air path heating. Among considered dual-fuel control strategies in-cylinder pressure control have proven to give very promising results in reducing cycle to cycle variations [17]. Even greater potential is expected from applying model based control [18]. Both strategies require development of fast and reliable mathematical models.

Simulations of dual fuel natural gas (NG)/diesel combustion have been reported with different approaches and for different purposes. The research works include detailed 3-D CFD simulations [12, 13], or faster reaction kinetic based multi-zone simulations [14-16]. Engine control development, however, requires much faster approaches. Despite long computation time, only a handful of models from that category have undergone complete experimental verification, which diminishes their reliability.

Simpler approaches had been also proposed. Wiebe fit models were proposed, *e. g.* [19]. Furthermore artificial neural network [20, 21] or gene expression programming [22] algorithms were applied to support creating high level correlations of engine parameters. These approaches are suited for developing the control algorithm [23], but only for the engine on which the model has been verified. Furthermore, the mentioned approaches are not based on the physical nature of phenomena occurring in the engine, and thus are unable to assist in comprehending them.

There are very few research results available on the process of NG combustion in modern, supercharged, dual-fuel engines [10, 24]. In particular, the possibility of the division of an initial dosage of diesel fuel has not yet been explored. Divided injection allows the control of the combustion process, reduction of toxic emissions and noise [25, 26]. In such a system, usually a very small portion of diesel fuel (pilot dose) is injected early, at the compression phase, to improve the combustion conditions of the main dose, which is injected slightly after pilot dose ignition.

To compensate on those drawbacks, in the attempt to create a fast and reliable dual fuel combustion model which can be used for model based control development, as well as to give insight on the in-cylinder processes, the authors proposed their own approach. A 0-D single-zone model with Wiebe fit as diesel burn rate representative and single-step macro-reaction kinetics describing gaseous fuel combustion had been introduced [24].

The objective of this paper was to verify whether the simplified kinetics of chemical reactions adopted in the model developed by the authors allows for a sufficiently accurate representation of gaseous fuel combustion in a dual-fuel engine. The validation of the model was performed for several dual-fuel engine fuelling concepts: for single injection of liquid fuel with a common pilot dose and gaseous fuel ignition point, and for a liquid fuel dose injected in two stages.

The 0-dimensional dual-fuel engine model

Mikulski *et al.* [24] elaborated description of the mathematical model developed and presented the methodology of numerical calculations. In this publication the basic model assumptions are presented briefly for introduction only.

In the developed model it is assumed that, at any time, the load in the cylinder forms a homogeneous mixture of air, NG and diesel fuel. The proportions of individual components

change with the injection and combustion of combustible components, and are the functions of crank angle (CA).

In the model the heat exchange with walls is adopted as the sum of three streams flowing through the wall, cylinder head, and piston bottom.

While injecting the liquid fuel the thermodynamic parameters of the medium are changed. The effect of the mass stream of the fuel injected into the cylinder was modelled with the aid of the Mikulski *et al.* [27] original correlation based on a normal distribution.

The model assumes that both the liquid (diesel fuel) and gaseous fractions combust independently, using shared oxygen resources. The beginning of combustion is common for both fuels and determined by the ignition delay angle of diesel fuel, calculated using the correlation proposed by Assanis, *et al.* [28], since it describes better than others the gas effect on the total self-ignition delay.

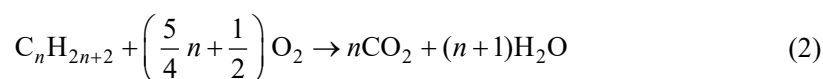
The diesel fuel combustion process is represented in the model with the Wiebe function. It allows for studying the effect of the diesel fuel combustion process on the gaseous fraction combustion.

The Wiebe fit has been validated for single fuel – mineral diesel (MD) operation in one of the earlier works [29] resulting in a simple and explicit correlation for diesel combustion duration, $\Delta\alpha_{MD}$ [CA], with respect to fuel consumption, G_{MD} [kg h⁻¹]:

$$\Delta\alpha_{MD} = 5.52G_{MD} + 18.57 \quad (1)$$

In the present work the same correlation has been used to describe liquid fuel combustion along with the Wiebe function exponential coefficient of 0.4 (also derived from single fuel validation). This expresses the assumption of the model, that both liquid and gaseous fuels combust separately within the cylinder chamber, utilising the common supplies of oxygen.

The natural gas combustion model was based on one-step macro-reactions of oxidation of the main components of the mixture: methane (CH₄), ethane (C₂H₆), and propane (C₃H₈). This leads to a system of three reactions of global forms:



for $n = 1...3$. In this case, the global reaction speed equation takes the form:

$$\frac{d[C_nH_{2n+2}]}{dt} = A_n \exp\left(-\frac{E_{a_n}}{RT}\right) [C_nH_{2n+2}]^{a_n} [O_2]^{b_n} \quad (3)$$

The values of constants present in the previous equation for methane, referred to in the literature, depending on the calculation algorithm adopted amount to:

– variant I:

$$A = 1.3 \cdot 10^9, \quad E_a = 48.4 \text{ kcal/mol}, \quad a = -0.3, \quad b = 1.3 \quad [30]$$

– variant II:

$$A = 8.3 \cdot 10^6, \quad E_a = 30.0 \text{ kcal/mol}, \quad a = -0.3, \quad b = 1.3 \quad [30]$$

Materials and methods

Data sets for verification

To validate the developed model the results of in-cylinder pressure measurements of a dual-fuel engine were applied. The ADCR (manufacturer code) Diesel engine unit was supplied by Andoria Motors and adopted for DF feeding by installing an after-market gaseous fuel injection system in a single point fashion, upstream of the engine intake manifold. The main parameters of the test engine were summarized in tab. 1.

Table 1. Technical details of dual-fuel ADCR engine

Type	4-stroke, turbocharged, intercooler
Fuel injection	Liquid – common rail, direct injection, multiple injections capability; Gaseous – single point, intake manifold injection
Engine layout	4 cylinder inline, vertical
Bore/Stroke	94/95 mm
Disp. volume	2636 cm ³
Compression ratio	17.5
Rated power [rpm]	85 kW/3700 rpm*
Max. torque [rpm]	240 Nm/1800-2200 rpm*
Fuels	Diesel CN = 52, LHV = 42.7 MJ/kg; natural gas LHV = 38.6 MJ/kg

* For single fuel operation

The validation involved the comparison of the model calculation results with the recorded mean pressure curve, averaged from 50 successive work cycles. Both the test bench and the methodology of the pressure measurements were described in detail in [10], and will not be broadly discussed here.

The tests were conducted at two rotational speeds:

- 1500 rpm – at which the engine controller injects two doses of diesel fuel (the pilot dose and the main dose), and
- 3400 rpm – at which the controller injects a single dose of fuel regardless of the load.

The engine tests were conducted at these rotational speeds for different engine loads and different BR of individual fuels (from 100% diesel to the minimum amount of diesel for which pre-set operating parameters could be maintained). For model validation, test runs were selected at which the acceptable engine operating stability was achieved, as determined by break mean effective pressure (BMEP) variations not exceeding 5%. This criterion limited the scope of validation to low-medium engine load conditions (BMEP range 2.4-7.2 bar).

Since the gas combustion takes place in very lean mixture conditions (air/gas equivalence ratio, λ_{NG} , in a range from 1.8 to 10.9, tab. 2), it can be assumed that the gas burns completely. In specified conditions, however, not all the gaseous fuel takes part in combustion, whereby the amount of unburnt CH₄ can reach up to 50%. This is due to the fact that, when the mixture is very lean, only the part of the gas which remains within the diesel fuel

flame zone will ignite [10]. It is therefore important to determine the amount of gas involved in the reaction.

This was done by comparing the fuel energy capacity for single fuel operation, Q_{SF} , with the cumulative energy capacity of diesel fuel and NG (Q_{DF_MD} and Q_{DF_NG} , respectively) introduced to the engine while operating in dual-fuel mode in corresponding operating point. This way gaseous fuel conversion efficiency was assessed:

$$\xi_{NG} = 100 \frac{Q_{DF_MD} + Q_{DF_NG}}{Q_{SF}} \quad (4)$$

and introduced as a modelling parameter.

The scope of the validation and the basic model input parameters are shown in tab. 2.

Table 2. The scope of the validation and the basic model input parameters taken from experimental measurements

No.	n [rpm]	BMEP [bar]	BR [%]	G_{air} [kg h^{-1}]	G_{MD} [kg h^{-1}]	G_{NG} [kg h^{-1}]	λ_{NG+MD} [-]	λ_{NG} [-]	ξ_{NG} [%]
1	3400	2.4	80	243	6.1	1.3	2.3	10.9	98
2		4.7		300	9.1	2.2	1.8	7.9	87
3		7.2		324	12.5	3.6	1.4	5.2	68
4	1500	4.7	80	106	0.23	1.0	5.2	6.1	65
					3.07		1.8	6.1	
5			50	102.5	0.32	2.1	2.5	2.8	78
					1.79		1.7	2.8	
6			30	99.5	0.36	2.8	1.9	2.1	86
					0.84		1.7	2.1	
7			17	98	0.28	3.2	1.7	1.8	91
	0.42	1.6			1.8				

Verification procedure

Verification was done by comparing the results of model calculations with recorded average pressure taken from 50 subsequent engine duty cycles. As fit quality indicator a straightforward difference between model predicted pressure and cycle averaged experimental pressure, for each CA, was introduced (model fit error). The previous approach was chosen to comply with measurement result cycle-to-cycle variation estimation [29].

The result of eq. (1) was used as diesel fuel combustion duration for the liquid fuel burn rate model as a basic approach. The model was then fine-tuned using this parameter until reaching the minimum of the averaged model fit error. The tuning strategy took to account the results of earlier experimental research [27] concluding that the presence of gaseous fuel causes prolongation of diesel combustion duration. The optimised $\Delta\alpha_{MD}$ was therefore searched within the boundaries of +20 CA from the basis value. Diesel combustion duration was therefore the only fitting parameter used in the present study.

During the first phase of validation, the accuracy of model calculations at the points of the single injection was validated for the engine rotational speed 3400 rpm, various loads, and for BR of 80%. It was thereby possible to determine which of the two available data variants (I or II) describing the CH₄ combustion rate, as per eq. (3), represents the process in the dual-fuel engine more effectively.

The model performance at higher CNG shares was validated for a more complex case, *i. e.* double injection. Since the greatest range of the gaseous fraction shares at which the engine operated steadily was at the rotational speed 1500 rpm and partial loads, the measurement results for those operating points of the engine were used for validation.

Results and discussion

Model validation results – single injection

First, the calculation results of the model for two data variants describing the CH₄ combustion rate according to the eq. (2) were compared. It was observed that for the model with variant I, due to the higher activation energy, the combustion process intensifies for much higher temperatures, compared to model II (fig. 1). As a result of, while maintaining the initial diesel fuel combustion angle, CH₄ combustion begins too late for the case I. Reducing the diesel fuel combustion angle results, in this case, in faster temperature increase in the cylinder and, thus, accelerated ignition.

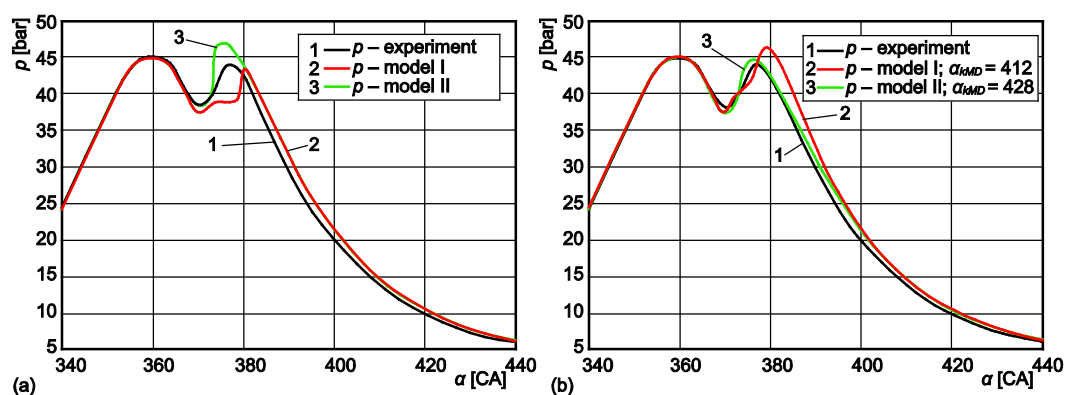


Figure 1. Comparison of calculation results for various variants of constant values, with the average pressure curve, fuelling with MD + CNG; $n = 3400$ rpm; BMEP = 2.4 bar, BR = 80%:
(a) $\alpha_{end} = 422$ CA, (b) optimised end points of diesel combustion

The results presented in fig. 1(a) demonstrate that, for this assumption, the diesel fuel combustion is too fast, which overstates the pressure curve. While applying to the model the data according to variant II, for the calculated diesel fuel combustion angle, the gaseous fuel ignition occurs almost immediately after liquid fraction starts to release energy. A slight extension of the diesel fuel combustion end time leads to a considerable improvement in model representation accuracy, fig. 1(b). The prolonged diesel fuel combustion period, compared to an identical dose in the single-fuel operation, can be explained by the reduction of oxygen concentration in the mixture being combusted. Optimisation of the combustion angle for higher rates in the dual-fuel model is therefore well-founded in theory.

Similar behavior in both models was reported for the other measurement attempts. A slight increase in the diesel fuel combustion angle caused improved calculation results. The results of the model II calculations for various engine loads, after optimization of the diesel fuel combustion angle, are presented on fig. 2.

The adopted kinetic combustion model of CH₄ slightly overstated the pressure curve compared to the values recorded in the tests, which was as expected. Since, in fact, CH₄ oxidation to CO₂ and water occurs in a series of multiple partial reactions, the overstated values of the combustion rate were obtained applying one global reaction. The maximum pressure reproduction error did not exceed 12%, and was present only in a narrow range of combustion angles. In other CA ranges the representation error was comparable to the standard deviation value defined for the pressure measurements.

Regardless of momentary deviations from the measurement value, the calculated pressure curve equalizes quickly with the experimental data when the gas combustion process is finished. This proves the thesis that the gas is not fully combusted.

Analysing heat release rates for the modelled cases, fig. 3, more rapid combustion characteristics of gaseous fuel compared to diesel was observed. At high BR the gaseous fuel combustion duration did not exceed 11 CA, tab. 2. This value is realistic when confronted with experimental results [2]. The decreasing of this parameter was observed with increasing load, which was as expected through strong dependency of the reaction rate on in cylinder temperature, eq. (3).

For small loads (50 Nm) a delay period between diesel and gaseous fuel ignition was observed. This was a kinetic effect predicted by eq. (3) and independent from diesel ignition delay predicted by the Assanis correlation. The activation energy needed to light on the gaseous combustion mechanism was reached after a major part of liquid fuel had already reacted. The Assanis correlation, implemented in the model, predicted the diesel fuel ignition delay very well, taking to account the influence of gaseous fuel addition, tab. 3.

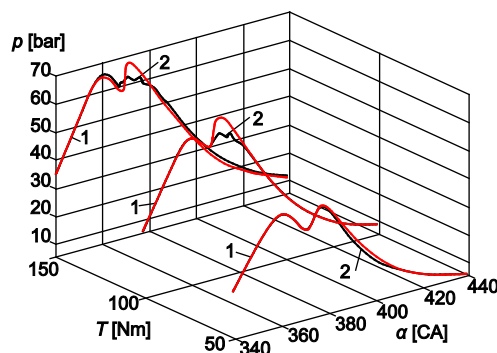


Figure 2. Comparison of the model calculation results (1) for the dual-fuel operation (optimised diesel fuel combustion end values) with the mean pressure curve (2):
 $n = 3400$ rpm, BR = 80%, various engine loads

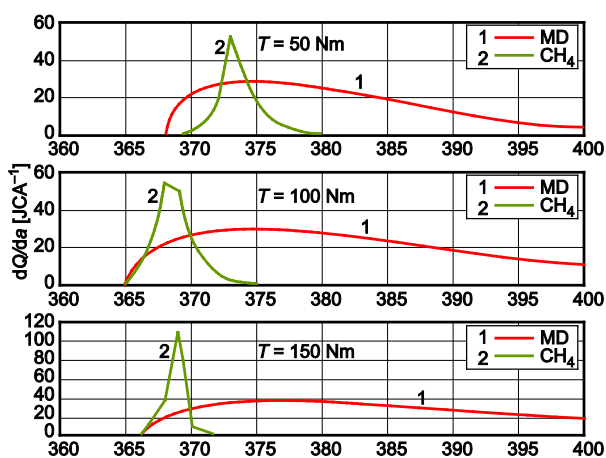


Figure 3. Modelled heat release rates of diesel and CH₄ fuel (optimised liquid fuel combustion duration):
 $n = 3400$ rpm, BR = 80%, various engine loads

Table 3. Combustion parameters for the verified cases for single injection mode

Test case	Measurement		Model			
	α_{id}	α_{start}	α_{id}	α_{end}	$\Delta\alpha_{MD}$	$\Delta\alpha_{CH_4}$
	[° CA]					
1	15	369	14.6	428	59	11
2	12	366	11.1	450	84	10
3	9	365	7.9	465	100	7

Model validation results – multiple injections

Initial validation attempts for the dual-fuel operation with double injection demonstrated that in the case of the 20% gaseous fuel share the CH₄ ignites from the main (second injection) diesel dose, which resulted in a very high consistency of the calculation results. A comparison of the curves is shown in fig 4.

The assumption, that the entire gas volume ignites from the combustion of the pilot or main dose of diesel fuel, was however not valid for some test cases. Two combustion concepts applied in the model calculations are compared in fig. 5, the assumption that all of the gaseous fuel ignites from the combustion of pilot (first) diesel injection and the assumption that the energy released from initial diesel dose is insufficient to cause gaseous fuel ignition and the combustion of the gas fraction starts when the main diesel dose ignites. Analysing the model calculation results, it can be concluded that the CH₄ combustion concepts described can not satisfactorily represent the pressure curve in the case being studied. Similar behavior was reported for the other measuring points.

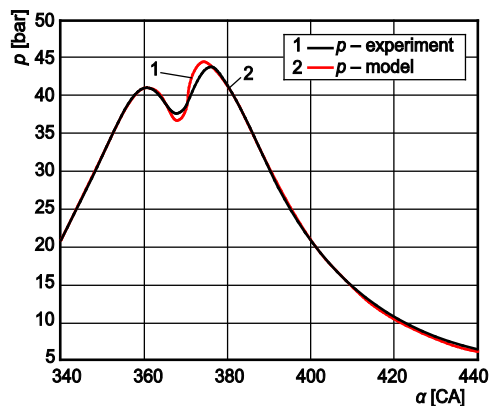


Figure 4. Comparison of the calculation results with mean pressure curve: $n = 1500$ rpm, BR = 20%, single CNG ignition point from main (second) diesel injection

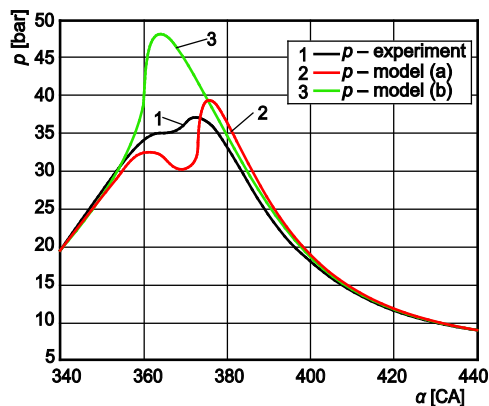


Figure 5. Comparison of the calculation results of the dual-fuel modes with mean pressure curve: $n = 1500$ rpm, BR = 50%. (a) The CH₄ ignition with first diesel injection. (b) The CH₄ ignition with second diesel injection

The only explanation for such behavior appears to be two separate CH₄ combustion processes taking place, *i. e.* some part of the gas volume ignites from the pilot dose, and another from the main one.

The third concept was then validated. It was assumed that the percent of total gaseous fuel mass attributable to the first phase is equal the pilot to main diesel dose proportion.

The amount of gas being combusted increases in both phases with the gas concentration, in spite of the generally lower dose of the diesel fuel combusted, since the gas reaches the flammability limit.

The implementation of two separate gas combustion points resulted in a significant improvement of the results of model calculations. The model with such a specification represented the pressure curve surprisingly well, particularly for higher doses of gaseous fuel, fig. 6. Two combustion phases were clearly marked in the model curve, while the pressure increase was constant in the recorded curve. This results from the fact that the actual CH₄ combustion time is longer and both combustion processes overlap. The overlapping of both combustion processes is well represented for a minimum dose of diesel fuel and illustrated on the heat release rate plot, fig. 7.

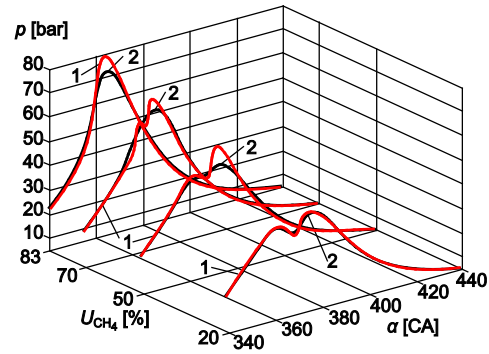


Figure 6. Comparison of the model calculation results (1) for dual-fuel operation with the mean pressure curve (2): $n = 1500$ rpm, BMEP = 4.7 bar, various BR, two CNG ignition points

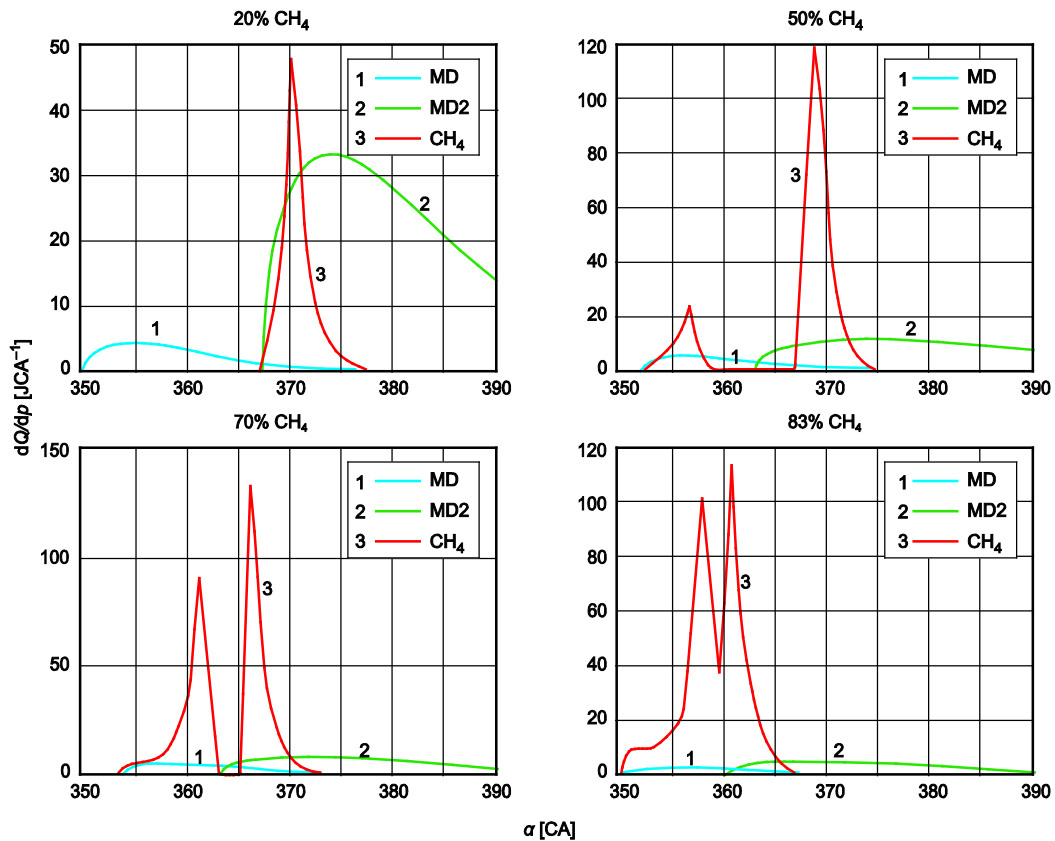


Figure 7. Heat release rates, $n = 1500$ rpm, BMEP = 4.7 bar: various BR, divided injection, two CNG ignition points

The heat release rate from CH₄ combustion was increasing with increasing CNG share in the fuel dose, reaching a maximum at the value of 120 J/CA. This is consistent with the elementary knowledge on gaseous mixtures which implies the existence of a limiting boundary for combustion speed.

The momentary maximum representation error did not exceed 15% for any of the measuring attempts, yet this value is obviously higher compared to the calculations for the single-fuel operation, tab. 4.

Table 4. Cycle averaged model fit errors vs. measurement results cycle to cycle variations; for all discussed test points

Test	n [rpm]	BMEP [bar]	BR [%]	Measurement		Model
				δp_{avg} [%]	δp_{max} [%]	δp_{avg} [%]
1	3400	2.4	80	7.6	19	6.1
2	3400	4.7	80	3.9	13.2	3.1
3	3400	7.2	80	4.5	13.8	3.7
4	1500	4.7	80	1.8	6.1	2.4
5	1500	4.7	50	5.4	17	6.1
6	1500	4.7	30	5	13.4	4.9
7	1500	4.7	16.5	3.2	10.7	6.2

Conclusions

The research results presented in this section demonstrated that the non-repeatability of the engine increases in the dual-fuel operation. Stable operation at higher gaseous fuel doses can be achieved only for lower rotational speeds. The model applied was also found to have correctly represented the pressure curve in the cylinder. The momentary error did not exceed 15% of the pressure value in the cylinder, and was found only in a narrow range of CA, tab. 4. The error is present during the combustion phase and due to that, significantly influences relevant control quantities (like CA of 50% mas burned, max pressure, and indicated mean effective pressure) prediction accuracy. Still this is considered to be sufficient taking to account measured engine cycle to cycle variations. Also note, that the gas combustion model adopted results strictly from the fundamental laws of thermochemistry and, contrary to the diesel fuel combustion model applied, it is fully autonomous. Furthermore, the model quickly tended to align with the actual curve after the combustion process was finished. This proves that the assumptions as to the total energy released in the combustion of the gaseous fraction are valid.

The pressure curve in the cylinder is largely affected by the ignition point of the liquid and gaseous fuels. For the liquid fuel, similarly as reported for the single-fuel operation, the model represents the delay of the main dose ignition very well. However, it fails when predicting the ignition of the pre-ignition dose. This results from the nature of the Assanis correlation applied, which is an empirical formula, and was validated for larger fuel doses injected at higher temperatures and pressures than observed for very early pilot injection.

The present work supplements the earlier works by the authors on model development [14] and partial validation for single fuel operation [29]. The presented model has

proved to be valid for broad engine operating conditions. The summary of the range of model validity along with approximation errors is presented in tab. 5.

Table 5. Overall stages of the verification with range and maximum errors per stage

Stage	Scope				Max. error			Computation time (avg) ** [s]
	n [rpm]	BMEP [bar]	p_{max} [bar]	BR [%]	Momentary		Cycle avg. [%]	
					[bar]	[%]		
Motoring*	750	0	27	0	1.1	5	6.6	0.008
SF SI*	2300-3400	2.4-9.5	49-92	100	6.5	8	8.4	0.12
SF MI*	1500	1-9.5	36-87	100	3.7	6	6.8	0.37
DF SI	3400	2.4-9.5	35-48	80	6.5	11	6.1	1.12
DF MI	1500	2.4-7.2	40-72	20-80	8	15	6.2	1.42

* Results from previous work [29]

** The CPU time on Intel Core i7 processor – running single core with MATLAB 2014b

Achieved accuracy vs. computation efficiency allow to conclude that the model is capable of supporting major phases of DF combustion engine development, *i. e.*: concept study support (some trend prediction capabilities using the model had already been shown in [27]), control development (the model can anticipate system reaction on air-path and injection system excitations and therefore support designing control strategies, also transients prediction is possible when combine with a proper air-path model) and model-assisted calibration (the model accuracy allows for pre-determining controller parameters which can serve as basis for experimental fine-tuning calibration). For model based control the model is still too slow for direct implementation. Achieved computation times however, tab. 5, show good potential for code optimisation towards real time embedded systems which is already significant taking to account complex combustion mode and high prediction accuracy. At the current state suitable calculation times can be achieved by using a map-based approach [18] with the model serving as efficient map-generator.

Nomenclature

E_a – activation energy, [J]
 G_{air} – air consumption, [kg h^{-1}]
 G_{MD} – diesel consumption, [kg h^{-1}]
 G_{NG} – natural gas consumption, [kg h^{-1}]
 p – pressure, [bar]
 Q – cumulative energy capacity, [J]
 T – engine load, [Nm]
 U_{CH_4} – amount of gaseous fuel, [%]

Acronyms

BR – blend ratio, [%]
 BMEP – break mean effective pressure, [bar]
 CA – crank angle, [°]
 CN – cetane number
 CNG – compressed natural gas
 CPU – central processing unit
 DF – dual-fuel
 LHV – lower heating value, [MJkg $^{-1}$]

MD – mineral diesel
 MI – multiple injections
 NG – natural gas
 SF – single fuel (diesel)
 SI – single injection

Greek symbols

α_{id} – ignition delay, [CA]
 α_{start} – start of diesel combustion, [CA]
 α_{end} – end of diesel combustion, [CA]
 $\Delta\alpha_{MD}$ – diesel combustion duration, [CA]
 $\Delta\alpha_{CH_4}$ – methane combustion duration, [CA]
 δp_{avg} – the CA averaged error, [%]
 δp_{max} – maximum error, [%]
 ζ_{NG} – te NG conversion efficiency, [%]
 λ_{NG} – air/gas equivalence ratio, [-]
 λ_{NG+MD} – air/(gas+ MD) equivalence ratio, [-]

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