THE ANN APPROXIMATION OF THE CH_4 COMBUSTION MODEL: THE MIXTURE COMPOSITION

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Abstract

The calculation of the changing of the combustion mixture composition during the combustion process of the CH_4 is presented of the paper. Correct calculation results of the mixture composition during the combustion process in combustion chambers of internal combustion engines is important to define the heat release calculation, modeling and simulation of the combustion phenomena. The paper presents results of calculations for the GriMech 3 kinetic mechanism of the methane combustion for different thermodynamic parameters and the composition of the combusted mixture. Results of the kinetic calculation of combustion process are qualitatively consistent with the data available in literature. The second purpose of research was the approximation of obtained results with the trained artificial neural network. Input data needed to approximate mole fractions of considered in the GriMech 3 mechanism combustion process chemical species consisted of 52 mole fractions of initial chemical species and temperature and pressure process. For all considered chemical species the mean square error did not exceed a value of 1·10-2 %, but the maximum error for a single value of 43 species excess even more than 100% of the value of mole fraction values taken from kinetic calculations. Single values of errors disqualify the neural network application for modeling of mole fractions of chemical species.

Keywords: *modeling, internal combustion engines, approximation, artificial neural network, combustion process, chemical species*

1. Introduction

Hydrocarbon fuels are still the most widely used source of energy in the energy machines [4]. The obtainment of such energy takes place by conversion of the chemical energy to a heat release during the combustion process. The resulting heat release is then transformed into other forms of useful energy. Therefore, it is necessary to continue a development of a research on increasing the efficiency of the combustion processes and accompanying physical and chemical phenomena. The aim of the research is to increase the energy production efficiency of hydrocarbon fuels but also to limit the toxic compounds amount emitted to the atmosphere. Lowering the cost of investigations is possible with using mathematical models, allowing simulation phenomena's occurring during the combustion process without the necessity of measurements on real objects [11]. The steady increase the computing power of computers makes models based on finite element method commonly used. Mentioned methods rely on dividing the fuel combustion phenomena in the smaller elements (division according to the geometry of the combustion chamber is possible, but also with other physical parameters such as velocity or temperature) [12]. This division is made in such a way that the mathematical description of phenomena in these finite elements was as simple as possible. Parameters, resulting from the finite element calculation, coupling them with the boundary conditions. This procedure simplifies the analysis and computation of complex phenomena as the combustion process, however, requires considerable computing power. The reason for this is multiplicity of finite elements used, often exceeding hundreds of thousands and the number and complexity of the phenomena taking place simultaneously during the combustion process.

Hydrocarbon fuel is supplied to the energy machine in the liquid or the gas form. This process requires a preparatory treatment prior to the combustion in the combustion chamber. Preparation is often done directly in the combustion chamber. The reasons of that procedure are increase the efficiency of the machine and the economic aspect. In the combustion chamber often a variety of physical and chemical phenomena happens, running parallel with the process of the combustion. In the case of the internal combustion diesel engine [6], during the process of the air compression in the cylinder with a piston the injection of liquid hydrocarbon fuel into the combustion chamber occur. At the same time followed the fuel fragmentation, the evaporation, the turbulent mixing with air, the thermal dissociation, the self-ignition and the combustion of the mixture by chemical reactions of the oxidation in air. The rate of chemical transformations and their progress depends on the local concentrations of chemical species involved in the combustion process and local thermodynamic conditions [3]. Due to the movement of the piston, the process of fuel delivering and occurring of individual phenomena's takes place dynamically and heterogeneous in different areas of the combustion chamber. For these reasons, the accuracy of the model of the combustion process depends on the number and size assumed to calculation finite elements. The accuracy of calculations also depends on the description of phenomena occurring in the same elements. In the case of modeling the turbulent combustion phenomena in the combustion chamber of engines complexity of the phenomena enforces the high cost of the modeling. So often it is reasonable to simplicity the model, depending on the intended purpose and accuracy of the modeling.

In the work [8] author attempted to the heat release model from the methane combustion process based on the GriMech 3 kinetic mechanism [1], developed by a research unit from the University of Berkeley. Obtained results appear to be qualitatively consistent with the available results of similar studies and general knowledge about the phenomena occurring in the combustion processes. The result of the modeling were continuous functions of the heat release from the fuel combustion, depending on mole fractions of considered chemical species of the combusted mixture, temperature, pressure and time of combustion. The obtained values of the heat release the next should be used to determine individual energy balances for the finite element modeling of instantaneous energy states of different areas over the engine cylinder or the other combustion chamber [7]. The complexity of calculations carried out, however, difficult to use even such a simple model for finite element calculations. For this reason, author try to made approximations of obtained results using an artificial neural network (ANN). During approximation the assumption was made that properly trained ANN able to provide correct results for similar thermodynamic parameters. The calculation of ANN's individual weights requires significantly less computing power than the algorithm based on the kinetic model of the combustion process.

The inputs to the built ANN's are mole fractions of chemical species taken into account in the GriMech 3 kinetic mechanism. For this reason, it is necessary to obtain actual values of mole fractions of chemical species for different thermodynamic conditions.

The paper presents the results of kinetic calculations of mole fractions of chemical species taken into account in the GriMech 3 kinetic model of the methane combustion. Obtained results of calculations were used to build, train and test different configurations of ANN's approximating mole fractions of chemical species for different configurations of combusted mixture, changing the value of humidity of air, changing pressure and temperature of the combustion process. Author assume that obtaining satisfactory results of using the ANN to approximation of results from GriMech 3 mechanism will apply in the future, more complex models of hydrocarbon fuels combustion.

2. Initial data

According to the considerations set out in the work [8], to determine the heat release we require input data in the form of mole fractions of chemical species considered in the GriMech 3 kinetic mechanism of methane combustion process [1]. GriMech 3 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.

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. According to mentioned data it's possible to calculate forward and reverse constant rates of all considered reactions between 52 chemical species. The useful formula is Arrhenius equation and formula of dependence between equilibrium constants for all reactions and molar enthalpy and entropy and thermodynamic parameters. Determination of the rate of change of molar concentration for all chemical reactions highlighted the sum of molar concentrations of all chemical species for a given moment of time. A fuller description of the calculation algorithm is presented in the work [8]. The calculations are made using a spreadsheet for the data presented in Tab. 1.

Tab. 1. Parameters used to GriMech 3 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 corresponds to the 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 (4.5 g_{H2O}/kg of air) to 95% at 30°C (30g_{H2O}/kg of air). Time interval corresponds to the rotation of the crankshaft by 1° at the engine working with 1000 rpm. The calculations were made for the different quantity of charge air. According to stoichiometric conditions the quantity of charge air was set on 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 of chemical species were calculated. For the selected temperature and pressure the forward and reverse constant rate of all reactions were calculated. Using these parameters molar concentrations of chemical species after the time equal $1{,}5\times10^{-5}$ second were calculated by summation of molar concentrations for all reaction products. During the calculations the assumption was made that in the above mentioned period of time temperature and pressure are constant. Obtained results were input to the next stage of the calculation after an identical period of time, so that the 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, which consisted of 52 input mole fractions of chemical species, temperature and pressure, 52 output mole fractions of chemical species from all considered reactions. After removing repeated cases 232222 of data sets were using to the ANN training.

3. The ANN training

As mentioned earlier obtained results of calculations have been modified in such a way that all duplicate data sets were removed. The reason for this approach is the need to avoid false the ANN training in case of repeated administration to training the same data sets [9]. The problem of

approximation of mole fractions of chemical species from the chemical kinetic calculation process is possible to solve by using perceptron neural networks [9]. Such networks consist of a minimum of three layers:

- the input layer, corresponding to the input data,
- the output layer corresponding to the output data,
- one or more hidden layers.

Each layer is made of neurons (in the case of perceptron network, perceptrons) processing the input signal at the output using by an algorithm whose parameters are changed during the ANN's training process. A more accurate description of the perceptron network is presented in the work [8].

The present study included the building, the training and the testing of ANN's allow for the approximation of 52 mole fractions of chemical species derived from the combustion of methane over Δt time. Each ANN 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, neurons in the output layer corresponding to the 52 mole fractions of chemical species after Δt time and from 15 to 60 neurons in the hidden layer. During the study we tested the following configurations:

- ANN with 52 outputs for each mole fractions of chemical species and one hidden layer,
- ANN with 52 outputs for each mole fractions of chemical species and two hidden layers,
- 52 ANN's with one output for each mole fractions of chemical species and 38 neurons in 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 [5, 10]. As the activation function the logistic function of all hidden layers and linear function for output layers of ANN's were applied. The calculations are made using the Matlab and Neural Network Toolbox software on the Galera server in The Academic Computer Centre in Gdańsk.

4. Results

Figure 1 shows examples of kinetic calculation results according to GriMech 3 mechanism of the methane combustion for following thermodynamic parameters 1100 K of temperature and 4 MPa of pressure, humidity of charge air equal 10g of water for 1 kg of air and air-fuel excess ratio equal 2.5.

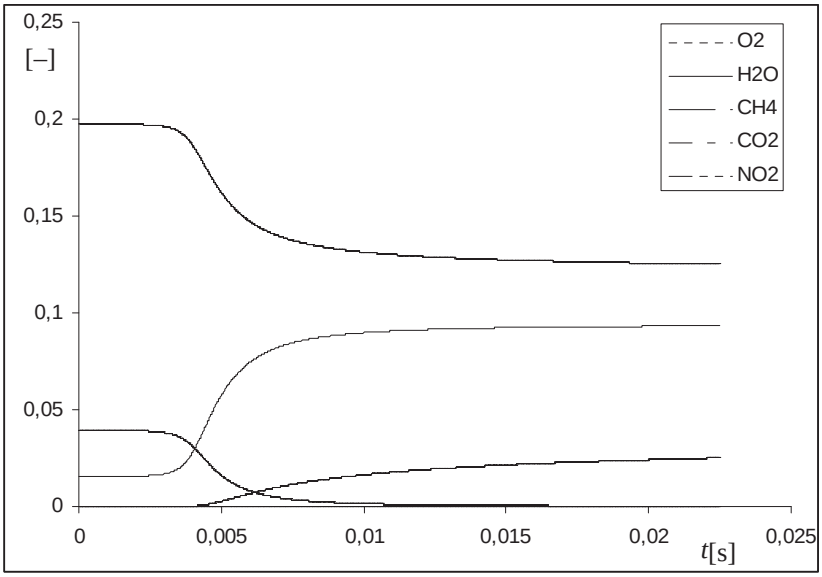

Fig. 1. Chosen results of kinetic calculations for temperature 1100 K, pressure 4 MPa, humidity of air 10g_{H2O}/kg of air and air fuel excess ratio 2.5

According to the presented results the fastest reactions, corresponding with the mole fraction of molecular oxygen, water and methane, for the chosen parameters were obtained approximately after 6ms. Further chemical reactions result only minor changes in the mole fractions. After about 17 ms the methane combustion is complete. The relatively low temperature of the combustion process not promote the formation of chemical species from the group of nitric oxides, that is why the maximum mole fraction of NO_2 in the combusted mixture is 2×10^{-11}. The graph for this chemical species overlap with x-axis of the coordinate system.

Figures 2 and 3 presents mole fractions of molecular oxygen and nitric dioxide for chosen thermodynamic parameters.

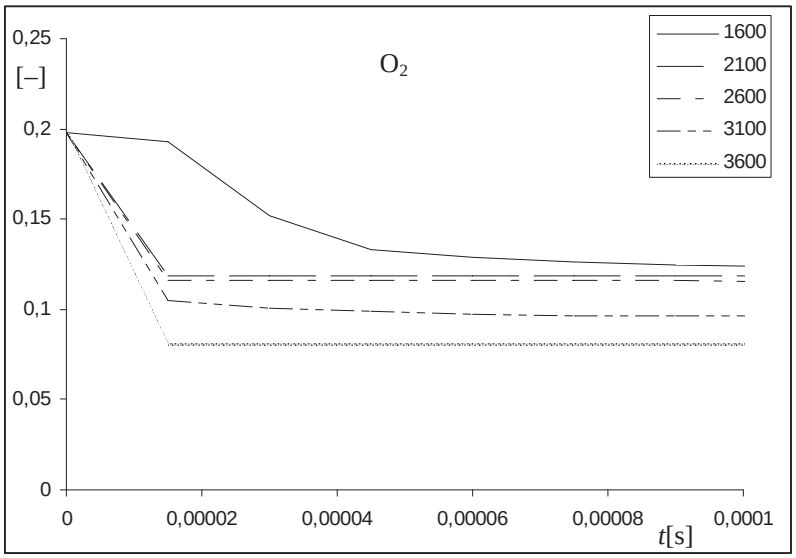

Fig. 2. Calculated mole fractions of O2 for pressure 4 MPa, humidity of air 10gH2O/kg of air, air-fuel excess ratio 2.5 and changed temperature

The requisition of oxygen in the combustion process can be an indicator of the speed of the combustion process. Fig. 2 shows the loss of molecular oxygen from the initial mole fraction value equal approximately 0.2 for chosen composition of the combusted mixture.

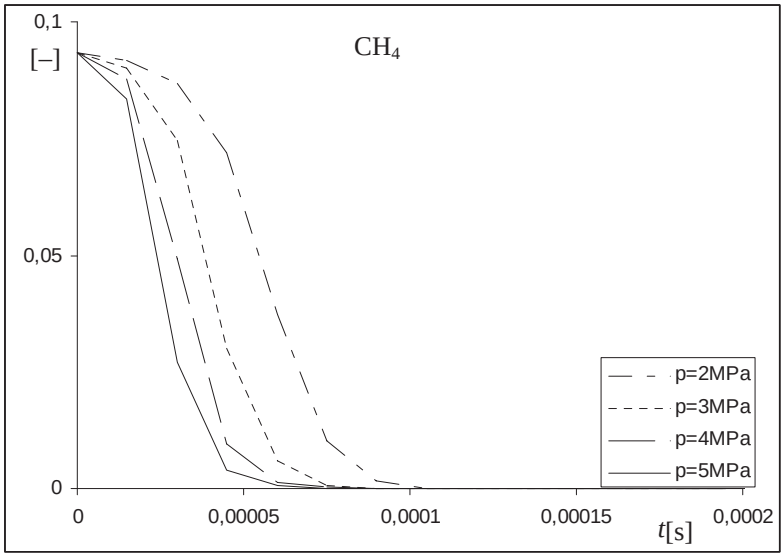

Fig. 3. Calculated mole fractions of CH4 for temperature 1600K, air-fuel excess ratio 1.0, humidity of air 10gH2O/kg of air and changed pressure

With the increase temperature of the combustion process the equilibrium fraction of these chemical species is obtain faster. The value of the equilibrium fraction of O2 decreases with increasing the temperature of the combustion. The reason of this situation is influence of the forward and reverse reaction rates on equilibrium fractions of chemical species and mentioned ratios strictly depends on temperature of the combustion process [6].

Figure 3 shows the effect of pressure on the combustion process on the example of the calculated mole fraction of methane. Along with the course of the combustion process mole fraction of methane decreases. The mole fraction equal of zero comes at a time that is shorter than the higher is pressure of the combustion process. According to the presented results, methane combustion rate is proportional to pressure of the combustion. Effect of influencing of combustion pressure on the rate of chemical transformation is associated with the reactions that cause changes in the quantity of chemical species (synthesis and species breaking reactions) [2].

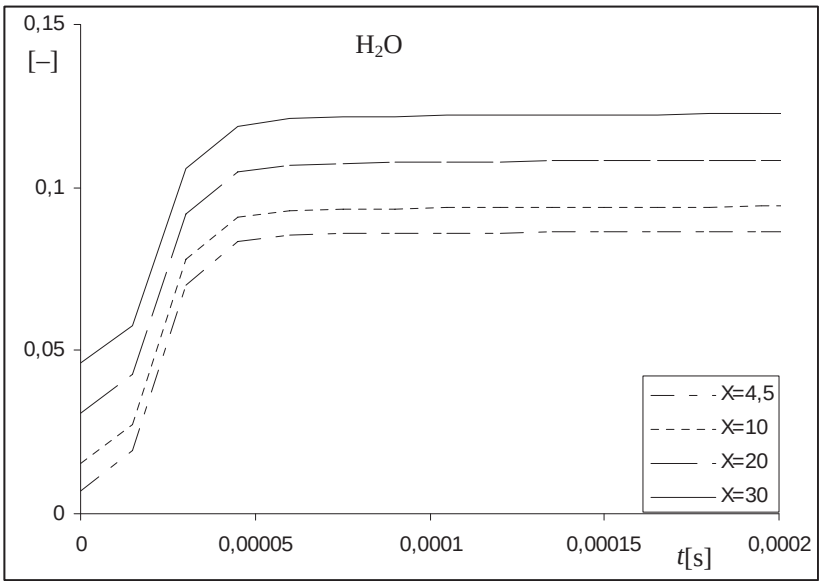

Fig. 4. Calculated mole fractions of H2O for pressure 5 MPa, temperature 1600 K, air-fuel excess ratio 2.5 and changed humidity of air

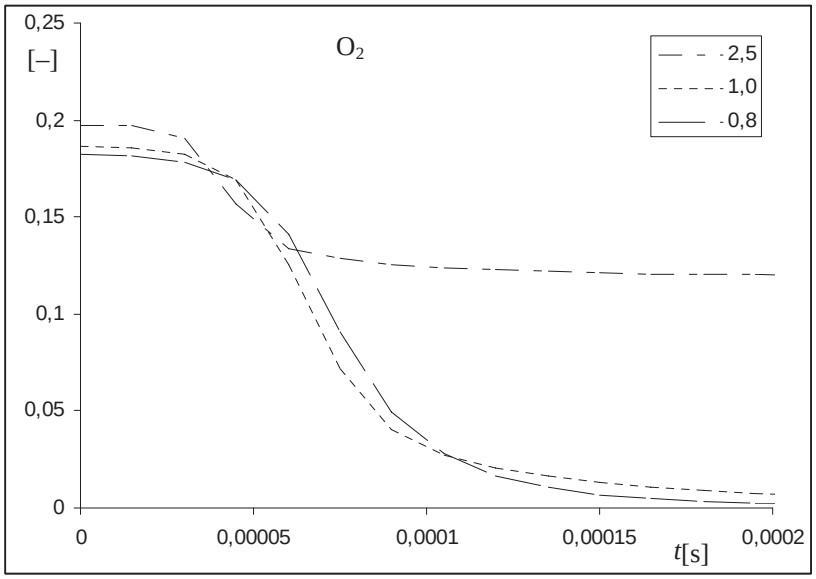

Fig. 5. Calculated mole fractions of O2 for pressure 2 MPa, temperature 1600 K, humidity of air 10gH2O/kg of air and changed air-fuel excess ratio

Fig. 4 presents the effect of the water content in the combustible mixture. The Fig. shows that increase water in charge air results in the final water content in the exhaust gases. It should be noted that, during the combustion process hydrogen-containing chemical species are combusted, inter alia, to form of water, thus the quantity of water in the combustible mixture during the combustion process increases. The content of air in mixture has a significant influence on the combustion process. According to the data in Fig. 5, the combustion process is the fastest with largest of air-fuel excess ratio. It should also be noted that the value of air-fuel excess ratio is determined by the participation of oxygen at the end of the combustion process.

Presented results of kinetic calculations of the combustion process in accordance with the GriMech 3 mechanism have been used to train various configurations of ANN's to approximation of mole fractions of all considered chemical species. During the initial phase of the ANN's training we tried to properly train a single ANN with 52 output neurons, one for each chemical species, however, we failed to obtain satisfactory results for ANN with one and two hidden layers. For this reason we decided to training 52 separate ANN's with one neuron output for each chemical species and 38 neurons in the hidden layer.

Fig. 6 shows sample results of mole fraction calculations of nitric oxide as a function of a mole fraction approximated by the ANN. According to the presented results there is a linear relationship between the results obtained. The mean square error for the network was $3 \cdot 10^{-4}$ % for both, the test data and the validation data. The maximum error for a single result was 1.6%.

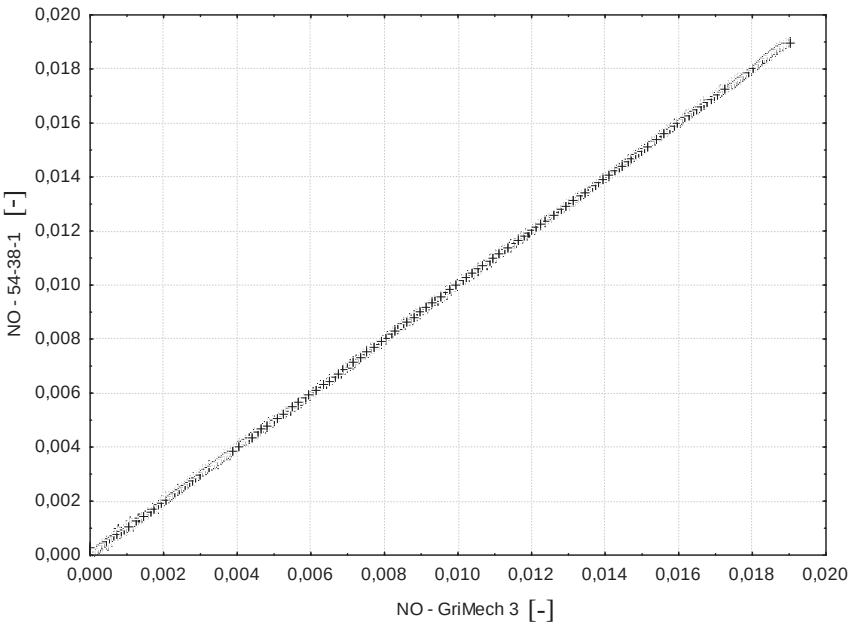

Fig. 6. NO mole fractions calculatedaccording to GriMech 3 mechanizm and approximated by 54–38–1 ANN

Similar results were also obtained for the remaining 51 chemical species. In any case, the mean square error did not exceed a value of $1 \cdot 10^{-2}$ %, but the maximum error for a single value of 43 chemical species excess even more than 100% of the value of mole fraction values taken from kinetic calculations. Please note that the mole fractions of the chemical species are, in assumption, products of the combustion process in one finite element. For the combustion process modeling in engine cylinder which dynamic changes of pressure and temperature, it is necessary to use the mole fractions of chemical species as the input for modeling the subsequent phases of the combustion process until the end of the cycle. This way of modeling offers the possibility of a geometrical enlargement of calculation errors of mole fractions in next stages of calculations. Due to the fact that mentioned results are also the input data to the model of heat release from the combustion process, these errors also affect on the value of the output from this model. For this

reason it is necessary to assume a conclusion that the approximation errors for mole fractions of chemical species obtained from ANN's training, despite the small mean square errors have errors of single values so large. The single values errors disqualify the ANN's application in current form for modeling of mole fractions of chemical species.

5. Conclusions

The presented work apply the ANN's to approximate functions of the 52 mole fractions of chemical species during the methane combustion process, calculated by the Gri-Mech 3 kinetic mechanism of combustion. During the research kinetic calculations of all considered in the GriMech 3 chemical species 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 hidden layers and neurons. As a result of calculations of methane combustion process it is possible to formulate the following conclusions:

- results of the kinetic calculation of chemical species mole fractions considered in the GriMech 3 combustion process mechanism are qualitatively consistent with the data available in literature.
- the mean square error did not exceed a value of $1 \cdot 10^{-2}$ % for all ANN's approximations but the maximum error for a single value of 43 chemical species excess more than 100% of the value of mole fraction values taken from the kinetic calculations.
- the single values errors disqualify the ANN's application in current form for modeling of mole fractions of chemical species.

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