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The quantitative description of the conversion of fuel and oxidizer in the combustion of a methane-air mixture.

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Abstract

The results of the combustion process simulation of methane-air mixtures for different compositions of flammable mixture were analysed. The calculations were obtained by using Chemkin-Pro Release 15101. The equations describing conversion of fuel and oxidizer from the data of the simulation for the limited range of the initial mixture composition have been developed.

Introduction

The combustion of methane in air is a complicated process. The transformation of fuel into products proceeds with the participation of a lot of intermediate connections and elementary reactions [1]. Therefore, there are known only a few works relating to the investigation of the macro-kinetic description of the combustion process [2-6]. One of them is PhD thesis of Renata Kedzior [5], in which the effort to obtain the process description for the kinetic combustion of hydrocarbons in air for surroundings of flammability limits was taken. The obtained equation, with the typical form for a chemical kinetic expression (power function), indicates an autocatalytic character in the combustion process. This work has attempted to verify this premise in application and to describe the combustion process of methane-air mixtures in surroundings of a stoichiometric point.

Approach

The simulation of the methane in air combustion was realised in Chemkin-Pro Release 15101 [7]. The initial conditions of the process have been assumed arbitrary: 298K, 1atm. In the chosen model, a one-direction flow of reacting mixture has been considered. Warnatz's mechanism has been used in the simulation with 84 elementary reactions, which proceeds with the participation of 34 connections [8]. The process is simulated by assuming that there are convection and diffusion (thermal diffusion). The results of a simulation are, e.g. reactant mole fractions, rates of their formation and consumption, temperature, axial velocity and unburned fuel fraction. Based on the obtained results, equations describing a time-dependence conversion of fuel and oxidizer have been developed.

Results and discussion

The following differential equations have been developed as a power function of fuel (α) and oxidizer (β) conversion:

$$\frac{d\alpha}{dt} = A\beta^a(1-\alpha)^b(1-\beta)^c \quad (1)$$

$$\frac{d\beta}{dt} = B\alpha^p(1-\alpha)^q(1-\beta)^r \quad (2)$$

The obtained equations give very good accuracy in respect to simulation results. The proportionality coefficient and exponents of the power function are different for each developed equation and depend on the initial concentration of methane in the air.

Table 1 shows example values of the proportionality coefficient A and B (unit of inverse time) for a few compositions of flammable mixture. Presented values of power function coefficients should be regarded as a sample, as these values were not obtained through an optimisation procedure. In Table 1, the designations mean, respectively: Φ – equivalence ratio, α – conversion of fuel, β – conversion of oxidizer, R^2 – coefficient of determination for the obtained equation.

Table 1. Parameters of the equations (1) – (2) for 8 different compositions of methane-air mixture at initial temperature $T_i = 298K$ and pressure $P_i = 1atm$.

No	Composi tion	Fuel					Oxidizer				
		% vol.	A	a	b	c	R^2	B	p	q	r
1	11.0	24 530	1.16	1.83	-2.91	0.995	10 880	1.33	0.81	-1.47	0.996
2	10.1	29 150	1.18	1.50	-2.43	0.996	11 720	1.34	0.62	-1.15	0.997
3	9.5	30.760	1.23	1.31	-2.02	0.997	11 610	1.41	0.47	-0.73	0.998
4	9.26	31 560	1.26	1.17	-1.70	0.999	19 770	1.42	0.49	-0.8	0.998
5	8.78	26 290	1.25	1.29	-2.14	0.998	8 737	1.42	0.48	-0.85	0.998
8	4.81	104	0.99	0.49	-2.27	0.995	6.15	1.71	0.43	-2.04	0.998

The variability of equation parameters (1) and (2) with respect to the change of composition mixture shows difficulties associated with obtaining a correct equation for a wide range of compositions. Therefore, the range of composition mixtures has been limited to a relatively tight range but those (significantly) important for methane combustion. The selected range of compositions includes concentrations of fuel between 9.14% and 9.38% vol. methane in air. In this range, the equivalence ratio Φ includes values from 0.986 to 0.958, and the excess of oxidizer ratio from 6.85% to 20.9%.

Based on the results in Table 1, the following set of exponents for equations (1) and (2) has been obtained:

$$a = 1.25; b = 1.2; c = -1.8 \quad \text{equation (1)} \quad (3a)$$

$$p = 1.4; q = 0.5; r = -0.85 \quad \text{equation (2)} \quad (3b)$$

The proportionality coefficients have been determined for each composition individually.

Figure 1 shows the differences between the values of fuel conversion (α) calculated by the simulation and the approximate by equation (1) with constant exponents (3a) in the considered range of compositions.

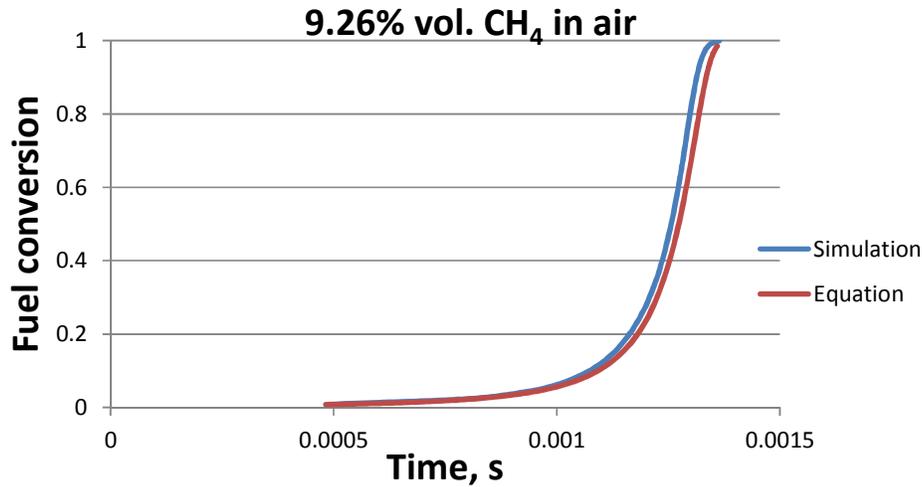


Figure 1. Comparison fuel conversion calculated by simulation and approximate equation ($A = 26500$) for initial concentration 9.26% vol. CH_4 in air. The initial value: time $4.825 \cdot 10^4$ s, fuel conversion 0,8%.

The results presented in Figure 1 indicate a possibility of acquiring an approximate description of fuel conversion. Similar results have been received for the oxidizer.

The power function form of the analysed equations is typical in chemical kinetic examples. The proportionality coefficients of developed equations are constant for the specified composition of the mixture. In the range of the equivalence ratio between 0.916 and 1.031, a dependence on those coefficients with respect to the equivalence ratio has been developed. The forms of those equations have been presented below:

$$A = (-3.547 + 6.378) \cdot 10^4 \Phi \quad (4a)$$

$$B = (-1.728 + 2.828) \cdot 10^4 \Phi \quad (4b)$$

Conclusions

The dependencies related to fuel and oxidizer conversion with time can be developed for each initial composition of methane-air mixture.

The right sites of the power function equations include the expressions dependent on a current fuel and oxidizer concentration (like a typical kinetic equation), but they also have an

expression which depends on an already transformed (reacted) fuel or oxidizer. This indicates an autocatalytic character of the combustion process. The results relating to lean mixtures, typical for a combustion process in the energy industry (the excess of oxidizer ratio about 20%), have been presented as an example.

In the equations, exponents are independent in respect to a composition (in a tight range) and the proportional coefficients are related to a composition through a linear function.

The developed equations correctly show fuel and oxidizer conversion obtained during simulation in a considered physicochemical model.

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