THE ANN APPROXIMATION OF THE CH_4 COMBUSTION MODEL: THE HEAT RELEASE

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Abstract

The calculation of the heat release from the combustion process of the CH_4 is presented of the paper. Correct calculation results of the heat released from combustion is important for design, modelling and testing phenomena in combustion chambers of internal combustion engines. The paper presents results of calculations for the kinetic mechanism of methane combustion GriMech 3 for different thermodynamic parameters and composition of the combusted mixture. The calculations were performed for all possible configurations of the variable temperature range from 1100K to 3600K, the variable pressure in the range of 2MPa to 5MPa, variable humidity of charged air from 10 to 30 grams of water per 1 kg of air and variable mole fractions of charge air. Results of the kinetic calculation of combustion process are qualitatively consistent with the data available in literature. The next stage of research was approximation of obtained results with the trained artificial neural network. Input data needed to approximate the energy of the combustion process consisted of 52 mole fractions of chemical species and temperature and pressure process. Approximation results have meant square error not exceeded 0.04% for the test data and 0.02% for the validation data. The maximum error for a single result was 1.9% compared to data obtained with chemical kinetic calculations.

Keywords: *modelling, internal combustion engines, approximation, artificial neural network, combustion process, heat release*

1. Introduction

The most widely used source of energy in transportation is the combustion process of hydrocarbon fuels in different types of internal combustion engines [3]. Energy machines, using this process, despite the continuous improvement are still imperfect and not very efficient, emitting into the atmosphere large quantities of toxic fluids [5]. For this reason, the intensive research on improving the efficiency of combustion and conversion energy processes carried out. Mathematical models are commonly used to designing and testing the processes of combustion of hydrocarbon fuels [16]. Most popular are models based on finite element method. This kind of method required of dividing the combustion chamber or combustion phenomenon for smaller elements, in which the phenomenon of mixing and combustion of fuel and the exchange of mass and energy with the environment are subject to mathematical description [18]. However, this kind of methods requires large computational power due to the complexity of phenomena occurring in the combustion chambers. Example is operating of the diesel engine [6]. During the process of compressing air in the cylinder with a piston the liquid hydrocarbon fuel is injected into the combustion chamber. During this process, the following phenomena occur simultaneously: atomizing fuel, its evaporation, turbulent mixing with air, self-ignition and combustion of the mixture with chemical reactions of oxidation. The rate of chemical transformations and their progress largely depends on local concentrations of chemical species involved in the combustion process and the local thermodynamic conditions [2]. According to the movement of the piston, the supply of fuel and the course of the various phenomena of the combustion process take place in a dynamic and heterogeneous in different areas of the combustion chamber. For this reason, the

accuracy of the combustion process model depends on the quantity and size of used finite elements and the accuracy of the description of phenomena occurring in the individual element. However, constantly increasing computational power of computers is still too small for a comprehensive modelling of combustion with using of the direct numerical simulation methods (DNS) [13]. Therefore, mathematical models used are largely simplified, depending on the purpose of modelling [17]. In the case of models aimed at increasing the efficiency of the combustion processes commonly used are limitations of the mathematical description of the kinetic combustion process. Such a description is often introduced to a few chemical reactions in each finite element. For modelling the combustion process which purpose is reduce emissions of harmful substances in exhaust gases, the reduction of the number of finite elements or phenomena of the heat transfer, mixing of fuel used, etc is often used. The simplification, however, is a compromise between quality and cost of the modelling.

The result of the kinetic modelling of the combustion process is a continuous function of the heat release from the combustion of fuel, depended on mole fractions of combustible mixture chemical species, temperature, pressure and time of the combustion. Values of such functions in modelling of the combustion process should be carried out to determine energy balances of individual finite elements [8]. The resulting heat release function can be used to modelling instantaneous energy states of individual finite elements in various types of engine combustion chambers. In order to reduce the required computational power, without significant reducing the accuracy of modelling possible is approximation of the heat release function. Useful approximation tool is an artificial neural network (ANN) [11].

The paper presents an example of approximation of heat release functions from the combustion process with using the ANN. The result of the research is built and trained the ANN, permitting the appointment of the heat release based on the kinetic model of the combustion process using as input data temperature, pressure and composition of the combustion mixture.

2. Chemical kinetic calculations

The data used for training and testing of ANN's is obtained from calculations using the kinetic model of the GriMech 3 mechanism of the combustion process [1]. This model is an optimized detailed chemical reaction mechanism capable of natural gas flames and ignition. This model was chosen for reasons of its simplicity and review more than 140 publications [7]. It was assumed that obtaining satisfactory results of using the ANN to approximation results from GriMech 3 mechanism will apply in the future, more complex models of hydrocarbon fuels combustion.

Model GriMech 3 includes a description of chemical reactions between 52 chemical species, its thermodynamic data and necessary coefficients for determining the quickness of reactions.

Based on Hess's law it's possible to designate the total energy, derived from the chemical reaction mechanism. Assuming isothermal-isobaric combustion for reaction we can write:

$$\Delta Q_i = \sum_{k=1}^{K} \nu''_{ki} \left[H_k^T - H_k^0 + \Delta H_{fk} \right]'' - \sum_{k=1}^{K} \nu'_{ki} \left[H_k^T - H_k^0 + \Delta H_{fk} \right], \tag{1}$$

where:
ΔQ_i - the combustion energy from the i-th reaction,
T - temperature,
ν'_{ki} - the stoichiometric coefficient of k-th reactant species in the i-th reaction,
ν''_{ki} - the stoichiometric coefficients of k-th product species in the i-th reaction,
H_k^T - the molar enthalpy of the k-th species at temperature T,
H_k^0 - the standard state molar enthalpy of the k-th species,
ΔH_{fk} - the enthalpy of formation k-th species.
for all reactions in GriMech 3 chemical kinetic mechanism:

$$Q = \sum_{i=1}^{I} \Delta Q_i \,. \tag{2}$$

To determine the heat release is necessary to set quantities of each chemical species. For this purpose, the constant rate of i-th reaction was calculated with using Arrhenius equation:

$$k_i^{'} = A \cdot T^{\beta} \cdot \exp\left(-E/RT\right), \tag{3}$$

where:
A, β - constant coefficients,
E - the activation energy,
R - the universal gas constant,
and constant rate for reverse reaction:

$$k_i^{''} = \frac{k_i^{'}}{K_{ci}}, \tag{4}$$

where:
K_{ci} - the equilibrium constant for the i-th reaction, determined by the following equation [14]:

$$K_{ci} = \left(\frac{p}{R \cdot T}\right)^{\sum_{k=1}^{K}\left(\upsilon_{ki}^{'} - \upsilon_{ki}^{''}\right)} \exp\left(\sum_{k=1}^{K}\left(\nu_{ki}^{'} - \nu_{ki}^{''}\right)\frac{S_k^0}{R} - \sum_{k=1}^{K}\left(\nu_{ki}^{'} - \nu_{ki}^{''}\right)\frac{H_k^0}{R \cdot T}\right), \tag{5}$$

where:
S_k^0 - the standard state molar entropy of the k-th species,
p - pressure,

Obtained results allowed calculating rates of molar concentration change of chemical species by the following equation:

$$q_i = \left(\sum_{k=1}^{K}\left(\left(a_{ki}\right) \cdot \left[X_k\right]\right)\right) \cdot \left(k_{fi}\prod_{k=1}^{K}\left[X_k\right]^{\nu^{'}{}_{ki}} - k_{ri}\prod_{k=1}^{K}\left[X_k\right]^{\nu^{''}{}_{ki}}\right), \tag{6}$$

where:
a_{ki} - the enhanced third-body efficiency of the k-th species in the i-th reaction,
X_k - the molar concentration of the k-th species.

Determination of the rate of change of the molar concentration for each chemical reaction highlighted the sum of molar concentrations of all chemical species for a given moment of time and heat released from the combustion process.

The calculations are made using a spreadsheet for the data presented in Tab. 1

Tab. 1. Parameters used to kinetic calculations and ANNs entry

Parameter	Value	Unit
pressure	2, 3, 4, 5	MPa
temperature	1100, 1600, 2100, 2600, 3100, 3600	K
Air humidity	4.5, 10, 20, 30	g_{H2O}/kg of air
Air-fuel excess ratio	0.8, 1, 2.5	–
Time interval	1.5×10^{-5}	s
Fuel	CH_4	

Combustion process parameters presented in Tab. 1 correspond to temperature and pressure in the combustion chamber of the marine diesel engine. Chosen air humidity correspond the engine charge air humidity from 20% at 20°C to 95% at 30°C. Time interval corresponds to the rotation of the crankshaft by one degree at the engine working with 1000 rpm. The calculations was made for the quantity of charge air enough to burn the fuel dose in the cylinder (air-fuel excess ratio equal 1) and with excess and deficiency of air. Such conditions may arise in different areas of the engine combustion chamber.

The sequence of calculations was as follows: for selected parameters from Tab. 1, initial molar concentrations and mole fractions of chemical species were calculated. For selected temperature and pressure the forward and reverse constant rates of all reactions were calculated. Using these parameters the molar concentrations of chemical species after the time equal 1.5×10^{-5} second were calculated by summation of molar concentrations of all reaction products. The total heat release from the combustion process was the sum of energy of each reaction [10, 14]. During calculations the assumption was made that in the above-mentioned period of time temperature and pressure are constant. Obtained results were the input to the next stage of the calculation after an identical period of time, so that calculation results for different initial concentrations of combustion mixture were obtained. Moreover, such an approach allows for the automation of calculations. In one series of calculations 1500 successive calculations were performed. The calculations are made for all possible configuration parameters set out in Tab. 1.

Using the presented algorithm more than 405 thousands data sets were collected. All data sets consists of 52 input mole fractions of chemical species, temperature and pressure, 52 output mole fractions of chemical species and the heat release from all considered reactions. After removing repeated cases more than 232 thousands of data sets were using to (ANN) training.

3. The artificial neural network training

Removing repeated cases is necessary to avoid the ANN training mistakes resulting from repeated administration of identical training data sets [11]. Approximation of functions, describing the heat release from the combustion processes and functions of mole fraction changes of chemical species according to combustion process conditions is a regression problem [11]. To address these issues the perceptron networks and radial basis networks may by use. The both of these networks were tested by the author at work [9]. The work led to the formulation of conclusion that would allow the selection of the perceptron neural network for further research. The perceptron neural network consists of input layer neurons, the hidden layer or layers and the output layer. Input and output layers consists of neurons, one for each input and output parameter of the model. Hidden layers can include any number of neurons. Each of the neurons in the network converts input signals with summing them using the weighting factors according to the following formula:

$$y = f\left(\sum_{i=1}^{n} w_i x_i\right), \tag{7}$$

where:
f - the nonlinear function, called the activation function,
x - the input signal,
w - the weight of the input signal,
n - the number of the input signal,
y - the output signal.

The ANN training relies on match weights of neurons to achieve the intended output signal or signals. Data sets from chemical kinetic calculations, standardized to values in the range from -1 to 1, were used to ANN training. Randomly selected 60% of data sets were used as the training data, 20% as a validation data and the rest 20% as a test data. The presented study included the building,

the training and the testing of ANN's to allow for calculation the total heat release obtained from the methane combustion process at the interval of time. Each of trained ANN's consisted of 54 neurons in the input layer, corresponding to 52 initial mole fractions of chemical species and temperature and pressure of the combustion process and one neuron in the output layer corresponding to the summarize heat release from the combustion process and from 15 to 60 neurons in the hidden layer.

The Broyden–Fletcher–Goldfarb–Shanno (BFGS) method was used to training all considered ANN's. This is one of the fastest quasi-Newton learning methods of ANN [4, 15]. As the activation function the logistic function of all hidden layers and the tangent hyperbolic function for output layers of networks were applied. The calculations are made using the Matlab and Neural Network Toolbox software on the Galera server in The Academic Computer Centre in Gdansk.

4. Results

Figure 1 shows examples of kinetic calculation results of the total heat release, derived from the combustion of methane in air with variable pressure and constant temperature, constant humidity of air and constant air-fuel excess ratio. According to presented dependencies the pressure increasing causes the acceleration of the combustion process and generates larger maximum heat release. The maximum heat release followed after 4ms from start of the combustion at 5 MPa pressure and more than 11 ms for the combustion at 2 MPa pressure at the same temperature. Completion of the combustion process takes place after a 9 ms and 20 ms, respectively. A similar relationship was obtained in the case of temperature changes and constant pressure, constant humidity and constant air-fuel excess ratio of the combustion process.

Figure 2 shows the effect of water content in charge air at the speed of the combustion process. Due to imperceptible differences between individual results graph has been enlarged at the area of the maximum energy. The reference area is lowest graph from the Fig. 1, which corresponds to the graph of the Fig. 2 for relative humidity equal 10 grams of water per 1 kg of air. According to results, increasing humidity of charge air decreases the maximum energy but accelerate the combustion process.

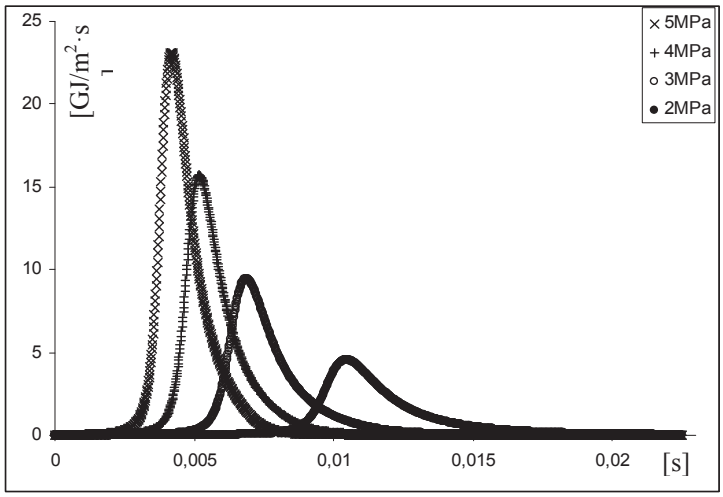

Fig. 1. The example of the kinetic calculation effects of heat release from combustion process in temperature 1100 K, humidity of air 10 g water on 1kg of air and air-fuel excess ratio equals 0,8

Figure 3 shows the effect of the amount of charge air on the heat release from the combustion process. Increasing of air content in the mixture causes a significant drop of the maximum heat release but accelerates the combustion process.

As mentioned earlier obtained results of calculations using the kinetic equations were approximated with ANN.

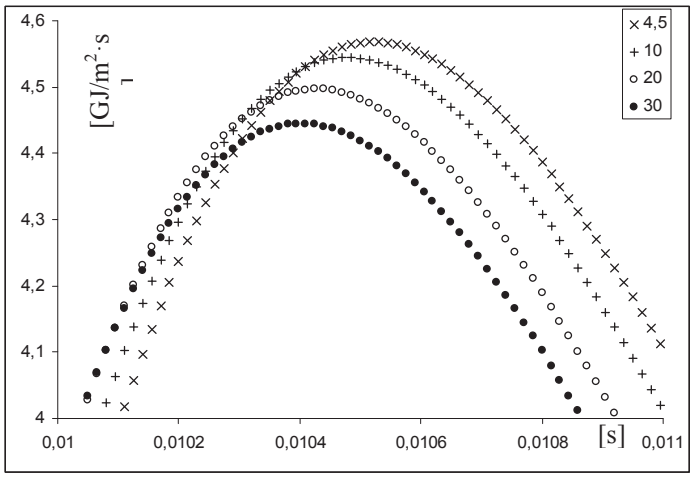

Fig. 2. The example of the kinetic calculation effects of the heat release from combustion process in temperature 1100K, pressure 2MPa and air-fuel excess ratio 0.8

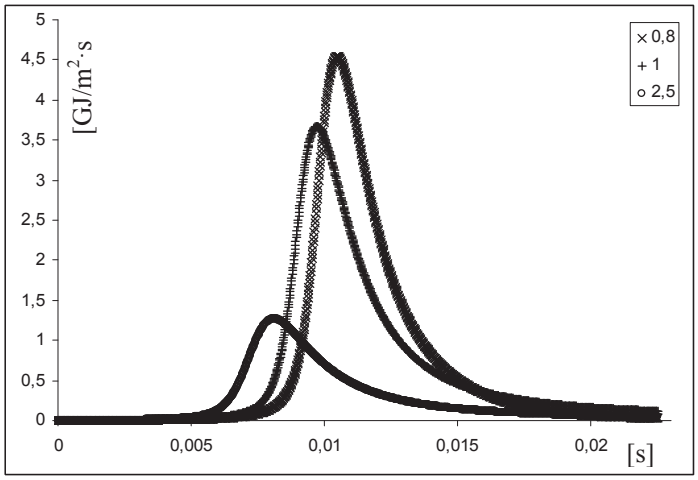

Fig. 3. The example of the kinetic calculation effects of the heat release from combustion process in temperature 1100K, pressure 2MPa humidity of air 10g water on 1kg of air

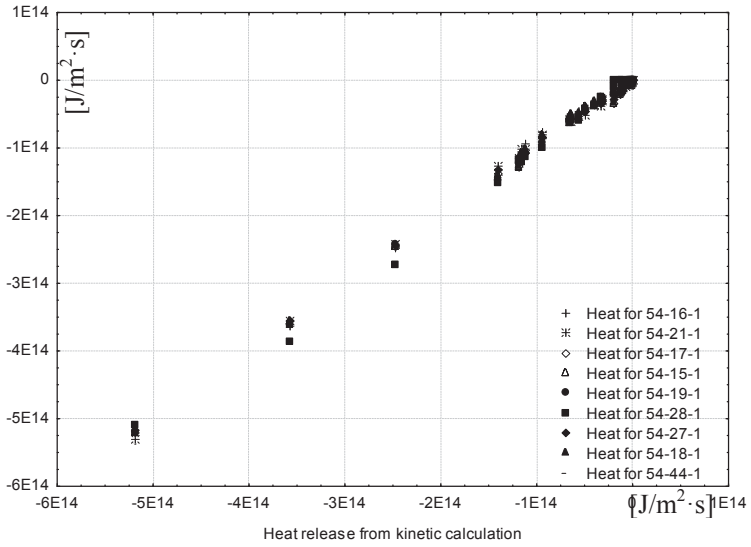

Fig. 4. The best ANN approximations of the kinetic calculations of the heat release for all considered parameters of the combustion process

Figure 4 presents a comparison of results of heat release calculations of the methane combustion process using nine neural networks with the smallest mean square error as a function of the heat release from the combustion process calculated with the GriMech 3 kinetic calculations (horizontal-axis) for all considered test data. Names of networks consist of numbers of neurons in the input layer, the hidden layer and the output layer consequently. According to presented results greatest differences between results obtained from ANN's were obtained for the negative heat release. The negative heat release corresponds to low thermodynamic parameters and it means the endothermic process at the start of the fuel oxidation. On the start of the combustion process the thermal decomposition of fuel is happen and low thermodynamic parameters are not enough to exceed the activation energy of all considered reactions. It should be noted that results of negative values do not exceed 35% of all test results. With the increase in temperature the combustion process became exothermic and differences between results obtained from ANN's and kinetic calculations were declined. Least mean square error was obtained for network with 19 neurons in the hidden layer (54-19-1). It was 0.04% for the test data and 0.02% for the validation data. Such low values of errors were made possible because of the large amount of data available. The maximum error for a single result was 1.9%.

5. Conclusions

The presented work apply ANN's to approximate functions of the total heat release from the methane combustion process, calculated with the Gri-Mech 3 kinetic mechanism of combustion. During the research kinetic calculations of the heat release were made for various thermodynamic parameters of the combustion process. These data were used to build and test various configurations of ANN's, which different numbers of neurons in the hidden layer. As a result of kinetic calculations of the methane combustion process in accordance with the GriMech 3 mechanism it is possible to formulate the following conclusions:

- increase pressure and temperature of the combustion process increases the maximum heat release and accelerates the combustion process. The maximum heat release followed after 4 ms from start of the combustion at 5 MPa pressure and more than 11 ms for the combustion at 2 MPa pressure. Completion of the combustion process takes place after a 9 ms and 20 ms, respectively,
- increase the humidity of charged air caused a slight reduction the time of the combustion process and reduces the maximum heat release,
- increase air content in the combustible mixture, according to air-fuel excess ratio, caused a significant reduction of the heat release in the combustion process. Time of the maximum heat release was shortened at unchanged time of the combustion.

The second purpose of this study was obtaining the ANN, allowing the approximation of the total heat release obtained from the combustion process. As a result of the activities the appropriate ANN was prepared. Training the ANN's allowing the approximation the heat release for the all considered parameters of the combustion process with the mean square error not exceeding 0.04%, and with a maximum error 1.9% for single result. The input data to the model of the combustion process were temperature and pressure and 52 mole fractions of chemical species involved in the combustion process according to the GriMech 3 mechanism.

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