The single-zone numerical model of homogeneous charge compression ignition engine performance

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Abstract. The single-zone model of methane-air mixture combustion in the Homogeneous Charge Compression Ignition engine was developed. First modeling efforts resulted in the selection of the detailed kinetic reaction mechanism, most appropriate for the conditions of the HCCI process. Then, the model was completed so as to simulate the performance of the four-stroke engine and was coupled by physically reasonable adjusting functions. Validation of calculations against experimental data showed acceptable agreement.

1. Introduction
Homogeneous Charge Compression Ignition (HCCI) is currently under widespread investigation. To limit the speed of combustion, lean mixtures are used. If the mixture is too rich, the pressure rises too rapid and generates knock-related problems. On the other side, lean equivalence ratios of the fuel/air mixture inducted into the cylinder provide low nitric oxides (NOx) and particulate emissions, low fuel consumption. The HCCI process seems promising when running the engine using gas as fuel, especially using natural gas.

However, several problems with the HCCI combustion concept reappear throughout the majority of investigations – two combustion control aspects. First, the ignition event and the ignition timing are not controlled. Second, the rate of heat release is not controlled too. It occurs due to insufficient understanding of HCCI technology. In conjunction with extensive experimental researches, computational models provide a good basis for exploring the HCCI combustion phenomena. Yet a direct numerical simulation of fluid mechanics combined with the detailed chemical kinetic model is computationally complex. The typical method of the solution of the problem is simplification either in fluid mechanics or in the chemistry part of the model. An example of the latter approach is the single-zone model, developed in Volgograd State Technical University. The simulation of chemical kinetics is based on the law of mass action and the Arrhenius rate expression. This approach enables one to explore numerically the influence of the inlet air-fuel ratio, the initial mixture temperature and the in-cylinder pressure on the ignition timing that is directly dependent on the pre-flame chemical reactions.

In this paper, we present the investigation arranged as follows. The first section is the development of the first stage of the ignition event model – self ignition in the constant volume adiabatic reactor. The results obtained made it possible to choose the most acceptable kinetic reaction mechanism of methane burning. The second section is the development of the one-zone numerical model of the HCCI running process incorporating the kinetic model mentioned above. The third – the analyses of the preliminary results of the study, related to the validation of the model predictions against...
measurements, enabled us to propose a physically determined method to define heat release and, thus, the basic constants of the model more accurately.

2. Modelling description

2.1. Selection of the kinetic reaction mechanism
At the first step of the study, the computational model of ignition and combustion in the constant volume adiabatic reactor [1] is developed. Thus, we excluded the influence of such factors as variable volume and wall heat transfer. The model represents the set of equations including the law of mass action and the Arrhenius rate expression to define the rates of three types of reactions:

\[ \frac{dc_i}{d\tau} = \sum_j W_{ij}, \]  
\[ W_{ij} = \pm k_{ij} c_{\alpha}, \]  
\[ W_{ij} = \pm k_{ij} c_{\alpha} c_{\beta}, \]  
\[ W_{ij} = \pm k_{ij} c_{\alpha} c_{\beta} c_{M}, \]  

where \( W \) denotes the reaction rate of chemical specie \( i \) in reaction \( j \); \( \alpha, \beta \) stands for \( i \) values of species involved in mono-, bi- and three molecular reactions; \( \tau \) – the time; \( c_i \) – the molar concentration of the specie; \( c_M \) – the molar concentration of active centers; \( k_j \) – the reaction rate constant of the \( j \)-th reaction. Equation (2) is used for calculating the rates of monomolecular reactions; equation (3) – for bimolecular reactions; and equation (4) – for three molecular reactions.

2.2. The model of HCCI performance
The next step was the study of heat release evolution in the variable volume reactor using the developed model of the kinetic reaction mechanism. The model also includes the set of equations: the energy conservation balance and the ideal gas equation:

\[ \frac{dQ}{d\varphi} + \frac{\alpha_w (T_w - T)}{\pi n} \frac{A}{p} \frac{dV}{d\varphi} + c_m c \frac{dT}{d\varphi}, \]
\[ pV = mRT, \]

where \( p, V, T \) denote the in-cylinder pressure, the volume and the temperature in the combustion chamber; \( \varphi \) – the crank angle; \( m, R \) – are respectively the mass and the individual gas constant of the air-methane mixture; \( c_v \) – the specific heat capacity of the mixture at constant volume; \( Q \) – heat release during the combustion process (calculated by the model depicted above); \( \alpha_w \) – the heat transfer coefficient; \( T_w \) – the cylinder wall mean temperature; \( A \) – the heat transfer area of the combustion chamber.

To date, the calculation of heat transfer coefficient \( \alpha_w \) is based on Woschni’s formula [2]. However, taking into account the results of investigations presented in [3], Woschni’s formula was modified to enhance the accuracy of heat loss prediction for the HCCI engine operation:

\[ \alpha_w = 819.5 \cdot \frac{p^{0.8} \cdot w^{0.8}}{T^{0.73} \cdot D^{0.2}}, \]  
\[ w = 2.28 \cdot c_m, \]  
\[ w = 2.28 \cdot c_m + 3.24 \cdot 10^3 \cdot \frac{V_s \cdot T_1}{6 \cdot p_1 \cdot V_i} \cdot (p - p_0), \]

where \( p \) – the in-cylinder pressure; \( w \) – the mean bulk speed; \( D \) – the engine bore; \( T \) – the mean in-cylinder gas temperature; \( c_m \) – the mean piston speed; \( p_1, T_1, V_i \) – the pressure, the temperature and the
volume in the compression beginning, respectively; \( V_s \) – the displaced volume; \( p_0 \) – the in-cylinder pressure under motoring conditions. Two formulas are used for calculating: (7) for a compression process, (8) for combustion and expansion.

3. Results and discussion

3.1. A kinetic mechanism

In our opinion, the combustion process in HCCI engines can be presented as three sequential stages: the stage of pre-flame reactions, the stage of active burning and the post-burning stage. For overcoming the combustion control problems mentioned above, the main attention should be paid to studying of the first stage.

By means of the model, the evolution of ignition and burning processes of the air-methane homogeneous mixture in the constant volume adiabatic reactor was explored. The aim of the study was to determine the choice of a kinetic reaction mechanism that shows best agreement of calculated pre-flame stage duration with corresponding experimental data. The necessity of these investigations is based on the fact that the majority of chemical kinetics models observed do not take into account the peculiarities of the HCCI process.

The experimental data that serve as the baseline to compare the simulation results are generalized in reference [4]. The validation criterion of the model predictions against experiments is pre-flame stage timing \( \tau_I \). Goldsborough [5] has shown that this stage is over when the magnitude of current pressure exceeds the initial by one more than 5%.

In figure 1, the effect of the initial mixture temperature on duration of the pre-flame reactions stage is shown, which was obtained from the experimental data [6] (lines 1–5) and from calculations with two versions of the kinetic reaction mechanism: one — by V. Ya. Basevich [6] (line 6) and the other is developed in San Diego University [7] (line 7). The latter chemical kinetics model is often used to simulate the combustion processes in the flame front of the air-methane mixture. Both experimental and computed data are taken for a stoichiometric mixture (\( \alpha = 1.0 \)) at initial pressure \( p_0 = 15 \) bar. Initial mixture temperature \( T_0 \) varied from 800 to 2000 K, corresponding to the conditions in the combustion chamber when the piston reaches TDC. Line 1 reveals the experimental data obtained by D. W. Walker et al [8] for air-methane mixture self ignition while the initial temperature varied from 800 K to 2000 K. Line 2 corresponds to the experimental data of self ignition delay of mixtures of pure methane, oxygen and argon for the initial temperature of 1250 K to 2500 K obtained by K. S. Krishman et al [9]. Lines 3 and 4 show the experimental data for self ignition delay of the oxygen-methane mixture including ballast gases (\( N_2 \), Ar or \( He_2 \)) obtained by E. L. Petersen et al [10]. In the experiments mentioned, shock pipes were used.

![Figure 1. Comparison of calculations results with experimental data.](image-url)
Obviously, values of pre-flame timing obtained by the Basevich kinetics mechanism show good agreement with measurements for the observed initial temperature range, while those by San Diego University diverge dramatically at temperatures less than 1700 K. Hence, the kinetics mechanism developed by Basevich was used in further calculations.

3.2. Simulation of HCCI performance

Numerical simulation of compression and combustion events of the HCCI-engine ‘Volvo TD100’ [11] was performed. The experimental data involved in the model were as follows. The engine was run at the speed of $n = 1000$ rpm using the air-methane mixture at fuel-air ratio $\alpha = 3.12$. The initial temperature and pressure at IVC were obtained by extrapolation of those from [11] at 60 CAD BTDC. The results of calculations and experimental data are presented in figure 2.

As can be seen from figure 2, the model simulates the indicator process only qualitatively. Similar divergence of experimental data and calculations occur in some other researches [12, 13]. Experimentally observed burning rates of lean air-fuel mixtures are significantly lower than the calculated ones. Moreover, as the experimental data show, this divergence follows the increase of burnt gas fraction in the reacting mixture.

![Figure 2. Experimental (line 1) and calculated (line 2) pressure profiles.](image)

In our opinion, the reason of the mentioned divergence is the specifics of HCCI performance that is burning of extra lean fuel/air mixtures. We can point out two main factors that have influence on the burning rate. The first – comparison of calculated and experimentally observed pre-flame reactions timing leads to the conclusion that this divergence follows the increase of $\alpha$. The latter shows that the surplus air in the air-fuel mixture reduces the rate of burning reactions at the first and second burning stages. The second factor that decreases burning rates is the increase of the burnt gas fraction in the reacting mixture during active burning and post burning stages. In the next section, the modification of the model taking into account phenomena mentioned is presented.

3.3. Model modification

It is known [14] that duration $\tau_t$ of the pre-flame reactions stage when the self ignition of the air-fuel mixture occurs depends exponentially on the reciprocal value of temperature $T$ and activation energy $E_a$ of burning reaction:
\[ \tau_f \sim \exp \left( -\frac{E_a}{R_u \cdot T} \right), \]  

where \( R_u \) is the universal gas constant.

So the impact of the air-fuel ratio on the pre-flame stage timing can be taken into account by varying the activation energy magnitude by including adjusting function \( k_\alpha \) in the argument of the exponential function. We suppose that the adjusting procedure of the activation energy should be implemented for all calculations of pre-flame and subsequent burning reactions, that is for all elementary reactions of the kinetic scheme. As the magnitude of the pre-flame reactions rate depends almost linearly on the air-fuel ratio and \( k_\alpha \) is a multiplier to the argument of the exponential function, its correlation with the air-fuel ratio is assumed to be logarithmic:

\[ k_\alpha = a_i \cdot \ln(\alpha) + 1. \]  

It provides, in particular, \( k_\alpha = 1 \) for \( \alpha = 1 \). Using the experimental data mentioned above, the magnitude of \( a_i = 0.1341 \) is calculated.

The slowdown of fuel burning as a sequence of the increase of the burnt gas concentration is also considered by the adjusting function. Function \( k_C \) simulating the burnt gas fraction impact is involved in the Arrhenius rate expression as an additional pre-exponential multiplier. The relationship between \( k_C \) and the instantaneous burning products fraction in the reacting mixture is represented as a power function:

\[ k_C = 1 - \left( \frac{C_b}{C_{b_{end}}} \right)^x, \]  

where \( C_b, C_{b_{end}} \) denote the instantaneous and final burning products fraction both calculated for the instantaneous state; \( x \) – the exponent. The analysis of the experimental data determined the value of exponent \( x \) as 0.16.

\[ \alpha = 2.43 \quad \alpha = 2.61 \quad \alpha = 2.87 \]

**Figure 3.** Comparison of experimental and computed (using the modified Arrhenius equation) pressure profiles obtained for the Volvo TD100 engine.  

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– Experimental  

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– Computed.
Thus, taking into account both adjusting functions, the rate constant for each chemical reaction incorporated in the kinetics mechanism is computed by the modified Arrhenius equation:

\[
k = k_C \cdot A \cdot T^n \cdot \exp \left( \frac{-E_a}{R_m \cdot T} \right).
\] (12)

In figure 3, the experimental pressure profiles obtained on the Volvo TD100 engine [11], and the results of calculations with the modified Arrhenius equation are presented as an example. Both experimental and computed profiles are obtained for 1400 rpm and three air-fuel ratios \( \alpha \) (2.43; 2.61; 2.87). As shown in the figure, the calculated profiles are in good agreement with experimental ones.

4. Conclusion

By means of the developed mathematical model numerical researches were performed which enabled the choice of the kinetic reaction mechanism of methane-air mixture burning, which is most appropriate for the conditions of the HCCI process. Being completed to simulate the performance of the four-stroke engine, the model must be coupled with physically reasonable adjusting functions to obtain acceptable quantitative agreement of calculations with experimental data.

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