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Numerical study on flame propagation in n-heptane/air mixture with the use of a gradient LES combustion model

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Abstract

This paper presents the results of numerical simulations with a combustion model using Large Eddy Simulation (LES). The objective is to check whether the proposed combustion model is capable of representing the laminar reacting flow. The numerical results are compared with flame front propagation data gained from experiments. The combustion model is based on the gradient method, which determines flame propagation. The gradient is calculated from the mass fraction of fuel or products. Laminar burning velocity is described by empirical correlation. Flame generated turbulence is used in this study to represent the nonlinear flame propagation effects in the laminar reacting flow. From the results it is concluded that flame generated turbulence can be used for laminar reacting flows and is important for representation of the combustion process in numerical simulations. The gradient combustion model for turbulence reacting flow is capable of proper representation of the flame front in laminar reacting flows. The gradient combustion model for LES did not increase the time needed for calculation, making it an attractive method in full engine cycle simulations.

Keywords: Combustion, LES, Sub-grid scale (SGS), n-heptane, constant volume chamber

1. Introduction

Reynolds Averaged Navier-Stokes (RANS) methods are standard in simulations of internal combustion engines [1, 2]. In RANS methods, the local instantaneous value of a computed dependent variable represents an ensemble- or phase-average over many engine cycles at a specified spatial location and crank phasing. Two-equation ($k - \varepsilon$) closures have been used to model turbulent transport, with standard equilibrium wall functions. Shortcomings of RANS models have been documented by many researchers [3, 4]. This method allows accurate prediction of the mean characteristics of stabilized engine operation, and is therefore widely used for identifying promising engine configurations before proceeding to the test phase. These techniques are inherently unsuited to predict inconstant phenomena [5]. A better candidate for predictions of this sort is Large Eddy Simulation (LES) [6]. The governing equations are spatially filtered. Explicit account is taken of flow structures larger than the filter width, which is of the order of the mesh spacing, while the influence of unresolved scales is modeled using a subgrid-scale (SGS) model.

Since statistics of small-scale turbulence are expected to be more universal than those of large scales, LES offers the promise of wider generality and reduced modeling uncertainty. Turbulence

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model formulation and calibration traditionally have been carried out in statistically stationary and/or homogeneous flows for simple geometric configurations [7].

2. Combustion model

For adequate basic representation of the combustion process there is a need to control the energy and species source term of the continuity equation. The energy source term is represented by the product of the reaction rate and the lower heating value:

$$\overline{S_e} = \overline{S_c} \cdot H_c \tag{1}$$

where $\overline{S_c}$, kg/m^3/s, is the source term for the species transport equation (reaction rate) and H_c is the fuel lower heating value, J/kg. The source term of the species transport equation is represented by:

$$\overline{S_c} = \rho_u \cdot S_t \cdot \mid \nabla \widetilde{c} \mid \tag{2}$$

where ρ_u is density of the unburnt mixture, S_t is turbulent burning velocity determined from the sub-grid-scale, $\mid \nabla \widetilde{c} \mid$ is gradient of the fuel or products mass fraction [8]. The equation describing the turbulent burning velocity takes the form [9–11]:

$$S_t = S_u(Y_{Fuel}, T, p) \cdot (\psi \cdot \chi_{Karl_{Max}}) \cdot exp\left(\frac{u'}{S_t}\right)^2 \tag{3}$$

where S_u is laminar burning velocity calculated as a function of temperature, pressure and mass fraction of fuel, χ_{Karl} is the Karlovitz factor representing the flame generated turbulence and u' is local velocity fluctuation. In this study the value of χ_{Karl} will be changed by various ψ values.

The influence of turbulence on the combustion process is introduced by fluctuation of local velocity $u' = u'_{SGS}$. For the laminar flows $u' = 0$ so this factor can be neglected in the simulations, but it is represented by the exponential function which means that for laminar flows this part of Eq. 3 is close to 1. Knowing that, the sub-grid scale unresolved root mean square velocity is defined by:

$$u'_{SGS} = \sqrt{2/3 \cdot k_{SGS}} \tag{4}$$

with k_{SGS} as the subgrid scale unresolved kinetic energy defined by

$$k_{SGS} = \frac{v_t^2}{L_{SGS}^2} = \frac{\mu_t^2}{\rho^2 \cdot L_{SGS}^2} \tag{5}$$

it follows that:

$$u'_{SGS} = \sqrt{\frac{2}{3}} \cdot \frac{\mu_t}{\rho \cdot L_{SGS}} \tag{6}$$

Using the SGS Smagorinsky-Lilly mixing length with $C_s = 0.157$:

$$L_s = 0.157 \cdot V^{1/3} \tag{7}$$

the sub-grid-scale residual velocity can be modeled for highly turbulent flows by

$$u'_{SGS} = \sqrt{\frac{2}{3}} \frac{\mu_t}{\rho\left(0.157 \cdot V_{CV}^{1/3}\right)} \tag{8}$$

The proposed combustion model is easy to adapt to other SGS turbulence models. There is no direct connection to the mechanism of chemical reactions and the process is described by means of one chemical reaction equation only.

The influence of initial pressure and temperature on the laminar burning velocity is given by the Eq. [12–15]:

$$S_u = S_{u0} \cdot \left(\frac{T_u}{T_{u0}}\right)^{\alpha_t} \cdot \left(\frac{p_u}{p_{u0}}\right)^{\beta_p} \tag{9}$$

where S_{uo} is the maximum laminar burning velocity. The initial conditions are described by T_{u0}, p_{u0}. T_u and p_u are temperature and pressure for the calculated time step in the volume, respectively. α_t and β_p are the coefficients which depend on the fuel and equivalence ratio. The values of coefficients are presented in Table 1.

Maximum laminar burning velocity is a function of the equivalence ratio. The correlation for n-heptane/air mixtures was derived by the authors with the use of the experimental results of Chong et al. [16]. The initial conditions in the experiments were 400 K and 0.1 MPa. Any other fuel can be simply introduced into the code by changing the equation for S_{u0}.

Table 1: Values of the α_t and β_p coefficient used for the calculations

α		β	
		$\Phi \leq 1$	$\Phi \geq 1$
C_7H_{16}	$1.783 - 0.375 \cdot (\Phi - 1)$	$\frac{-0.17}{\sqrt{\Phi}}$	$-0.17 \cdot \sqrt{\Phi}$

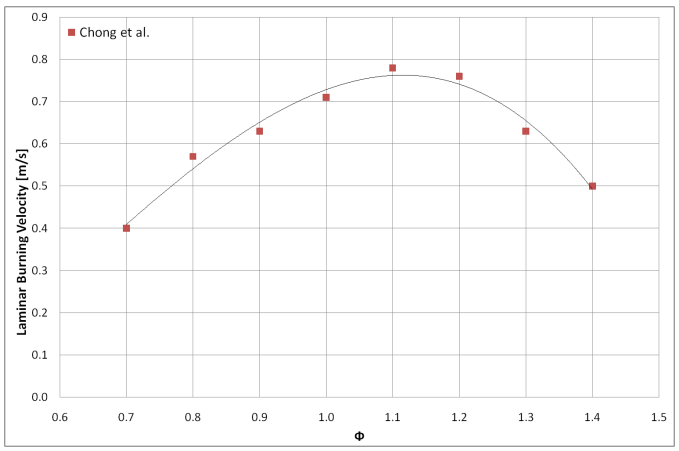

Figure 1: Maximum laminar burning velocity as a function of Φ for n-heptane/air mixture

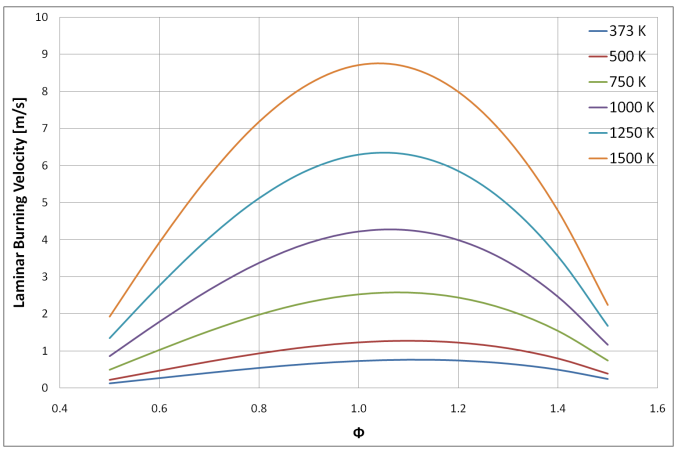

Figure 2: Influence of temperature increase on laminar burning velocity as a function of Φ for n-heptane/air mixture

$$S_{uo} = -1.8182\phi^3 + 3.2749\phi^2 - 0.5216\phi - 0.2068 \tag{10}$$

Experimental results and the Eq. 10 are presented in Fig. 1.

Figures 2 and 3 present the influence of temperature and pressure on laminar burning velocity. During the studies in constant volume bomb the influence of the temperature and equivalence ratio on the calculated laminar burning velocity S_u is higher than the pressure effect. Eq. 9. describes the laminar burning velocity with no influence of the nonlinear flame propagation effects. If these effects are not included in Eq. 3 the flame propagation would probably not correctly represent the experimental results. This issue was checked during the study. Eq. 3 for the case without nonlinear flame propagation effects takes the form:

$$S_t = S_u(Y_{Fuel}, T, p) \cdot exp\left(\frac{u'}{S_t}\right)^2 \tag{11}$$

As shown in Eq. 3 the representation of the nonlinear flame propagation effects is controlled by the use of empirical coefficient ψ and maximum Karlovitz factor $\chi_{Karl_{Max}}$. The nonlinear effects for the laminar reacting flows will be represented by the flame generated turbulence theory for turbulence reaction flows. Expansion coefficient E is used to calculate the maximum turbulence generated by the flame front itself. The maximum Karlovitz factor is defined by [17]:

$$\chi_{Karl_{Max}} = \frac{E-1}{\sqrt{3}} \tag{12}$$

The expansion coefficient represents the ratio of the unburned mixture density to the burned mixture density:

$$E = \frac{\rho_u}{\rho_b} \tag{13}$$

Additionally, empirical coefficient ψ is the only one which can be used to adjust the simulation results to the experimental ones. The values of ψ ranged from 0 to 1. The value of expansion coefficient E is calculated with the use of the GASEQ code for the reaction of fuel with one mole of air under constant pressure conditions. In Eq. 3 the laminar burning velocity is multiplied by the Karlovitz factor and the value $\psi = 0$ means no reaction. Figure 5 shows the influence of ψ on Karlovitz factor χ_{Karl}. For values of ψ lower than 0.5 the flame generated turbulence slows down the combustion process. Figure 4

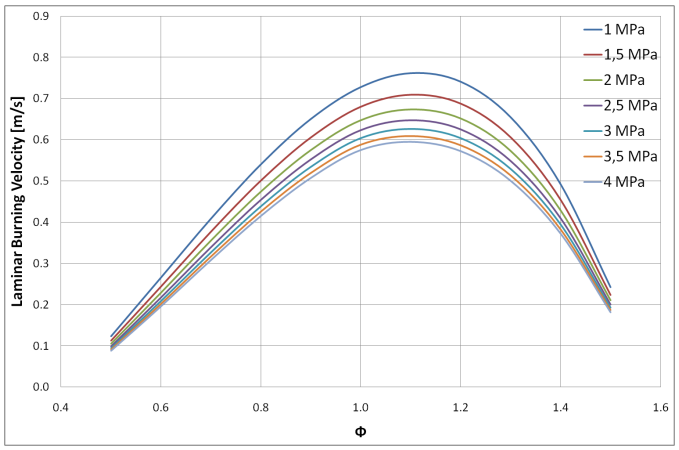

Figure 3: Influence of pressure increase on laminar burning velocity as a function of Φ for n-heptane/air mixture

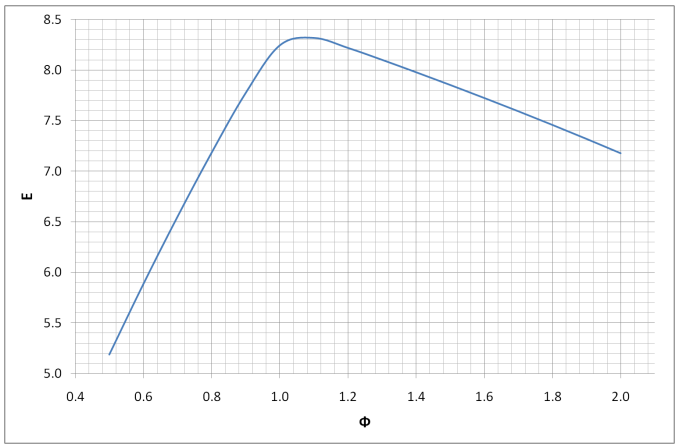

Figure 4: Expansion coefficient for n-heptane/air mixture as a function of Φ

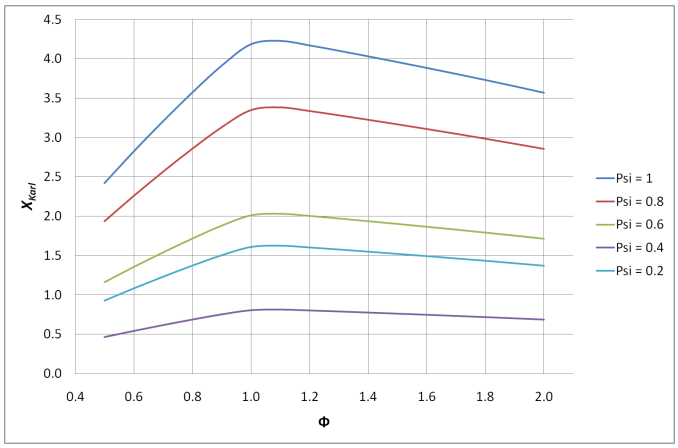

Figure 5: Influence of ψ coefficient on the Karlovitz factor for n-heptane/air mixture as a function of Φ

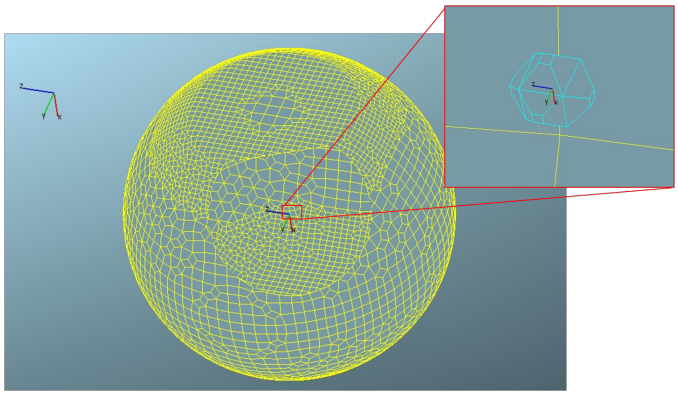

Figure 6: Discrete model of mesh with close up of ignition center

presents the expansion coefficient. For the simulations, E is taken for the stoichiometric mixture.

3. Comparison of results

The experimental results were taken from Jarzembeck et al. [18, 19] research for n-heptane/air combustion in a constant volume chamber. Initial conditions were T = 373 K, p = 1 and 2.5 MPa, equivalence ratio Φ = 0.8, 1.0 and 1.2. Ignition took place in the center of the chamber and was 0.3 ms long. Experimental results represent the laminar flame propagation. As was described earlier, the combustion model is dedicated for turbulent reacting flows. The nonlinear flame propagation effects of the laminar flow have no special representation in the combustion model. Whether the flame generated turbulence term included in the code is able to properly simulate the nonlinear laminar effects phenomenon will be checked during the simulation.

The numerical flame front position was taken from the 3D results of the simulation for the gradient of temperature. The sphere combustion chamber for the simulation had a similar design to the experimental one, with a diameter of 100 mm. 50 mm diameter "view windows" are included in the mesh. The discrete form of the model is presented in Fig. 6.

The turbulence is simulated with the use of LES, which provides a more precise representation of the velocity fluctuation. The combustion process is represented by the gradient model prepared by the authors and adjusted for the use of n-heptane fuel. Experimental results were obtained for ψ = 1, 0.5 (Eq. 3), no flame generated turbulence effect (Eq. 11). Experimental and numerical flame front

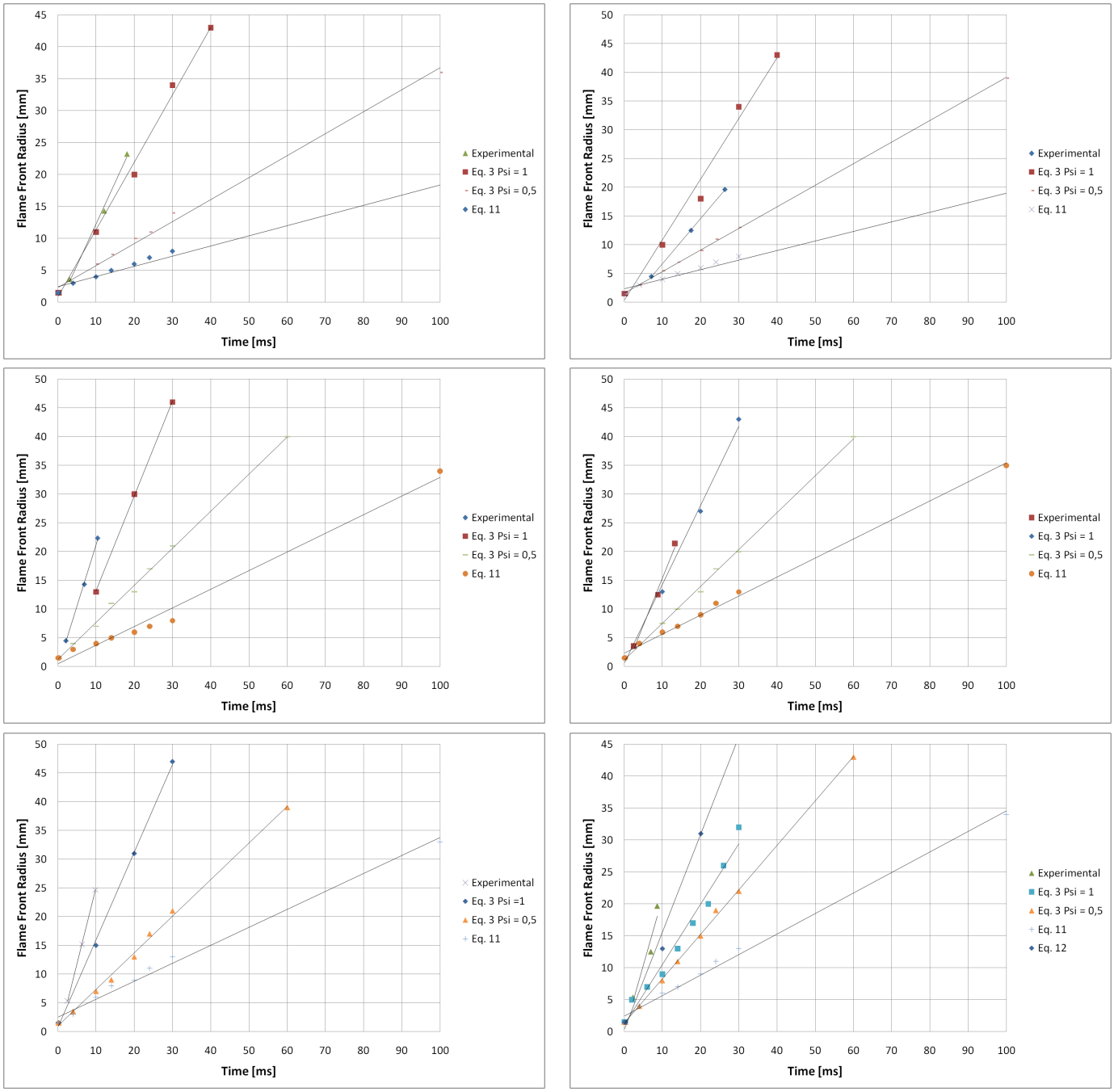

Figure 7: Flame front propagation experimental and simulation results for n-heptane/air mixture

Table 2: Calculated expansion coefficient for n-heptane/air mixture as a function of Φ

Φ	Number of fuel moles	Unburnt mixture density	Burned mixture density	E
0.5	0.010	11.99	2.31	5.19
0.6	0.011	12.05	2.05	5.89
0.7	0.013	12.10	1.85	6.55
0.8	0.153	12.16	1.69	7.18
0.9	0.017	12.21	1.57	7.77
1	0.019	12.26	1.49	8.24
1.1	0.021	12.32	1.48	8.32
1.2	0.023	12.37	1.50	8.22
1.3	0.025	12.42	1.53	8.10
1.4	0.027	12.47	1.56	7.98
1.5	0.029	12.53	1.60	7.85
1.6	0.031	12.58	1.63	7.72
1.7	0.032	12.63	1.66	7.59
1.8	0.034	12.68	1.70	7.46
1.9	0.036	12.73	1.74	7.32
2	0.038	12.79	1.78	7.18

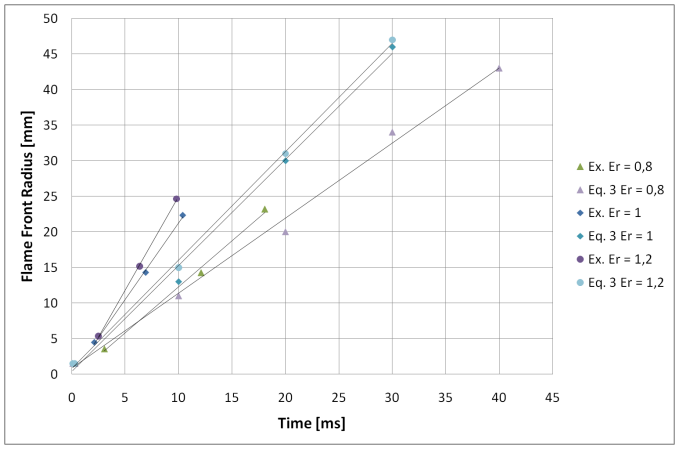

Figure 8: Flame front propagation experimental and simulation results for n-heptane/air mixture. Initial temperature 373 K, pressure 1 MPa. $\psi = 1$

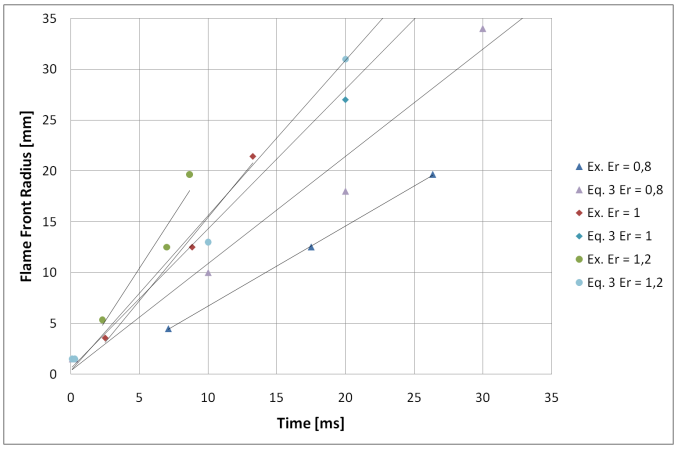

Figure 9: Flame front propagation experimental and simulation results for n-heptane/air mixture. Initial temperature 373 K, pressure 2.5 MPa. $\psi = 1$

propagation results are presented in Fig. 7.

Good agreement with the experimental results was found for Eq. 3 $\Psi = 1$ for all calculation cases. This means that nonlinear flame propagation effects are an important part of the burning velocity calculation for the mixture and cannot be neglected. In Figures 8 and 9 the experimental and Eq. 3 $\Psi = 1$ results are presented. The results are correct for every case. Differences in velocity as a function of the equivalence ratio give correct values, faster reactions for rich mixtures, slower for lean mixtures.

4. Conclusion

Results obtained from the presented simulations are satisfactory for the proposed combustion model based on the gradient method. It was found that the nonlinear propagation effects cannot be neglected in the simulations. The representation of these effects by flame generated turbulence is satisfactory when

compared with the experimental results. It is clearly shown that the best results are obtained for Eq. 3 $\psi = 1$ which means that the combustion model can also represent the laminar reacting flows because the fluctuation in velocity is included in the exponential function. The presented gradient combustion model is capable of representing the laminar reacting flows.

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Nomenclature

α_t	Empirical coefficient
β_p	Empirical coefficient
χ_{Karl}	Karlovitz factor
$\mid \nabla\tilde{c} \mid$	Gradient of the fuel or products mass fraction
Φ	Equivalence ratio
ψ	Empirical coefficient
ρ	Density
H_C	Fuel lower heating value
k_{SGS}	Sub-grid scale unresolved kinetic energy

L Length scale

p Pressure

S_C Source term of the species transport equation

S_E Source term of the energy equation

S_t Turbulent burning velocity

S_u Laminar burning velocity

T Temperature

u' Local velocity fluctuation

u'_{SGS} Sub-grid scale residual velocity

V Volume

v Molecular viscosity

Y Mass fraction of the species

0 Initial conditions

b Burned mixture

max Maximum

sgs Sub-grid scale

t Turbulent

u Unburned mixture