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THE ANN APPROXIMATION OF THE CH_4 COMBUSTION MODEL

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Abstract

The paper presents results of research on the possibility of approximation of the results of calculations using the GriMech 3 kinetic mechanism by an artificial neural network (ANN). Application of kinetic mechanisms for modeling of combustion process in the finite element method requires considerable computing power which is associated with high costs of modeling. It is therefore necessary to seek alternative solutions in this area. The paper focuses on the possibility of application of ANN to approximate the total heat release from the combustion of methane. We built and trained ANN allows the approximation of the total heat release from the combustion process with a mean square error not exceeding 0.04% and the individual error for one result equal to 1.9%. Inputs for this model are the temperature and pressure of the combustion process and 52 mole fractions of chemical species in combusted mixture taken into account in the GriMech 3 kinetic model. For this reason, we tried to build and train the ANN approximating the mentioned mole fractions of chemical species. During the study we tested different configurations of ANN's, containing different numbers of hidden layers and different numbers of neurons in the output and the hidden layer. The best results were obtained for the approximation of the ANN with one hidden layer containing 38 neurons. It was built and trained 52 ANN's, one for each chemical species. Unfortunately, even for obtained small values of mean square errors of approximation, errors of individual results often exceed 100% of the results obtained from the kinetic calculations. For this reason, the application of ANN in the presented form to approximate mole fractions of chemical species is impossible.

Keywords: *combustion process, model, combustion engines, methane, kinetic calculation, GriMech 3*

1. Introduction

The development of alternative energy sources is not as yet resulted in a significant reduction of hydrocarbon fuels consumption. Still, hydrocarbon fuels are the most widely used in power machinery of the world [2]. In energy machines the energy generation from hydrocarbon fuels is obtained by changing the chemical energy into heat release during the combustion process and then into mechanical energy. Therefore, studies on the improving efficiency of the combustion process and accompanying energy changes reducing the amount of emitted to the atmosphere toxic compounds are a necessity. The high cost of experimental research makes that to the study of combustion processes and design of combustion chamber components of energy machines are also commonly used mathematical models [11]. The steady increase the computing power of computers makes models based on finite element method popular. The basis of these methods is dividing the combustion phenomena in the smaller elements (it's possible the division according to the geometry of the combustion chamber or other physical parameters such as velocity or temperature) [12]. This division is made in such a way that the mathematical description of physical phenomena in these finite elements were as simple as possible. Elements are "connected" each other by

boundary equations. This procedure simplifies the analysis and computation of complex phenomena as the combustion process, however, requires considerable high computing power because of the multiplicity of finite elements used (often exceeding hundreds of thousands elements), and the number and complexity of the phenomena taking place simultaneously during the combustion process.

The use of hydrocarbon fuel required to provide it to the energy machine in the liquid or gas form. This process requires a preparatory treatment before combustion the fuel. Preparation is often done directly in the combustion chamber, which is caused by economic considerations and increasing the efficiency of the machine. That is why in the combustion chamber often take place parallel a variety of physical and chemical phenomena. In the case of diesel engine working [4], during the process of air compressing in the cylinder with a piston simultaneously take place injection of liquid hydrocarbon fuel into the combustion chamber, its atomization and evaporation, turbulent mixing with air, self-ignition and combustion of the mixture by chemical reactions of oxidation in air. The rate of chemical transformations and their progress depends largely on local concentrations of substrates involved in the combustion process and the local thermodynamic conditions [5]. Due to the movement of the piston, the process of delivering fuel and progress of considered individual phenomena takes place in a dynamic and heterogeneous conditions in different areas of the combustion chamber. For these reasons, the accuracy of the model of the combustion process depends on number and size of finite elements established to calculations, but also on the accuracy of the description of phenomena occurring in the same elements. In the case of modeling the phenomena associated with turbulent combustion in the combustion chamber of the diesel engine the complexity of the phenomena enforces of the high cost of modeling. So often it is reasonable simplification to the model, depending on the intended purpose and accuracy of modeling.

In work [7] author has attempted to model of combustion process of methane based on the GriMech 3 kinetic mechanism [1], developed by scientific unit from University of Berkley. Our results appear to be qualitatively consistent with available results of similar studies and the general knowledge about the phenomena occurring in combustion processes. The results of modeling are continuous functions of heat release derived from the fuel combustion, depending on the concentrations of individual chemical species of the combustible mixture, temperature, pressure and time of combustion and mole fractions of established chemical kinetic model. The obtained values of mole fractions, together with the heat release function should be in the next stage used to determine individual energy balances in all finite elements of the combustion phenomena to modeling the instantaneous energy states of different areas of the engine cylinder or other combustion chamber [6]. The complexity of the calculations carried out, however, difficult to use even such a simple model for finite element calculations. For this reason, author tried made approximations of obtained results using the artificial neural network (ANN). During the preparation of approximation author made assumption that properly trained ANN able to provide correct results for other, similar thermodynamic parameters and calculation of individual weights of the network requires significantly less computing power than the algorithm based on the kinetic model of combustion.

The paper presents the results of approximation of the GriMech 3 modeling results of the methane combustion process using the ANN. The calculation results are presented for different mole fractions of fuel and oxidizer in the combusted mixture, different humidity of air and different pressure and temperature of combustion.

2. The selection of ANN parameters

The data used to approximate the relationship between the mole fractions of chemical species and the heat release from the combustion process of methane in humidity air have been determined

on the basis of calculations based on the GriMech 3 kinetic mechanism. Calculations were performed for selected values of temperature and pressure of the combustion process and selected mole fractions of methane and air. The calculations are made for all possible configurations of parameters given in Table 1.

Tab. 1. Parameters used to kinetic calculations according to GriMech 3 mechanism

Parameter	Value	Unit
Pressure p	2, 3, 4, 5	MPa
Temperature T	1100, 1600, 2100, 2600, 3100, 3600	K
Air humidity X	4,5; 10; 20; 30	g_{H2O}/kg of air
Air-fuel excess ratio λ	0,8; 1; 2,5	–
Time interval Δt	$1{,}5\times10^{-5}$	s

The obtained calculation results include a total of 432,000 data sets. Each data set contains the input data in the form of 52 mole fractions of chemical species adopted in the GriMech 3 kinetic mechanism and temperature and pressure of combustion process as well as output in the form of 52 mole fractions of combustion products and the total heat release from the CH_4 combustion after Δt time. The course and results of calculations are presented in the work [7].

Obtained results of calculations have been modified in such a way that removed all of data sets, which are duplicate. The reason for this approach is the need to avoid false ANN training in case of repeated administration to train the same data sets [9]. After presented modification process data sets received 232,222 cases, which were used to ANN's training. The training process allow approximate of the results obtained by calculation based on GriMech 3 kinetic mechanism of combustion.

Approximation of functions, describing the amount of total heat release from combustion processes and functions of changes of mole fractions of chemical species depending on the conditions of the combustion process is classified as regression problem [9]. To address these issues are usually used perceptron neural networks or radial basis neural networks. The use of both of networks has been tested by the author at [8] work. Results of work permitted to formulate conclusions that would allow to select the perceptron neural network for further research. Perceptron neural network, which structure is presented in Figure 1, consists of input layer, hidden layer or layers and output layer.

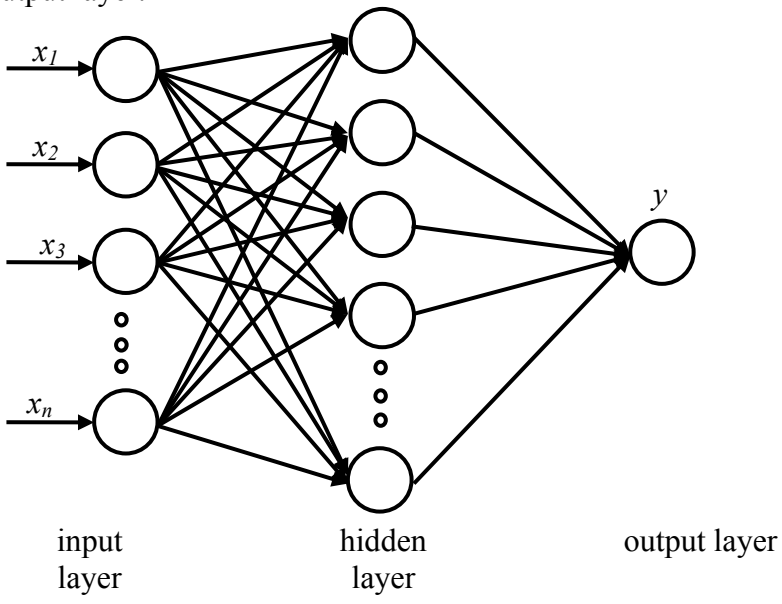

Fig. 1. The scheme of ANN

The input and output layer consists of neurons, one for each input and output parameter of the approximated model. Hidden layers can include any number of neurons. Each of the neurons in the network converts input signals by summing them using the weight factors according to the following dependency:

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

were:

f – the nonlinear function, named 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 rely on matching weights of input signals so as to achieve the intended output signal or signals. The study used data from the GriMech 3 kinetic calculations, standardized to the values in the range from -1 to 1. To ANN training process 60% of randomly selected data sets were used as training data, 20% as a validation data and the remaining 20% as test data. The present study included the building, training and testing of ANN's to allow for the designation of 52 mole fractions of chemical species and the total heat release derived from CH_4 combustion process after Δt time. All trained ANN's consists of 54 neurons in the input layer, corresponding to 52 initial mole fractions of chemical species and temperature and pressure of the combustion process, neurons in the output layer corresponding to the output signals and from 15 to 60 neurons in the hidden layer. During the study the following configurations of ANN's were tested:

– a neural network with one output for the total heat release from CH_4 combustion process;

– a neural network with 52 outputs for each mole fractions of combustion products and one hidden layer;

– a neural network with 52 outputs for each mole fractions of combustion products and two hidden layers;

– 52 neural networks with one output for each mole fraction of combustion product and 38 neurons in one hidden layer.

To ANN training the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method of back propagation weights setting was used, as one of the fastest quasi-Newton methods of ANN training [3], [10]. As the activation function we applied the logistic function for all hidden layers of ANN's and a linear function for the output layers to all ANN's approximating the mole fractions of chemical products of combustion and hyperbolic tangent function for the output layer network approximating the total heat release from the CH_4 combustion process. The calculations are made using the Matlab software with Neural Network Toolbox on the Galera server in The Academic Computer Centre in Gdańsk.

3. Results of approximation

During the training all configurations of ANN's, after a random distribution of data sets on training, testing and validation sets, input data were made available to input neurons. Random adopted weights of neurons allow to calculate the summarize heat release from all considered in the GriMech 3 kinetic mechanism chemical reactions or mole fractions of chemical species. Values of mentioned parameters were compared with the appropriate output values of heat an

mole fractions, obtained from the kinetic calculations. After administration of all training data errors of approximation was calculated. Errors were input data to algorithm of modifying weights of all neurons in ANN in accordance with the BFGS back propagation method of training. All presented steps of training named one epoch. After this we start the next epoch of ANN's training by random redistribution of data set, and re-modification of neurons' weights until a satisfactory accuracy with the validation data. In all cases the number of training epochs not exceeded 200.

3.1 Sum of heat release from combustion process

As mentioned earlier, the approximation of sum of heat release from fuel combustion was used perceptron network with 54 neurons in the input layer, corresponding to 52 values of mole fractions of al considered in GriMech 3 kinetic mechanism chemical species, temperature and pressure of the combustion process, and one neuron in output layer corresponding to the total heat release from all chemical reactions. During the training process we considered ANN's containing from 15 to 60 neurons in one hidden layer.

Figure 2 shows a comparison of the results of calculations of total heat release from the combustion process using nine ANN's with the smallest mean square error as a function of total heat release calculated by kinetic calculations (x-axis) for the test data. The names of the ANN's derived from the number of neurons of sequentially the input layer, the hidden and the output layer.

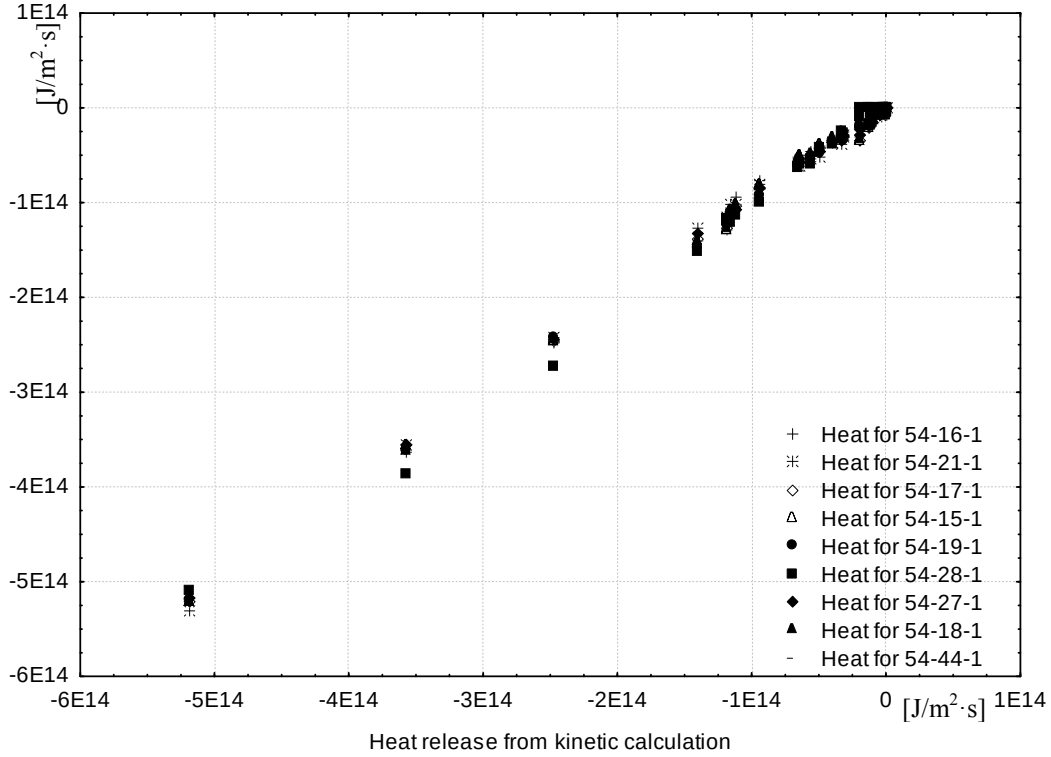

Fig. 2. The best ANN approximations of the kinetic calculations of the total heat release for all considered parameters of the combustion process

According to the results presented on figure 2, the biggest differences between the results obtained from each ANN's and results from kinetic calculations were obtained for the negative heat release. The negative heat release from the combustion process means, that the fuel oxidation process is endothermic. That process is possible for low thermodynamic data of fuel dissociation.

It should be noted that the results of the negative values of heat release do not exceed 35% of all test results. With the increase in temperature the combustion process became exothermic and the differences in results between different networks was minimal. Smallest mean square error was obtained for networks with 19 neurons in hidden layer (named 54-19-1). It not exceed of 0.04% for 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 and low number of training epochs. The maximum error for a single result was 1.9% ant it was in endothermic area of the combustion process.

3.2 Mole fractions of chemical species

Using ANN approximation of heat release from one finite element is only possible when we know changes of mole fractions of all considered in established kinetic mechanism chemical species during the combustion process. During the initial phase of the ANN training for approximation of mole fraction we tried to properly train a single network with 52 output neurons, one for each chemical species. In the course of the calculations, however, failed to obtain satisfactory results for both the application; ANN with one and two hidden layers. For this reason it was decided to training separate 52 ANN's, having in each case, one neuron output for each chemical compound. The best results with minimum approximation error we obtained for ANN's with 38 neurons in hidden layer.

According to mentioned situation we obtained 52 networks, trained for all considered mole fractions of chemical species after Δt time of the combustion process. All trained networks consist of 54 neurons in the input layer, 38 neurons in the hidden layer and one neuron in the output layer. Figure 3 shows sample results of calculations of the mole fractions of nitric oxide as a function of mole fraction of this chemical species approximated by obtained ANN. According to the presented relation there is a linear relationship between the obtained results. The mean square error for the network was $3 \cdot 10^{-4}$ % for both test and validation data. The maximum error for a single result was 1.6%.

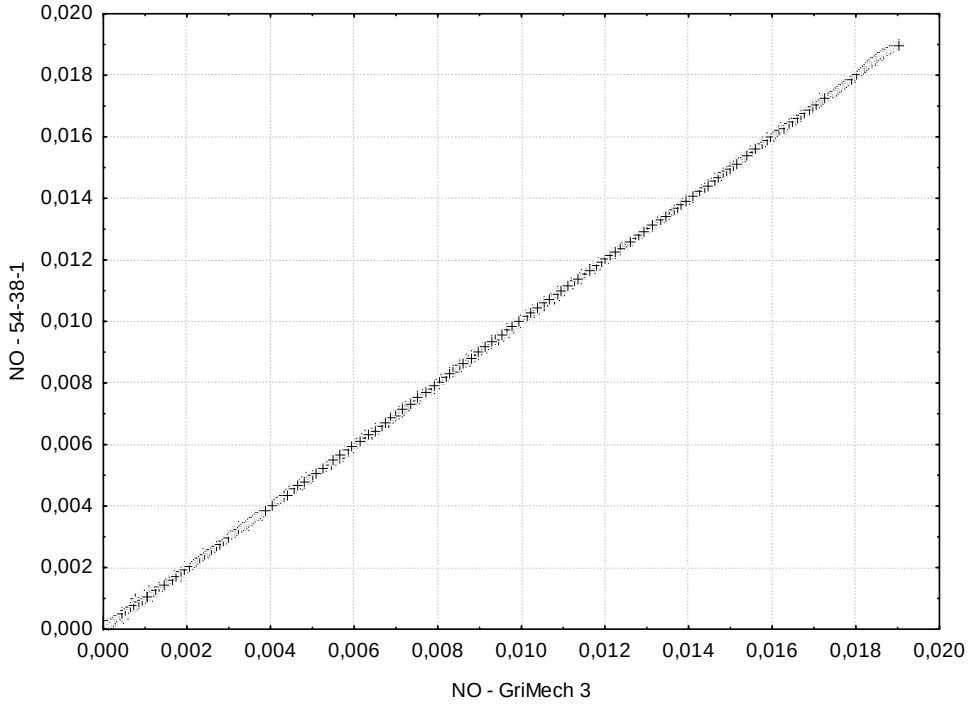

Fig. 3. Mole fractions of nitric oxide calculated by GriMech 3 mechanism and approximated by 54–38–1 ANN

Similar results we were also obtain for the remaining 51 considered chemical species. In any case, the mean square error of approximated by trained ANN mole fractions did not exceed a value of $1 \cdot 10^{-2}$ %, but the maximum error for a single value of the mole fractions of 43 chemical species excess even more than 100% of the value of mole fractions calculated by the GriMech 3 kinetic mechanism of the combustion process. Please note that the calculated mole fractions of chemical species are products of the combustion process in a finite element. For modeling the combustion process in engine cylinder, which the dynamic changes in pressure and temperature, it is necessary to use the calculated mole fractions, as input for modeling the subsequent phases of the combustion process until the end of the work cycle of diesel engine. Such a model creates the possibility of a geometric rise of the calculation error of mole fractions. Due to the fact that these mole fractions are also input data to the model of heat release from the combustion process in one finite element, these errors also affect the value of the output from this model. For this reason it is necessary to adopt a conclusion that the obtained approximation errors of mole fraction values of chemical species in relation to the calculated values taken from the kinetic mechanism calculation, despite the small mean square errors, have individual values errors too large. Obtained individual error results for mole fractions of 43 chemical species are too large and disqualify the application of ANN in their current form for modeling the combustion process.

4. Conclusions

The presented work was to apply the ANN to approximate functions of the total heat release from the combustion process and mole fractions of CH_4 combustion products, calculated using the GriMech 3 kinetic mechanism. During the research work we were built and train several ANN's configurations, differing in the number of neurons in the hidden and the output layer and the number of hidden layers. The result of this study was to obtain an ANN, allowing approximation of total heat release obtained from the combustion process with a mean square error not exceeding 0.04%, and with a maximum error 1.9%. The inputs to this model are temperature and pressure of the combustion process and 52 mole fractions of chemical species, considered in mentioned GriMech 3 kinetic mechanism. For this reason, we tried to set up and train an ANN, which allows approximation of mole fractions of these chemical species. As work progresses, however, failed to obtain a satisfactory ANN, allowing to obtain reliable results, enabling the use of ANN's in prace of modeling. Despite the small value of the mean square error, the errors of individual results often exceed 100% of the value obtained from the kinetic calculations. For this reason, it is necessary to conduct further investigations in order to seek an alternative methods of calculating of mole fractions of chemical species, enabling the reduction the cost of modeling in relation to the kinetic calculations.

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