Application of Artificial Neural Networks for Solution of Scientific and Applied Problems

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Abstract[1]

Examples of ANN using for solution of scientific and applied problems in field of combustion in particular for combustion diagnostic and experimental investigation as well as for industry control are presented in the paper.

1. Possibilities for a creation of new kinds of models for combustion wave (CW) propagation by means of ANN are presented. A goal of such kinds of models is solving of hard tasks of experimental investigation of propellants burning.
2. New ways for solving direct and inverse problems of optics by means of ANN are presented. These problems have to be solved for many optical and non-optical methods of combustion diagnostics for example for interferometric and shadow techniques, absorption spectroscopy, X-ray, etc.
3. Possibilities for a creation of ANN model for automatic control system of boiler unit during transient processes are presented. A database for training of ANN was obtained by means of system of finite-difference equations based on full dynamic non-linear mathematical model of boiler unit.

1. Introduction

Artificial neural networks [1] (ANN) can be considered as a universal tool for multidimensional approximation. The Kolmogorov-Arnold theorem dealing with capability of representation of multidimensional functions by means of superposition of functions of smaller number of variables is in the basis of ANN application. In more late formulation, the theorem consists in a capability of representation of multidimensional function by means of superposition of functions of one variable. It allows to use the ANN for problem solving of approximation of multidimensional functions in all cases, when usual methods of approximating either can not be utilized, or give poor results.

Program emulators of ANN are computer codes, in a basis of creation and application of which a training on examples (on a database of examples) lies. ANN represent some quantity of "neurons", each of which is an elementary processor realizing a mathematical function (a transfer function). The number of "neurons" can be various, a part of "neurons" may be connected with others and another part won't. ANN can be presented often as "neurons" formed in layers. The neurons in one layer are not concerned with each other, but they concerned with neurons of a previous and next layers by principle "each with each". Input information goes into the first layer, then into the second layer and so on. After passing each layer, information varies in accordance with synaptic weight of each "neuron" and its transfer function. The synaptic weight is a contribution of each "neuron's" calculation into a final result (output information). A task of ANN training consists of finding such synaptic weights at which input information will

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correctly be mapped in output information. A database for ANN training can be formed by means of various techniques. For example, a database for ANN training can be formed by means of real experimental data or data obtained by means of a numerical experiment organized specially and connected with a task to be solved.

ANN technologies do not negate, but rather include and extend statistical methods, methods of experimental design, and methods of solution regularization.

ANN have advantages in comparison with pure mathematical methods (analytical and numerical) in three cases:

1. When a task cannot be adequate formalized, as it contains units of uncertainty;
2. When a task can be formalized, but at the given time there is no mathematical apparatus for its solution;
3. When the task can be formalized and there is a mathematical apparatus for its solution, but the implementation of the calculations by means of available computing systems does not meet requirements of obtaining solutions in time, in size, in computer techniques used, etc.

A main advantage of ANN technologies for modeling is that they can be used to solve problems that have no obvious algorithmic solution. With ANN, legitimacies of a system behavior may be revealed on a basis of "inexact data" about the characteristics of the system. ANN are a universal tool for construction of numerical models such as "a black box" from which one it is possible to obtain multivariate non-linear dependences from incomplete discrete data. This is especially important when the system is characterized by many parameters and the determination of part of them is technically unfeasible. ANN are capable also, in some cases, to induce analytical models of real complex systems directly from experimental data. Therefore ANN can be used for construction of multifactor quantitative forecasts.

A main condition for successful application of ANN is a quality of a database used for training. However, certainly, there are also other conditions of successful application (ANN architecture, technique of ANN training and some of other methodical features of ANN using).

ANN have such properties as parallelism of information processing, adaptability to various conditions (learning capability and self training capability), good stability of calculation, reliability (potential fault tolerance owing to redundance of ANN architecture), that is very important in control systems.

Examples of ANN using for solution of scientific and applied problems in field of combustion of energetic materials in particular for combustion diagnostic and experimental investigation of combustion as well as for industry control are presented in this paper.

2. New Kinds of Models for Combustion

2.1. The First Analytical Solution of Combustion Wave Differential Equation

This part of our work is not directly connected with ANN however it was born directly during performance of this work as well as it is a base for creation of ANN model of combustion wave.

A propagation of a stationary combustion wave (CW) is described by a heat conduction equation which one is non-linear differential second-order equation. Together with an unknown function - temperature distribution, the equation includes unknown parameter - burning rate, which one is the main characteristic of CW that should be determined from the solution of a task (it may be considered as the task eigen value). A number of approaches were offered for obtaining approximated formulas of a burning rate till now. Many from these formulas were obtained by expansion of variables into series near to characteristic point. Different approximations of temperature distributions were applied. A number of iterative, variation, and asymptotic methods of the solution were designed [2]. Thus the different assumptions resulting into simplification of a heat conduction equation were made however the non-linear differential second-order equation had not been decided as a whole.

The complexity of the differential heat conduction equation describing CW propagation in a general case is that it contains addend, in which one the unknown function is in an exponent denominator (of an exponential multiplicand). In reference books on differential equations, for example [3], general views of such differential equation, and, accordingly, methods of its solution are not cited.

In this part of our work, a new method which one allows to obtain analytical solutions of such differential equations is offered for the first time. From the point of view of solution methods of differential equations, the method can be attributed to a method of a substitution. So, for example, analytical solution of differential equations of oscillations or Schrodinger equation is searched out.

In such approach, it is important to find an analytical function correctly describing behaviour of a task.

We suggest to present an unknown function of a differential equation (temperature distribution) by means of a sigmoid function. Thus the differential equation can be reduced to an algebraic equation from which one a burning rate and other important characteristics of CW can be derived and calculated.

The sigmoid function (SF) is the monotonically increasing, everywhere differentiating non-linear function:

$$f(x)=\frac{1}{1+e^{-ax}}$$

where a is the SF parameter, x – argument (Fig.1).

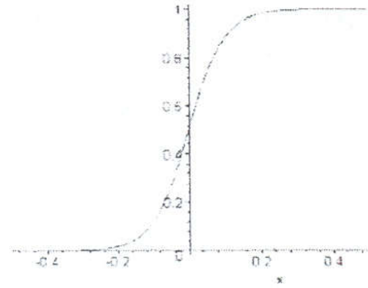

Figure 1. The Sigmoid Function f(x)

Let's consider possibilities of SF using for analytical solution of differential equations describing CW propagation on an example of a solution of equation (1) that describes a propagation of a one dimensional stationary CW in a homogeneous gaseous combustible mixture

$$\lambda \cdot \frac{d^2T}{dx^2} - u_n \cdot c_p \cdot \rho \cdot \frac{dT}{dx} + Q \cdot C \cdot k_0 \cdot e^{-\frac{E}{R \cdot T}} = 0 \quad , (1)$$

where λ and cp is heat conduction and specific heat values accordingly (we consider them as constant values here); T - temperature in a CW, un - linear velocity of a combustible mixture flow and ρ - density of a combustible mixture flow (we consider them as variable values here); Q - heat effect of chemical reaction, C - density of the not burnt out combustible mixture, which one can be expressed through a temperature, k0 - fore-exponential factor, E - activation energy, R - universal gas constant.

Here we have used a coordinate system connected with the moving CW, where Tx=0 = T_0 and Tx=∝ = Tmax , where T_0 - initial temperature of combustible mixture, and Tmax - maximum temperature of CW.

Let's write a sigmoid function as follows (Fig.2):

$$T = T_0 + \frac{T_{max} - T_0}{1 + e^{-ax}} \quad , \quad (2)$$

We can see that this function corresponds to "idealized" distribution of temperature in a stationary one-dimensional CW precisely, i.e. the function reflects characteristic features of the task correctly. Let's write a density change of the not burnt out combustible mixture as follows

$$C = \rho_0 \cdot \left(\frac{T_{max} - T}{T_{max} - T_0}\right) = \rho_0 \left(\frac{e^{-ax}}{1 + e^{-ax}}\right) \quad (3)$$

and variable density as follows

$$\rho = \frac{\rho_0 \cdot T_0}{T} = \frac{\rho_0 \cdot T_0 (1 + e^{-ax})}{T_0 \cdot e^{-ax} + T_{max}}$$

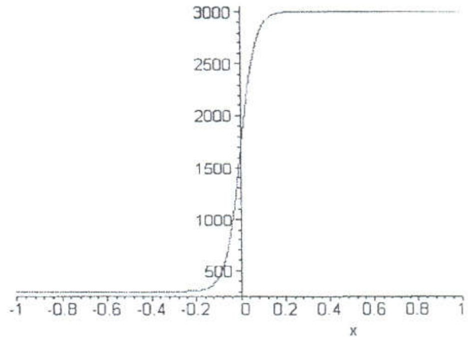

Figure 2. The Sigmoid Function T(x)

Then we can take the first and the second derivative of temperature, to substitute them in (1), to obtain algebraic form of (1), and to obtain the following analytical expression for linear velocity of a combustible mixture flow, i.e. to solve analytically the equation (1):

$$u_n = \frac{\lambda a}{c_p \rho_0 T_0} \cdot \frac{(e^{-ax}-1)(T_0 e^{-ax}+T_{max})}{(e^{-ax}+1)^2} + \frac{Q k_0 (T_0 e^{-ax}+T_{max})}{a c_p \cdot T_0 (T_{max}-T_0)} e^{-\frac{E(e^{-ax}+1)}{R(T_0 e^{-ax}+T_{max})}} \quad (4)$$

The preliminary analysis depict that the solution correctly describes dependences of the linear velocity of a combustible mixture flow from gradient of temperature (parameter a), thermal (heat conduction, thermal capacity) parameters of a combustible mixture, heat effect of chemical reaction, etc. Comparison of the solution (4) for $x = 0$ and $x = \propto$ with the well known solutions[2] depicts that they coincide for SF parameter $a \approx 10^4$.

In our opinion, such way of obtaining of the analytical solutions can be promising in many cases described by differential equations of combustion such as (1), for which one the distribution of temperature is like sigmoid function. In case of a solution of non-stationary problems of combustion, this method allows to reduce a general problem to a task of solution of differential equation of the first order, i.e. essentially facilitate a solution general problem.

From the quantitative point of view, merit of the method include that it allows to calculate value of normal burning rate of a combustible mixture of a known composition as well as it allows to obtain analytical solutions as respects to others five parameters of a task (thermal capacity, heat conduction, initial density, heat effect, fore exponential factor). It could allow solving a task of choice of combustible composition which one can ensure a demanded burning rate and maximum temperature. It could set up also a task of determination of "real" values of thermal conductivity and thermal capacity in CW in real cases.

From the point of view of quantitative research of CW structure in real cases, it is very interesting is a solution of the important experimental problem of determination of a temperature distribution (and heat release rate or constant of chemical reactions rate) in CW.

Though the method offered does not allow directly to obtain an analytical solution concerning distribution of temperature (algebraic equations which one can be obtained from (1) by means of sigmoid function can not be analytically solved as respect to parameter a), the method allows to reduce this, very difficult in experimental sense, problem to a task of measurement of linear (or mass) burning rate. This task can be executed by means of modern experimental methods reliably enough. After measurement of real burning rate value, the algebraic equation that is obtained from (1), can be resolved with respect to parameter a and value of maximum temperature (at a known initial temperature) by means of approximate methods of a solution of algebraic equations.

However in our mind, the most eligible method for the solution of algebraic equations that could be obtained by means of sigmoid function is an using of ANN technologies (see the next section).

2.2. Artificial Neural Networks Models

A goal of such kinds of models is a solving of hard tasks of experimental investigation of burning.

A solution of the above mentioned hard task of determination of a temperature profile of CW by means of ANN CW model and measurement of burning rate of CW is represented as example below.

The scheme of construction of ANN CW model in a case of one-dimensional CW, described by Eq. (1) can be presented as follows.

At first, Eq. (1) should be converted in an algebraic form by means of sigmoid function (2). Then, as you could see above, the formula (4) can be obtained. Further, for x going to infinity, the following formula can be obtained:

$$u_n = -\frac{\lambda \cdot a \cdot T_{\max}}{c_p \rho_0 T_0} + \frac{Q \cdot k_0 T_{\max}}{a \cdot c_p \cdot T_0 (T_{\max} - T_0)} e^{-\frac{E}{RT_{\max}}}$$

This formula consists of all connection between all variables of CW. Further, changing values of sigmoid parameter a and values of thermal and kinetic variables of CW, it is possible to obtain values of burning rate appropriated to any set of the variables.

The "database" obtained can be used for ANN training and construction of ANN model as follows. The different sets of numerical values of burning rate, thermal and kinetic parameters install on an input of ANN. The appropriate numerical values of sigmoid parameter a install on an output of ANN. In total, we used about 500 sets of the above-mentioned values. By means of an appropriate procedure of ANN training, for example, by means of method "back propagation of errors" [1], ANN CW model have been obtained. This model is a model of type "black box" that involves all latent connections between all variables. The "black box" obtained can be used in experimental investigation for "measurement" of a temperature profile as follows. A real, experimentally obtained, value of burning rate and real (or approximate) values of thermal and kinetic parameters install on an input of ANN model. Then, the value of sigmoid parameter a, which one determines a temperature profile will be obtained on an output of ANN model.

A comparison of model results obtained with literature data concerning with real burning cases show good prospects of ANN using for determination of temperature profiles in CW, and, also, possibilities for solutions of other problems, for example, for determination of degree of burn-out of reactants, real thermal parameters of medium during a CW propagation, formal effective kinetic parameters of chemical reactions of combustion, for experimental investigations of CW structure in a case of burning of a micron size particle (or a nano size particle!), for determination of temperature surface in a case of real propellant burning, etc.

We are planning to execute these concrete tasks in a future and invite those who are interested to join work.

Apart from a way of "algebraization" of differential CW equations, there are also capabilities of construction of CW ANN models by means of a base of real experimental data concerning burning characteristics. This could help to create CW ANN models in conditions of real burning.

It is interesting to mark here that ANN allow to solve algebraic equations that can not be solved analytically. Eg. (4) can not be solved analytically relative to sigmoid parameter a. However the database formed by means of Eq. (4) can be used for ANN training from the point of view of determination of sigmoid parameter a.

From the point of view of perspective problems, capabilities of solutions of which require additional serious research, it is possible to mark here problems of determination of a real CW structure for powders and propellants as well as for a case of combustion of micro and nano-particles (in these cases the distribution of temperature in a CW cannot be presented by means of the only sigmoid function). The problems of determination of temperature profiles and heat release rate, concentration of reactants and products (both in pseudo one dimensional case and two dimensional case of a cylindrical symmetry as well as for real three dimensional case) as well as a determination of a surface temperature or maximum temperature in stationary mode and their time history during ignition could be relative to these perspective problems. Problems dealing with an analysis of models of combustion described by means of systems of partial differential equations could be relative to these problems also.

3. Modeling of Deflagration-to-Detonation Transition for Pulse Detonation Engine. ANN Discovery Possibilities

As an example of ANN discovery possibilities, the results obtained on the basis of data of Santoro R.J. *at al* [4] are presented in Table 1. A deflagration-to-detonation transition under various experiment conditions was studied in [4]. The data that were presented in [4] had many blanks (about 60%). A task of filling them by means of ANN was set. The results of ANN discovery are underlined and the data of [4] are not underlined. The data of the discovery of the N2/O2 meanings (the level of nitrogen dilution of combustible mixture) for borders between S (successful detonation) and F (failure detonation) received with the help of ANN are presented in the last line of Table 1.

Table 1. Experimental Results of Deflagration-to-Detonation Transition upon Various Experimental Conditions

N_2/O_2	1.117-meter predetonator tube				2.031-meter predetonator tube		
	78% BR flat disk						
	0 cm	5 cm	10 cm	15 cm	5 cm	10 cm	15 cm
0.00	S	S	S	S	S	S	S
0.75	S	S	S	S	S	S	S
1.50	S	S	S	S	S	S	S
2.25	S	S	S	S	S	S	S
2.40	S	S	S	S	S	S	S
2.50	S	S	S	S	S	S	S
2.60	S	S	S	S	S	S	S
2.70	S/F	S	S	S	S	S	S
2.80	F	S	S	S	S	S	S
3.00	F	S	S/F	S/F	S	S	S
3.20	F	F	F	F	S	S	S/F
3.40	F	F	F	F	F	S/F	F
3.60	F	F	F	F	F	F	F
3.76	F	F	F	F	F	F	F
Borders	2.65 - 2.72	3.09 - 3.13	2.94 - 3.05	2.92-3.04	3.31-3.34	3.35-3.45	3.22 - 3.27

4. New Models for Solving Direct and Inverse Problems of Optics

These problems have to be solved for many optical and non-optical methods of combustion process diagnostics for example for interferometric and shadow techniques, absorption spectroscopy, X-ray, etc.

A problem addressed in our work was a determination of integral and local characteristics of a flame by means of an ANN without measuring a lot of values of function of phases difference distribution on an interferogram plane, $S(x,y)$, i.e. by using an incomplete set of $S(x,y)$.

A task of integral equations solution, i.e. a task of determination of an integrand by means of determination of integral meanings distribution was considered. Possibilities for using of incomplete information about integral meanings distribution are shown. In particular, possibilities for using even the only value of a function of integral meanings distribution for determination of an integrand, i.e. a full distribution of local characteristics in an object (for example a determination of temperature field in a flame by means of interferometric techniques), as well as integral characteristics of an object (for example a total quantity of a heat in a flame) for a case of any known symmetry of an object are shown.

Let's consider the task of determination of an integrand by means of the only value of integral meaning on example of solving of Abel's integral equation for the case of cylindrical symmetry of an object. In order to solve this problem we used a dimensionless Abel's integral equation that corresponds to a cross-section of a flame in a case of flame interferometry:

$$S(p) = 2\int_0^{\sqrt{1-p^2}} (n_0 - n(r))dz, \qquad (5)$$

where S is dimensionless phases difference, $z^2 + p^2 = r^2$, z is a ray's path in the object, p is an aim distance ($0 < p < 1$), and r is a variable radius (Figure 3), n_0 is a refractive index of undisturbed medium surrounding a flame and n(r) is a refractive index distribution in flame.

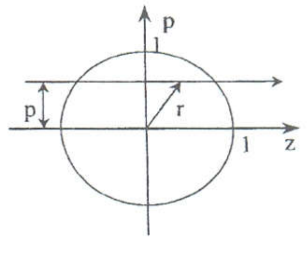

Figure 3. Geometrical Interpretation Corresponding to a Cross-Section of a Model Flame

ANN training database was obtained as follows. Using the equation (5), we determined the indefinite integrals $S(p)$ from the different integrands of a form $n_o - n(r) = 1 + ar - br^2$, where a and b are the given constants. In total we have used seven different integrands that reflect real distributions of a refractive index in flames. The values $n_o - n(r)$ were calculated for various values of r. The values of $S(p)$ were calculated for different values of p. The input data for ANN training were the values of $S(p)$, p and r. The values of $n_o - n(r)$ were the output data. In total, we used about 700 sets of the values $S(p)$, p, r and $n_o - n(r)$.

During using of the ANN model obtained, any value of dimensionless S and the corresponding value of p as well as the value of r are installed on input of ANN model and then the dimensionless value of n_o - $n(r)$ will be obtained on output of ANN. The real value of n_o - $n(r)$ can be obtained by means of a simple conversion factor and then can be converted in real temperature by means of well-known procedures [5].

As our results depict, the errors of determination of values of $n_o - n(r)$ do not exceed 5% in a case of cylindrical symmetry of an object.

In a case of integral flame characteristics, for example, a mass of cross-section or a quantity of heat in flame cross-section, which ones can be calculated by means of values of $\int S(p)dp$ [5], the input data for training ANN should be values of $S(p)$ *and* p. Value of $\int S(p)dp$ should be an output value.

This new approach is very important when an object cannot be visualized as a whole and in a case of optically thick object as well as in a number of other cases when ordinary methods of solution of inverse problems and direct tasks can not be used. Besides that this approach could principally expand possibilities of optical fiber methods as well as possibilities of laser-diode techniques for combustion diagnostics.

We would like to mark here that, in a case of homogeneous object, ANN allow to determine a form, size and orientation of an object by means of the only value of a function of signal distribution in a plane of the registration.

So, main advantages of ANN application for solving direct and inverse problems of optics are:

1. With ANN, one may calculate the distribution of local thermodynamic characteristics, including density of separate components, by means of measuring in one point of plane of signal registration;

2. ANN do not require additional real experiments in order to solve the inverse and direct problems. The ANN for solving of inverse and direct problems can be obtained by means of a database created with using relatively simple numerical calculations;

3. ANN can be used for all optical and non-optical methods, for which the measuring data are integrated on a line of registration;

4. ANN can be applied not only for objects with cylindrical symmetry but also for objects with other kinds of symmetry. All you need is to create a congruent database for ANN training.

In total, the results obtained depict that ANN allow to significantly extend possibilities of combustion diagnostics techniques. A joining of these possibilities with our approaches and computer codes for automatic processing and analysis of images allows to automate fully a determination of integral and local characteristics of an object as well as to use optical methods for creation of automated control systems.

5. Model of an Automatic Control System of a Boiler Unit

A problem of creation of automated control systems in modern engineering system is one of most actual. Improving of existing control systems as well as a creation of a new generation of automated control systems are the extremely pressing problems for redesign of old energetic devices and design of modern energetic devices. In particular, a special notice addresses on increase of a level of automation, reliability, safety and flexibility of control system.

The modern thermal manufacturing processes are characterized by essential nonlinearity of processes. Dynamics of separate links and an object as a whole is very complex from the point of view of control. An operator which one execute a function of control and decision making in case of transition from one mode to another mode, or for escaping an emergency situation, has many difficulties for implementation of optimal control because of a lot of information. Perspective way is an using of methods of artificial intelligence that can directly use expert's experience and human brain flexibility as well as strongly formulated mathematical models for decision making in complex situations.

This part of our work has been aimed on a development of principles of creation of a new model of automatic control system of a boiler unit in transient regimes (change of load, launch and stop of the boiler aggregate, etc) on a basis of ANN technologies.

This problem has been set for the first time. A search that has been conducted in scientific literature, in a base of patents of the Russian Federal Institute of Industrial Property, and also in an Internet has shown that examples of the solution of this problem are absent.

The following problems were set and solved for creation of a model of an automatic control system of a boiler unit:

1. A complete set of non-linear differential equations for the two-phase flow in cylindrical coordinate system circumscribing processes in a super heater was formulated. It described also a process of injection of water into a super heater during control procedure of vapor temperature in a super heater.

2. The obtained set of equations was converted into a system of finite-difference equations.

3. Adjustable and controlling parameters were selected by means of experimental data and experts' experience. The rate of a change of vapor temperature on an exit of the boiler aggregate was selected as a controlled parameter. The water mass flow via injector was selected as controlling parameter. The

analytical connection between them was determined by means of the mathematical apparatus of Lee derivatives.

The database for training of ANN was created by means of the obtained analytical connection and an optimal architecture of ANN was determined. The training of ANN was executed and a model of a control system as well as a skeleton diagram of a position of a gate valve governing a water discharge on injection were created.

The prototype of an automatic control system of temperature vapor in a super heater of a boiler unit TGME-464 was designed. It consists of the program emulator of ANN established on the personal computer, industrial microcontroller Philips P89LPC935, cable lines and switch gears. The prototype can be a deckhouse to a main system of the testing and control.

The obtained prototype can work both in a mode of advice, and in a mode of automatic control. It can be simply enough integrated in present control systems. The features of ANN technologies of control (property of adaptability to new conditions and ability to self training) provide simplicity of modernization and escalating of capabilities.

The creation of other control systems of dynamic behaviors on the basis of ANN, in particular, control systems of process of combustion in a furnace is hereinafter planned at the expense of regulation of supplies of gas both air in burners and recirculation of products of combustion.

6. Conclusions

- ANN could help to solve various complex tasks of combustion research in fields of experiment, diagnostics, testing and control.
- ANN technologies could be considered in a future as a powerful tool for solution of combustion problems that supporting high contact of theory, experiment and computer simulation

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