CLOSED VESSEL COMBUSTION MODELLING BY USING PRESSURE-TIME EVOLUTION FUNCTION DERIVED FROM TWO-ZONAL APPROACH

by

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In this paper a new method for burned mass fraction – pressure relation, x-p relation, for two-zone model combustion calculation is developed. The main application of the two-zone model is obtaining laminar burning velocity, S_L, by using a pressure history from a closed vessel combustion experiment. The linear x-p relation by Lewis and von Elbe is still widely used. For linear x-p relation, the end pressure is necessary as input data for the description of the combustion process. In this paper a new x-p relation is presented on the basis of mass and energy conservation during the combustion. In order to correctly represent pressure evolution, the model proposed in this paper needs several input parameters. They were obtained from different sources, like the PREMIX software (with GRIMECH 3.0 mechanism) and GASEQ software, as well as thermodynamic tables. The error analysis is presented in regard to the input parameters. The proposed model is validated against the experiment by Dahoe and Goey, and compared with linear x-p relation from Lewis and von Elbe. The proposed two zone model shows sufficient accuracy when describing the combustion process in a closed vessel without knowing the end pressure in advance, i. e. both peak pressure and combustion rates can be sufficiently correctly captured.

Key words: *combustion bomb, laminar flame speed, methane, two-zone model*

Introduction

Combustion modeling has become significant with the growing concern for decreasing fossil fuels reserves and preserving our environment. Important aspects of the modeling are to give information about combustion efficiency, green house gases emission, and pollutant reduction, as well as insight into combustion of alternative fuels. The most often researched gas fuels are methane [1, 2], hydrogen [3], and their mixtures [4-9]. A very important property of a fuel, which has been investigated, is laminar burning velocity, often denoted as S_L. One of the methods, commonly used for modeling combustion of perfectly premixed gas fuels, is the zonal approach. In the zonal approach, the domain of the combustion vessel is divided into zones, mutually connected with a mathematical function, based on the mass and energy conservation laws.

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The simplest is the two-zonal model, where the combustion vessel is divided into burned zone (containing combustion products) and unburned zone (containing fresh mixture), separated with infinitely thin flame front. Generally, pressure-time evolution in a closed vessel is a function of burnt mass fraction x and the laminar burning velocity S_L. Mathematically, it can be expressed as an ordinary differential equation, containing laminar burning velocity S_L as a parameter, and x as a variable. In order to solve it, the functional dependence between burned mass fraction and pressure, x-p relation, must be known.

Literature review

The first zonal model was developed by Levis *et al*. [10]. For the pressure raise function, which links the burnt mass fraction x and instantaneous pressure p, a linear relation was adopted. Bradley *et al*. [11] published a review paper in which they compared the linear x-p relation to the numerical multi zone model. The results appeared to be very close to the linear relation. Stone *et al*. [12] compared multi zone x-p relation with the linear one and concluded that observed difference in results is not exceeding more than 1.6%. Dahoe *et al*. [13], calculated laminar burning velocities for methane-air mixtures by using the linear x-p relation. In their work [14], Lujten *et al*. argued that Dahoe results for laminar burning velocities of methane-air mixtures are 5-8% larger due to the use of linear x-p relation. On the other hand, in their recent work, Farrell *et al*. [15] determined laminar burning velocities for 45 hydro-carbonates. In their research two methods were used: pressure history and schlieren. For the pressure history method non-linear x-p relation was used. The measurements showed that velocities obtained by pressure history method were systematically ~10% higher than results from schlieren method.

In both cases, for linear and non-linear x-p relation, the end pressure is necessary for the description of the combustion process, namely for determining laminar burning velocity. In this paper a new x-p relation is presented on the basis of mass and energy conservation during the combustion. It will be shown that by using this new relation, it is possible to correctly describe the combustion process in a closed vessel without knowing the end pressure in advance, *i. e.* both peak pressure and combustion rates can be obtained. In order to correctly represent this, the model proposed in this paper needs several input parameters. They were obtained from different sources, like the PREMIX software (with GRIMECH 3.0 mechanism) and GASEQ software covering combustion of methane flames, as well as thermodynamic tables. Enetta *et al*. showed that standard detailed scheme GRIMECH 3.0 can correctly predict pollutant emissions in an IC engine [16]. The proposed model is validated against the experiment by Dahoe *et al*. [13]. In this experiment a spherical vessel, with radius of 168 mm, was used. The vessel was filled with a stoichiometric mixture of methane and air at 1 bar and 298 K. Mixture was ignited at the center of the vessel. This experiment is very suitable due to the fact that with spherical geometry intensive cooling of the flame on the walls of the vessel can be avoided. On the other hand, the vessel is sufficiently small so we can exclude buoyant effects. This simplifies the problem, since the lack of heat loss in the proposed method becomes less significant and adiabatic conditions during the combustion can be assumed.

In practical applications, zonal approach is used for simulation of different phenomena occuring in internal combustion engines, like homogeneous charge compression ignition [17], NO_x formation [18] or knock [19]. Khalilarya *et al*. [20] divided combustion chamber into three zones: cylinder head, cylinder wall, and piston head for calculating the rate of heat loss to the engine coolant.

First, mathematical description of pressure raise function modeling is presented. This is followed by an error analysis of the presented model. The analysis shows that the maximum error of the model is 1.56%. In the end, the results of both models, based on linear *x-p* relation and new method, are compared with the experiment.

Pressure raise function modelling

Methgalchy *et al*., published a two-zone model [21] in which energy and mass conservation equation are simultaneously solved. In their later work [22] an analysis of possible disturbing effects was discussed. They concluded that effects like wall heat transfer, burnt gas temperature gradient, buoyant rise for small vessels, charge stratification, flame wrinkling, ignition energy input, and radiative heat loss had limited effects on the process in the vessel. Based upon this, in a closed vessel combustion bomb analysis, the following assumptions are introduced:
(1) fresh mixture is perfectly premixed and no levels of turbulence are present,
(2) during the combustion, pressure remains spatially uniform in the vessel,
(3) in each zone of the two zones temperature is equally distributed,
(4) there is no heat exchange between unburned and burned zone,
(5) overall mass and mean density in the vessel is constant during the combustion,
(6) the vessel is adiabatically insulated,
(7) buoyancy is negligible,
(8) flame front is spherically shaped and infinitely thin,
(9) flame stretching effect is neglectable,
(10) fresh mixture is compressed adiabatically during the combustion process, and
(11) by the end of combustion there is still a small unburned fraction of fresh mixture remaining in the system.

The model which is presented in this paper requires the introduction of combustion efficiency parameter η which describes the last assumption. This parameter has a role to limit combustion to the some predefined limit which is less than one. This limit is necessary, since in real applications some of the fuel remains unburned due to molecular dissociation and chemical kinetics. The main part of the method is pressure raise function. This function describes pressure-time evolution. In addition to that, several features are also described: laminar burning velocity, and ignition.

Pressure raise function

Pressure raise function is an essential part of the methodology, since it relates pressure change with time. Based on the above assumptions the differential equation for the pressure can be derived:

$$\frac{\mathrm{d}p}{\mathrm{d}t} = \frac{3}{R_v}\frac{\mathrm{d}p}{\mathrm{d}x}\left[1-(1-x)\left(\frac{p_{in}}{p}\right)^{1/\kappa}\right]^{2/3}\left(\frac{p}{p_{in}}\right)^{1/\kappa}S_L \tag{1}$$

Equation (1) is widespread in the literature, and its derivation is not given here [13, 14, 23]. The detailed derivation could be found in [14]. Progress variable used in eq. (1) is the burned mass fraction *x*. In literature one can find linear, eq. (2), and non-linear, eq. (3), formulations for *x* [3, 14]:

$$x = \frac{p - p_{in}}{p_{end} - p_{in}} \tag{2}$$

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$$x = \frac{p - p_{\text{in}}\left[\dfrac{\kappa_b - 1}{\kappa_u - 1} + \dfrac{T_u}{T_{\text{in}}}\dfrac{\kappa_u - \kappa_b}{\kappa_u - 1}\right]}{p_{\text{end}} - p_{\text{in}}\left[\dfrac{\kappa_b - 1}{\kappa_u - 1} + \dfrac{T_u}{T_{\text{in}}}\dfrac{\kappa_u - \kappa_b}{\kappa_u - 1}\right]} \tag{3}$$

Because of its simplicity and small error, linear function $x(p)$ (2) is in wide use. Since peak pressure is not known in advance, eq. (1) alone is not sufficient to describe pressure-time evolution during the combustion process. This is why relation between pressure and progress variable is found. By deriving eq. (2) we obtain:

$$\frac{\mathrm{d}p}{\mathrm{d}x} = p_{\text{end}} - p_{\text{in}} \tag{4}$$

For easier differencing eq. (3), the equation will be written in a more concise form:

$$x = \frac{p - p_{\text{in}}\,\mathrm{f}(p)}{p_{\text{end}} - p_{\text{in}}\,\mathrm{f}(p)} \tag{5}$$

where function of pressure can be written as:

$$\mathrm{f}(p) = \frac{\kappa_b - 1}{\kappa_u - 1} + \frac{\kappa_u - \kappa_b}{\kappa_u - 1}\left(\frac{p}{p_{\text{in}}}\right)^{\frac{\kappa_u - 1}{\kappa_u}} \tag{6}$$

Differencing eq. (5) yields:

$$\frac{\mathrm{d}x}{\mathrm{d}p} = \frac{p - p_{\text{in}}\,\mathrm{f}'(p)}{p_{\text{end}} - p_{\text{in}}\,\mathrm{f}(p)} + \frac{p_{\text{in}}\,\mathrm{f}'(p)[p - p_{\text{in}}\,\mathrm{f}(p)]}{[p_{\text{end}} - p_{\text{in}}\,\mathrm{f}(p)]^2} \tag{7}$$

with

$$p_{\text{in}}\,\mathrm{f}'(p) = \frac{\kappa_u - \kappa_b}{\kappa_u}\left(\frac{p}{p_{\text{in}}}\right)^{-\frac{1}{\kappa_u}} \tag{8}$$

Relation between p and x can also be found from the energy balance:

$$\delta Q = \mathrm{d}m\, q\, Y_{\text{fu}}\eta_{\text{fu}} \tag{9}$$

On the other hand, releasing the energy of amount δQ, mean temperature in the vessel rises for $\mathrm{d}\overline{T}$, so it could be written:

$$\delta Q = m\,\overline{C}\,\mathrm{d}\overline{T} \tag{10}$$

By equalizing eqs. (9) and (10), and adopting that $\mathrm{d}x = \mathrm{d}m/m$, one can obtain the following relation:

$$\mathrm{d}x\, q\, Y_{\text{fu}}\eta_{\text{fu}} = \overline{C}\mathrm{d}\overline{T} \tag{11}$$

By assuming that the mixture in the vessel is an ideal gas,

$$\frac{p}{\rho} = \overline{R}\,\overline{T} \tag{12}$$

and differencing the eq. (12) one obtains:

$$\frac{\mathrm{d}p}{\rho} = \mathrm{d}\overline{R}\,\overline{T} + \overline{R}\,\mathrm{d}\overline{T} \tag{13}$$

If one takes into consideration the fact that mean gas constant $\overline{R}$ is equal to $\overline{R} = R_u(1 - x) + R_b x$, and substituting this into (13), a differential equation yields:

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$$\frac{\mathrm{d}p}{\overline{\rho}} = \mathrm{d}x(R_\mathrm{b} - R_\mathrm{u})\overline{T} + \overline{R}\mathrm{d}\overline{T} \tag{14}$$

Inserting $\mathrm{d}\overline{T}$ from eq. (11), into eq. (12) yields,

$$\frac{\mathrm{d}p}{\overline{\rho}\,\overline{R}} - \frac{\mathrm{d}x(R_\mathrm{b} - R_\mathrm{u})\overline{T}}{\overline{R}} = \frac{\mathrm{d}x\, q\, Y_\mathrm{fu}\, \eta_\mathrm{fu}}{\overline{C}} \tag{15}$$

Finally, in order to obtain the pressure raise function, when eq. (13) is rearranged, and divided with $\mathrm{d}x$, a differential equation relating pressure and mass burnt fraction x can be obtained:

$$\frac{\mathrm{d}p}{\mathrm{d}x} = \frac{\overline{\rho}\, q\, Y_\mathrm{fu}\, \eta_\mathrm{fu}\, \overline{R}}{\overline{C}} + \overline{\rho}\,\Delta R\,\overline{T} \tag{16}$$

and eq. (1) becomes finally:

$$\frac{\mathrm{d}p}{\mathrm{d}t} = \frac{3}{R_\mathrm{v}}\left(\frac{\overline{\rho}\, q\, Y_\mathrm{fu}\eta_\mathrm{fu}\, \overline{R}}{\overline{C}} + \overline{\rho}\,\Delta R\,\overline{T}\right)\left[1 - (1-x)\left(\frac{p_\mathrm{in}}{p}\right)^{1/\kappa}\right]^{2/3}\left(\frac{p}{p_\mathrm{in}}\right)^{1/\kappa} S_\mathrm{L} \tag{17}$$

Simulation error analysis

In the following section an error analysis of the proposed model is presented. Error analysis is estimated on change in the output of the model with regards to the variation/deviation of the model input parameters about a mean within reasonable boundaries.

Pressure-raise function deviation analysis

For easier analysis eq. (1) can be written as:

$$\frac{\mathrm{d}p}{\mathrm{d}t} \propto \frac{\mathrm{d}p}{\mathrm{d}x} S_\mathrm{L} \tag{18}$$

Term $\mathrm{d}p/\mathrm{d}x$ is a pressure raise function, and has an influence on the peak pressure value, while laminar burning velocities, S_L, affect combustion time, and therefore the slope of the function. In the case of stoichiometric mixture of air and methane, gas constants of unburned, and burned mixture are approximately equal, $R_\mathrm{u} \approx R_\mathrm{b}$. Since the second term of eq. (16) on the right-hand side in the majority of cases is of lower order of magnitude than others, it could be neglected. The total differential of the eq. (16) is:

$$\mathrm{d}p' = \frac{\partial p'}{\partial \overline{\rho}}\mathrm{d}\overline{\rho} + \frac{\partial p'}{\partial q}\mathrm{d}q + \frac{\partial p'}{\partial \eta_\mathrm{fu}}\mathrm{d}\eta + \frac{\partial p'}{\partial Y_\mathrm{fu}}\mathrm{d}Y_\mathrm{fu} + \frac{\partial p'}{\partial \overline{C}}\mathrm{d}\overline{C} + \frac{\partial p'}{\partial \overline{R}}\mathrm{d}\overline{R} \tag{19}$$

where p' is due to conciseness:

$$p' = \frac{\mathrm{d}p}{\mathrm{d}x} \tag{20}$$

Because the mean fluid density and fuel share Y_fu are constants which can easily and accurately be obtained, their variance will be assumed to be zero. Variance of lower heating value of the fuel, fuel efficiency value, heat capacity, respectively, and gas constant are $\sigma_q, \sigma_\eta, \sigma_C, \sigma_R$ respectively. Applying these values into (19), one obtains:

$$\sigma_{p'} = \frac{\overline{\rho}\,\overline{Y}_\mathrm{fu}\overline{R}\eta_\mathrm{fu}}{\overline{C}}\sigma_q + \frac{\overline{\rho}\,\overline{Y}_\mathrm{fu}\overline{R}q}{\overline{C}}\sigma_\eta - \frac{\overline{\rho}\,\overline{Y}_\mathrm{fu}\eta_\mathrm{fu}\overline{R}}{\overline{C}^2}\sigma_C + \frac{\overline{\rho}\,\overline{Y}_\mathrm{fu}q\eta_\mathrm{fu}}{\overline{C}}\sigma_R \tag{21}$$

Table 1. Methane lower and higher heating value

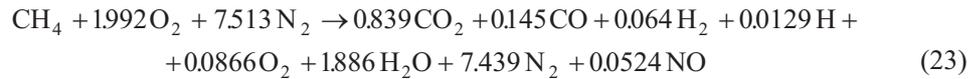|	$q_1^{[24]}$ [J]	$q_2^{[25]}$ [J]	$q_3^{[26]}$ [J]	q_m [J]	σ [%]
LHV	49853158	49812991	50014961	49893703	0.2143
HHV	55384386	56046628	55417030	55616015	0.6712

Heat value data deviation

In tab. 1, an error analysis for the fuel heating value is presented. As it is shown in the table, that value deviation does not exceed 0.21 and 0.67% in this case.

Deviation of heat capacity

In the case of the ideal stoichiometric combustion of methane at pressure of 1bar and temperature of 298 K, the equation is:

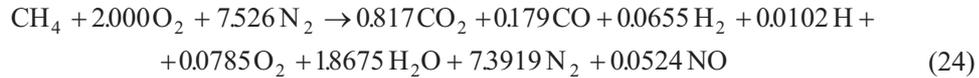$$CH_4 + 2(O_2 + 3.716N_2) \rightarrow CO_2 + 2H_2O + 7.432N_2 \qquad (22)$$
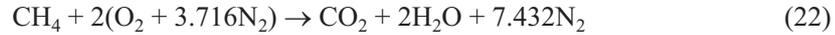
During the combustion process, there is a variety of chemical species on both reactants and products side. Combustion equation, which was obtained by PREMIX with GRIMECH 3.0 mechanism, and assumes constant pressure combustion, taking into account the most relevant species, has the following form:

$$CH_4 + 1.992O_2 + 7.513N_2 \rightarrow 0.839CO_2 + 0.145CO + 0.064H_2 + 0.0129H +$$
$$+ 0.0866O_2 + 1.886H_2O + 7.439N_2 + 0.0524NO \qquad (23)$$

with combustion temperature of 2300 K.

Similarly, by GASEQ software, for adiabatic flame and constant volume combustion, the following results are obtained:

$$CH_4 + 2.000O_2 + 7.526N_2 \rightarrow 0.817CO_2 + 0.179CO + 0.0655H_2 + 0.0102H +$$
$$+ 0.0785O_2 + 1.8675H_2O + 7.3919N_2 + 0.0524NO \qquad (24)$$

with combustion temperature of 2587 K.

All results in the paper representing constant pressure combustion were obtained with PREMIX, and all results representing constant volume combustion were obtained with GASEQ.

From tab. 2, 3, and 4 it could be concluded that ideal and real combustion products heat capacity, and gas constants do not vary much with temperature and difference in the composition. On the other hand, mean heat capacity, which is by definition:

$$C = \frac{\Delta q}{\Delta T} \qquad (25)$$

depends on released heat, and temperature differences. The amount of released energy has bigger

Table 2. GASEQ results

GASEQ V = const.	p_{end} [bar]	T [K]	η_{fu} [–]	R_u [Jkg^{-1}K^{-1}]	R_b [Jkg^{-1}K^{-1}]
	9.04	2587	0.9538	301	303.1

Table 3. Constant pressure specific heat capacity of the combustion products

	Ideal combustion		Real combustion	
	p = const.	V = const.	p = const.	V = const.
T [K]	~2300	~2600	~2300	~2600
C_{pb} [Jkg^{-1}K^{-1}]	1521	1539	1530	1532

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influence on mixture heat capacity, as it could be seen from eq. (25) and tab. 5. Heat capacity on the beginning of the combustion is equal to the fresh mixture constant pressure heat capacity, and on the end of combustion, to the burned gases constant volume heat capacity. For the simplicity of the model, heat capacity function will be assumed as a second order polynomial:

Table 4 Mean heat capacity of the mixture during the combustion

	Ideal combustion	Real combustion
Δq [J]	2744	2595
ΔT [K]	~2300	~2300
C [Jkg^{-1}K^{-1}]	1991	1131

$$\overline{C} = ax^2 + bx + c \qquad (26)$$

The conditions for determining value of constants a, b, and c are:

(1) at initial moment when $x = 0$:

$$\overline{C} = C_{pu} \qquad (27)$$

(2) at the end of combustion when $x = 1$:

$$\overline{C} = C_{vb} \qquad (28)$$

(3) and mid value during the combustion process:

$$\overline{C}_{ave} = \frac{1}{1-0}\int_0^1 \overline{C}dx = \frac{\Delta q}{\Delta T} \qquad (29)$$

The error was estimated as a truncation error of MacLaurin's series. If we take only first three terms from MacLaurin series and by knowing that x ranges from zero to one, the truncation error limits are:

Table 5. PREMIX results for constant pressure combustion of stoichiometric mixture of methane and air

PREMIX p = const.					
p [bar]	T_i [K]	T_b [K]	σ_{fin} [–]	R_u [Jkg^{-1}K^{-1}]	R_b [Jkg^{-1}K^{-1}]
1	298	2162	0.9287	302	305
2	363	2272	0.9523	301	304
3	408	2304	0.9557	301	303
5	432	2349	0.9526	301	303
10	575	2420	0.9400	301	304
Mean value	–	2301	0.9459	301.2	303.8
σ		95.7	0.0113	0.447	0.837

$$\varepsilon_C = O(x - 0)^3 \le O(1 - 0)^3 \le 10 \qquad (30)$$

For the heat capacity deviation, it was adopted a value of $\sigma_C = 10$ Jkg^{-1}K^{-1}, based on eq. (28).

Combustion efficiency deviation

As it has been emphasized in introduction, in the calculation of the pressure evolution combustion efficiency η_{fu} has a very big influence. In order to determine combustion efficiency, from the the maximum possible released energy (LHV of the fuel) the energy "trapped" in unburned combustible reactants is subtracted (hydrogen, and carbon-monoxide LHV values):

$$\eta_{fu} = \frac{m_{fu}LHV_{fu} - m_{CO}LHV_{CO} - m_{H_2}LHV_{H_2}}{m_{fu}LHV_{fu}} \qquad (31)$$

Assuming that constant volume combustion chamber can be represented as of finite number of constant pressure combustion chamber, an analysis of constant volume combustion can be performed with PREMIX. Table 5 presents results for the η coefficient obtained from PREMIX with GRIMECH 3.0 mechanism. Coefficients in tab. 5 are for pressures and temperatures of an adiabatic compression of stoichiometric mixture of methane and air. Mean value of η, and its standard deviation, together with gas constants, their mean value and standard deviation are also presented in the tab. 5.

Ignition modeling

Experimental research [9, 27, 28] confirmed that laminar flame speed is independent from ignition energy, when flame radius is greater than 5 mm. It can be calculated easily that the ratio of energy brought into the vessel by ignition (which is usually about 100 mJ [2, 6,13]), and released by combustion when flame radius reaches 5 mm, is less than 10%. Also, it was noted that until flame reaches radius of 25 mm the pressure raise is insignificant [6], and the condition in a vessel can be treated as an isobaric. Considering this, and also the fact that constant volume combustion of a stoichiometric methane-air mixture, reactants at 1 bar, and 298 K, combustion temperature is approximately 2600 K. From eq. (32), knowing the flame radius of 5 mm when flame front was formed, the value x can be calculated, and it amounts 2.62E-05. Also, from eq. (33) the temperature of unburned mixture was calculated, and it values 297.94 K:

$$r_{\mathrm{f}} = R_{\mathrm{v}} v \sqrt[3]{1 - (1 - x)\frac{p_{\mathrm{in}}}{p}\frac{T_{\mathrm{u}}}{T_{\mathrm{in}}}} \tag{32}$$

$$\frac{R_{\mathrm{u}}T_{\mathrm{in}}}{p} = x\frac{R_{\mathrm{b}}T_{\mathrm{b}}}{p} + (1 - x)\frac{R_{\mathrm{u}}T_{\mathrm{u}}}{p} \tag{33}$$

Results and discussion

Based on the assumptions introduced in the third chapter, it is possible to do an error analysis of the zonal model for the stoichiometric methane-air combustion. Section is divided into 3 parts: pressure raise function error, numerical integration error of the eq. (17), and comparisons of two zonal models with linear and modified pressure raise function, with experimental results from Dahoe *et al*. [4].
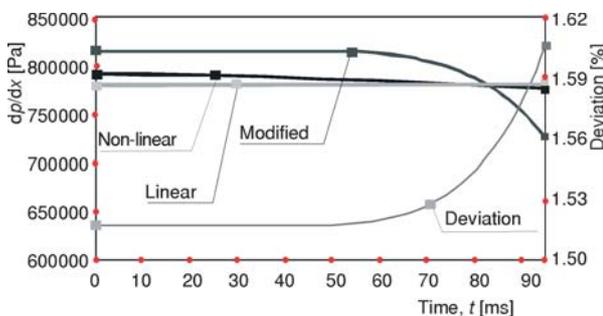

Figure 1. Comparison of dp/dx models and modified model´s standard deviation [%]

Pressure raise function deviation

By substituting required values, σ_{q}, σ_{η}, σ_{C}, σ_{R} in eq. (26), pressure raise function deviation was calculated. Heat capacity value C, is not a constant, and according to (26), it is a function of x, and hence also a function of time. fig. 1 presents a comparison of simulation results, a two-zone model with a linear pressure-raise function, and a two-zone model with

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new pressure-raise function and experiment. The deviation of the model is presented on the right axis.

Error of the numerical integration

For the simulation, laminar burning velocity S_L was adopted as:

$$\frac{S_L}{S_{L0}} = \left(\frac{T}{T_0}\right)^{\beta_1}\left(\frac{p}{p_0}\right)^{\beta_2} \tag{34}$$

where, values for S_{L0}, β_1, and β_2, were 0.4118 m/s, 1.89, and –0.45912, respectively [13]. Since numerical integration of eqs. (16) and (17) was done, it is necessary to consider the impact of the size of time step Δt on the result of simulation. For the integration Euler scheme was used, in which the magnitude of the errors arising from the method is proportional to Δt. Results of the numerical integration are presented in fig. 2 and tab. 6. Time step was varied from 0.005 to 10 ms. The ending criteria were the step, when x reaches, or overlaps the value of 1. From the results, it could be concluded, that substantial deviations occur when the time step is larger than 1 ms, which is 1.008% of the observed combustion time interval. As integration was done by Euler method for this time step, when $\Delta t =1$ ms, the numerical error of integration was of the order of magnitude of 1%. The error of integration for the time step of 1 ms was 2.680% for the peak pressure value, and 7.800% for combustion time. For the finest time step it was of 2.05 and 2.24%, for 0.005 and 0.05 ms, respectively . The results for all time steps are presented in tab. 6.

Comparison of the results

From the graphics in fig. 3, it can be seen that the peak pressure, obtained by the modified model, is slightly higher than the experimental value. Deviation, which is obtained in this way is acceptable, and is 1.6%, which is equal to the predicted one (fig. 1). The linear model, in the case of peak pressure, does not show any devia-
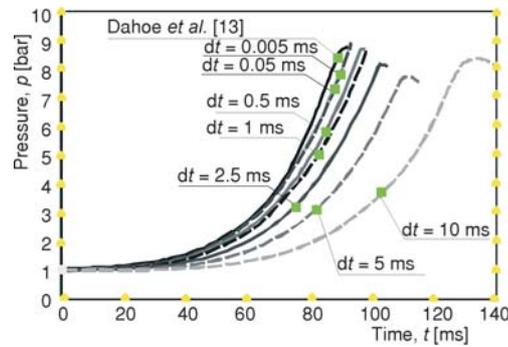

Figure 2. Results of numerical integration of the expression (1) for different magnitude of time steps from 0.005 to 10 ms [13]

Table 6. Results of numerical integration of pressure equation, depending on the time step

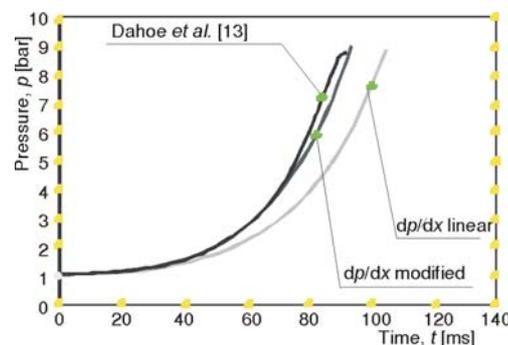| Δt [ms]	t_{comb} [ms]	$p_{max.}$ [bar]	x_{end}	$\varepsilon \propto$ [%]
0.005	94.085	8.930	1.000	0.005
0.05	94.300	8.922	1.001	0.054
0.5	97.500	8.967	1.001	0.544
1	99.000	8.535	1.006	1.088
2.5	105.000	8.096	1.001	2.721
5	115	7.585	1.014	5.4427
10	140	8.156	1.289	10.8854

Figure 3. Comparison of the experiment with modified pressure raise function model, and linear pressure raise function model [13]

Table 7. Comparison of peak pressure values and combustion time of experiment and models

	p_{end} [bar]	t_{comb} [ms]	ε_p [%]	ε_t [%]
Experiment	8.78	91.837	–	–
Linear model	8.78	105.29	–	14.64
Modified model	8.92	94.085	1.59	2.45

tion, because the peak pressure value is an input value in the eq. (2). As for the time of combustion, the value which was obtained by modified relation is higher for 13.45 ms or 14.64%. It should be noted that integration of expression (1) was done with time steps of $\Delta t = 0.005$ ms, and in the case of a modified relation was used Euler's method, and for the linear model fourth order Runge-Kutta. The main results are presented in tab. 7.

Here should be noted that the experimental results for combustion also input uncertainty. According to [13], results for stoichiometric mixture of methane and air combustion in a 20 l vessel, can vary from 8.4 to 8.78 bar.

Conclusions

This paper presents a new method for modeling the pressure raise function, dp/dx. When compared to the experiment (performed by Dahoe *et al.* [13]), the new method proposed here shows sufficiently accurate results in pressure evolution prediction, namely peak pressure, combustion rate and time till complete combustion. In comparison with the two zonal model with linear pressure raise function, combustion rate was far better predicted by the two zone model with modified pressure raise function. Based on the presented results, a modified dp/dx relation represents an effective tool in constant volume combustion calculation.

Acknowledgments

Nomenclature

$\overline{C}$ – mean specific heat capacity, [Jkg^{-1}K^{-1}]
C_{pb} – constant pressure heat capacity of burned
    – mixture, [Jkg^{-1}K^{-1}]
C_{pu} – constant pressure heat capacity of
    fresh mixture, [Jkg^{-1}K^{-1}]
C_{vb} – constant volume heat capacity of
    burned mixture, [Jkg^{-1}K^{-1}]
m – mass, [kg]
p – pressure, [Pa]
p_{end} – end pressure, [Pa]
p_{in} – initial pressure, [Pa]
Q – released heat, [J]
q – heat value of fuel, [Jkg^{-1}]
$\overline{R}$ – mean gas constant, [Jkg^{-1}K^{-1}]
R_b – burned mixture gas constant, [Jkg^{-1}K^{-1}]
R_u – fresh mixture gas constant, [Jkg^{-1}K^{-1}]

R_v – equivalent radius of an observed vessel, [m]
S_L – laminar burning velocity, [ms^{-1}]
S_{L_0} – laminar burning velocity at referent
    conditions, [ms^{-1}]
T – temperature, [K]
T_{in} – initial temperature, [K]
T_u – fresh mixture temperature, [K]
t – time, [ms]
t_{comb} – combustion time, [ms^{-1}]
x – burned mass fraction, [–]
Y_{fu} – mass share of the fuel in air – fuel mixture, [–]

Greek letters

β_1 – temperature exponent, [–]
β_2 – pressure exponent, [–]
ε_p – pressure estimation error, [Pa]

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ε_t – combustion time estimation error, [ms]

κ – adiabatic exponent, [–]

κ_b – adiabatic exponent of burned mixture, [–]

κ_u – adiabatic exponent of fresh mixture, [–]

η_{fu} – combustion efficiency, [–]

ρ – density, [kgm^{-3}]

σ – standard deviatio

σ_C – specific heat capacity deviation, [Jkg^{-1}K^{-1}]

σ_q – heat value deviation, [Jkg^{-1}]

σ_R – gas constant deviation, [Jkg^{-1}K^{-1}]

σ_η – combustion efficiency deviation, [–]

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