Solution of the Inverse Incorrectly Posed Problem by the Library Method

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Abstract: The presented study considers a range of problems to be interpreted as inverse problems. The complexity of solving incorrectly posed inverse problems due to their unique features and the lack of a universal method for their solution is highlighted. In this regard, the importance of considering the application of different methods on the example of specific problems is emphasised. The research analyses a method of solving the problem of determining the composition of gaseous hydrocarbon fuel in the process of its combustion in real time. It is emphasised that the way of measuring technological parameters allows to consider this problem as a complex problem of interpretation. The method of "library" (selection) as the most universal one is chosen. For its implementation the method of library formation in the form of a three-dimensional array is proposed, where the initial data for each solution of the direct problem are presented in the form of a single number, using the positional principle of recording decimal numbers. In the process of forming the working array, the method of comparing the oxidant excess ratio and the ratio of oxidant and fuel volume flow rates was used. This made it possible to use the results of the solution of the direct problem to determine the composition of fuel by the measured temperature of combustion products within the framework of the inverse problem. A method of searching for a solution among the elements of the working array based on the results of technological measurements of the combustion product temperature and the ratio of oxidant and fuel volume flow rates was developed.

1 INTRODUCTION

The solution of technical problems is based on a list of initial data. Their quantitative characteristics can be set and kept constant or determined by direct measurements during operation. But it is not always possible. For example, quantitative characteristics of the composition of substances in the process of work may change, and there is no possibility of their determination. Or in principle they are measurable, but cannot be provided with the necessary promptness. Also, the elements that determine the configuration of an object may be known, but their quantitative parameters are not known and are not directly measurable, etc. In all cases, an approach related to the solution of inverse problems can be used. In the process of its realisation it is necessary to determine, for example, the composition of initial substances or characteristics of elements included in the considered object by measured parameters of manifestation of some processes. In this case, the qualitative composition of substances (a set of chemical elements) or the list of elements and the order of their combination are known. It is necessary to determine their quantitative characteristics.

The generality of the approach to research by solving the inverse problem is accompanied by a variety of external conditions and, as a consequence, of possible solution methods. These methods depend on the problem to be solved. The type of method can be selected or developed in relation to a specific problem. For this reason, it is relevant to consider the application of each method on the example of solving a specific problem relevant in modern society. In this case, the method of determining the variable composition of the mixture of gaseous fuel in the process of its combustion is considered. Unlike certified fuel, the variable composition is due to the use of alternative sources of gaseous fuel, including those that do not generate greenhouse effect (gas generators, pyrolysis gases of woodworking waste, agricultural waste, coke, blast furnace gases, etc.).

The optimal combustion process of gaseous fuel of variable composition can in principle be organised on the basis of direct measurement methods.

Gas analysers. Mixtures of gases can be analysed for their qualitative and quantitative composition using chemical, physico-chemical and physical methods. The advantages of physico-chemical and physical methods over chemical methods are the rapidity of execution and the possibility of automating the analysis. Today, the most commonly used methods are gas chromatography [1]. Their main disadvantages are the sequential (not simultaneous) measurement of different gas components, long analysis time, and difficulties encountered in the detection of some components.

With the advent of small, reliable laser sources and highly sensitive multichannel photodetectors, the development of gas analysers based on the use of spontaneous Raman spectroscopy began. The development of such an instrument has been considered in the applied plan [2, 3], although it is still at the stage of laboratory development.

Extreme regulators. Despite the fact that they do not allow determining the composition of the combusted gas, they can theoretically be used to organise the combustion process with maintaining the temperature of combustion products at an optimal (maximum) level. All types of extreme regulators have a common disadvantage. When approaching the extremum point, the gradient of the measured parameter decreases (down to zero). This applies both to the case of determining the maximum temperature in the combustion chamber (furnace) [4] and to the case of determining the maximum temperature of the heat transfer medium [5]. The same property of the function is also manifested when determining the minimum (zero) concentration of carbon monoxide (CO) at the minimum concentration of oxygen in flue gases [6]. Taking into account that measuring instruments have a threshold of sensitivity, as well as there are noises in the measuring channels, at the point of extremum there is a maximum measurement error, which often excludes the possibility of using extreme regulators.

Determination of the reduced formula of the mixture. If the enthalpy and gross formula of a mixture of gases are known, some calculations of combustion process parameters are performed on the basis of chemical kinetics methods for a single substance [7,8]. In [9], a method for determining such a gross formula is proposed. It is based on the measurement of the temperature of combustion products (CP) and the flow rates of an unknown gaseous fuel and air. The formulated problem is an inverse one. On the basis of measurements of technological parameters, the composition of the combusted fuel is determined. In [9] it is shown that the solution of this problem exists and is unique. But the attempt to find the solution showed its instability. Thus, while this approach is promising, it leads to the necessity of solving the inverse, incorrectly formulated problem.

There is no single method for solving the whole variety of inverse incorrectly posed problems. Each of these problems requires an individual approach and contains an element of heuristics. As a result, there is a need to develop a new solution method capable of coping with the complexity and variability of such problems.

2 AIM AND OBJECTIVES OF THE STUDY

The aim of the study is to solve the problem of determining the composition of flared gas using the constraint method.

In order to achieve the objective, the following objectives were set:
- justify the choice of a method for solving the inverse incorrectly posed problem;
- develop a method of filling the library of solutions to a direct problem as a working three-dimensional array;
- to develop a method for finding a solution to a complex interpretation problem on the basis of using data from a working three-dimensional array.

3 METHOD FOR SOLVING THE PROBLEM

3.1 Justification of the Chosen Solution Method

To solve the inverse problem, you must first master the methods for solving the direct problem.

Let us consider the process on the example of solving the problem of determining the composition of flared gas.

During the solution of the direct problem, one of the initial parameters is the oxidant excess coefficient, denoted by α. However, a different parameter is used in the calculations:

$$\chi = \alpha \cdot \chi_o, \qquad (1)$$

where χ is the molar ratio of the components; χ_0 is the molar stoichiometric ratio of the components.

In the process of analysing the combustible and oxidising agent represented as ideal gases, the value of χ can be calculated on the basis of equality of molar volumes of any gases

$$\chi = \dot{V}_{ox} / \dot{V}_f . \qquad (2)$$

Here $\dot{V}_{ox}$ is the oxidiser (air) volume flow rate; $\dot{V}_f$ is the fuel volume flow rate. In other words, the value of χ (1) can be calculated on the basis of technological measurements of flow rates, while the chemical composition of the combustible fuel and oxidiser is not fixed. The model for solving the problem of determining the composition of combustible fuel is built on this property, using technological measurements of CP temperature and volumetric flow rates of combustible and oxidant (inverse problem).

Suppose that the fuel composition is known in advance in the form of the gross formula $C_{b_C} H_{b_H} O_{b_O} N_{b_N}$ with a list of chemical elements.

We will assume that during a certain period of time the fuel composition remains constant, ensuring the constancy of the values of the required parameters b_C, b_H, b_O, b_N, I_t in the process of their determination. The ratio between fuel and oxidiser is set with measurement of their volume flow rates ($\dot{V}_{ox}^1$ and $\dot{V}_f^1$). The temperature of the CP T^1 is measured during the combustion process. This data is used to form part of the model as a set of equations (in this case, 13 equations) that allow the determination of 12 partial pressures P_j^1 and one of the quantities sought, e.g., b_C. Then the volume flow ratios ($\dot{V}_{ox}^i$ and $\dot{V}_f^i$) are changed several times, and for each case the temperature of the PS is measured - T^i. These data serve as a basis for the formation of additional sets of equations necessary to determine the remaining required parameters - b_H, b_O, b_N, I_t. At the same time, the corresponding number of sets of partial pressures P_j^i of the CP is also determined. As a result, a system of equations is formed, consisting of five sets of 13 equations each (65 equations in total), designed to determine the five required quantities and the corresponding groups of partial pressures. Each group corresponds to different ratios of fuel and oxidiser volume flow rates.

In [10], the most universal approach to solving such a direct problem is outlined.

3.2 Method of Solving a Direct Problem

At the stage of preparation for determination of the gross formula of the fuel it is necessary to fill in the library of solutions for the direct problem with variation of six parameters. These parameters include the possible number of atoms of the corresponding elements in the gross formula of the fuel (b_C, b_H, b_O, b_N), possible values of the oxidant excess factor α and enthalpy of the fuel I_t .

The number of intervals can be chosen arbitrarily, and for concreteness we will take it equal to 100. This will allow tracking the change of each of the values b_C, b_H, b_O, b_N , in the interval 0.05...4.95 with a step of 0.05, the value α - in the interval 0.025...2.5 with a step of 0.025. It will require $(100)^6 = 10^{12}$ solutions of the direct problem with fixation of all results. At this stage, it is possible to reduce the dimensionality of the problem.

Thus the stoichiometric combustion process of ethane (and any other substance) can be organised both on the basis of its complete formula and at a normalised number of atoms.

$$2X2H6+7O2=4XO2+6H2O \qquad (3)$$

or

$$4X1H3+7O2=4XO2+6H2O.$$
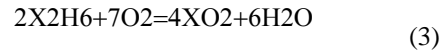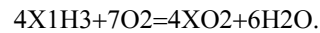
Here the normalisation is carried out by the number of carbon atoms. In the gross formula, the number of atoms is not necessarily an integer, and normalisation can be performed with respect to any chemical element. In this problem, carbon normalisation is applied, where the number of carbon atoms is fixed and equal to 1 and the gross formula is defined as follows:

$$C_1 H_{(b_H/b_C)} O_{(b_O/b_C)} N_{(b_N/b_C)} \text{ or } C_1 H_{d_H} O_{d_O} N_{d_N} \qquad (4)$$
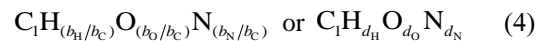
Thus, the number of solutions to the direct problem is reduced to $(100)^4 = 10^8$ realisations as a result.

At the next stage, the proposed method is used to convert the obtained results into a form convenient for further use in finding a solution based on the conducted process measurements of the CP temperature and volume flow rates of the fuel and oxidiser:

1) By varying dH, dO, dN and from (4), for each realisation of the solution of the direct problem, a certain fuel composition is set. For each case, the molar stoichiometric ratio of the components χ_0 is determined. The change in the value of the oxidiser excess ratio α is converted into a change

in the ratio of the measured process parameters $\dot{V}_{ox}/\dot{V}_f$.

2) At all possible combinations of initial data $\dot{V}_{ox}/\dot{V}_f$ (α), dH, dO, dN and It, arising at variation of their values, an attempt is made to solve a direct problem on definition of temperature of CP. In some cases, the ratio of fuel composition and enthalpy is incompatible, and such variants are excluded from consideration.

3) For the remaining (successful) realisations of the solution to the direct problem, the set of input data dH, dO, dN and It is represented as a single number using the positional principle of decimal number representation.

First, the data is written in normalised form:

$$\bar{d}_H = \frac{d_H - d_H^l}{d_H^r - d_H^l} \cdot 100. \qquad (5)$$

Here d_H - number of hydrogen atoms in the considered realisation of the direct problem; d_H^l, d_H^r - left and right boundaries of the considered interval of change in the value of the number of hydrogen atoms during the solution of the direct problem. The obtained values are combined into one number "E" by setting to its corresponding digits (Figure 1). Although the order of formation of this number can be any, let us assume that the value I_t is placed in the first two digits. As a result, complexes are formed in which each pair of values of the results of the solution of the direct problem (T and $\dot{V}_{ox}/\dot{V}_f$) corresponds to one number "E" with packed values of the initial data corresponding to them.

4) The calculation results (T and $\dot{V}_{ox}/\dot{V}_f$) are structured. Their max [Tr, ($\dot{V}_{ox}/\dot{V}_f$)r] and min [Tl, ($\dot{V}_{ox}/\dot{V}_f$)l] values are determined. The ranges of variation of these values are divided into a certain number of intervals. The number of intervals and the value of the step of change of each value are correlated with the technological accuracy of measurement (T and $\dot{V}_{ox}/\dot{V}_f$) in the process of fuel combustion.

5) The results of the solution (T and $\dot{V}_{ox}/\dot{V}_f$) of the direct problem and their corresponding initial data, summarised into a single number "E", are used to form a three-dimensional array (Figure 2).
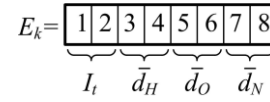
Figure 1: Diagram of positional representation in the form of a single number of normalized values of the initial data.
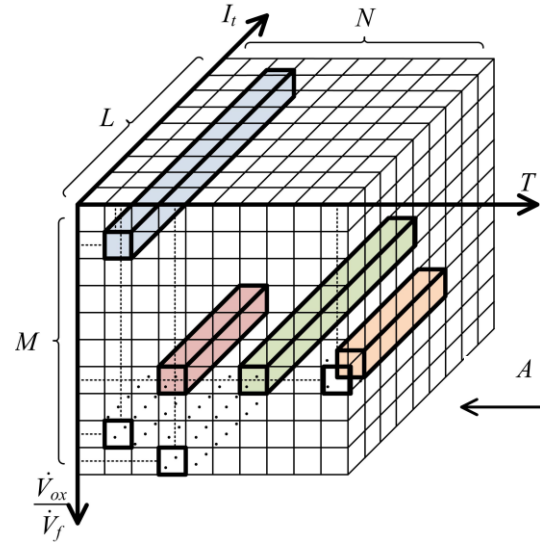
Figure 2: Diagram of forming a structured three-dimensional working array based on the initial data and the results of solving the direct problem.

6) Each cell corresponds to a vector of dimension L (Figure 2), the elements of which are numbers "E". The value of the number is determined by the value in the first (highest) digit. In this case, the values in the first digits are related to the enthalpy value. Therefore, the vector axis is labelled as enthalpy axis It .

Parameters L, M, N, are determined on the basis of the required accuracy of consideration of the corresponding values. Let's assume, for example, that N=M=100. In this case, 104 cells are formed on the plane T - $\dot{V}_{ox}/\dot{V}_f$. At the number of realisations of the solution of the direct problem 108 each cell can correspond to the results of ~108/104 =104 solutions. The same number of numbers "E_k" associated with these solutions are placed in the elements of the corresponding vectors.

7) In the elements of the vector are placed the values "E_k", which are in their respective boundaries:

$$E_k \in [(I_t^l)_k, (I_t^r)_k]. \qquad (6)$$

Since not all combinations of fuel composition ($\bar{d}_H$, $\bar{d}_O$, $\bar{d}_N$) can be realised with the

considered list of enthalpy values I_t, some elements of the vectors are unfilled. The elements of the vectors are ordered in ascending order. Examples of filling of some vectors are shown in Figure 2 and marked in colour.

3.3 Method for Finding a Solution to the Interpretation Problem

A method for determining a fuel composition using a generated working three-dimensional array includes the following steps:

1) The CP temperature Ti is measured for different values of the oxidiser-fuel volume ratio ($\dot{V}_{ox}/\dot{V}_f$)i . The number of measurements is determined by the number of quantities to be determined. So in case of fuel of the type (4) it is necessary to determine 4 quantities ($\bar{d}_H$, $\bar{d}_O$, $\bar{d}_N$, I_t) and, accordingly, to perform 4 sets of measurements.

2) Based on the measurements, 4 cells (highlighted by dashed lines in Figure 2) and associated vectors (highlighted in colour) are defined on the T - $\dot{V}_{ox}/\dot{V}_f$ plane of the working three-dimensional array. Each vector in E_k records all possible combinations of defined quantities ($\bar{d}_H$, $\bar{d}_O$, $\bar{d}_N$, I_t) that provide the temperature Ti at ($\dot{V}_{ox}/\dot{V}_f$)i .

3) The projections of the selected vectors on the plane $\dot{V}_{ox}/\dot{V}_f$ - It (view A, Figure 2), more precisely on the axis It (Figure 3) are determined.

4) Since the composition and enthalpy of the determined fuel remain constant at any ratios of changes in volume flow rates, the corresponding values of the numbers E_k in all vectors under consideration must be the same. Therefore, the area D of intersection of the set of elements of each vector is determined (Figure 3). The elements of vectors exceeding the area are removed. Further actions are aimed at reducing the width of the area to 1 element, which will determine the desired solution.

5) The selected numbers (area D, Figure 3) are rearranged in stack order. The values of the next value to be determined are transferred to the upper digits The value from the upper digits (Figure 1) is transferred to the end of the number.

The rearranged numbers are sorted, resulting in a scheme similar to the one shown in Figure 3.

6) The steps from step 4 are repeated until all values from the list of values to be determined (I_t, $\bar{d}_H$, $\bar{d}_O$, $\bar{d}_N$) have been used. With each pass the number of remaining numbers E_k decreases. In the end there remains one value E_k in which the determined parameters (I_t, $\bar{d}_H$, $\bar{d}_O$, $\bar{d}_N$) correspond to all measured Ti at the given $\dot{V}_{ox}/\dot{V}_f$. This is the solution.

Figure 3: Example of the projection of selected vectors.

4 EXAMPLES OF SOLVING PROBLEMS OF FUEL COMPOSITION DETERMINATION

4.1 Simulation of Process Measurements

Initial data in the form of process measurements were simulated by the results of solving the direct problem for the corresponding substances. Ethanol was chosen as the fuel. The choice of ethanol as a combustible material is justified by the availability of reference data [9] on its combustion process in oxygen (α, T, composition of the CP). This ensures the reliability control of the results in solving the direct problem. Two variants of initial data setting are considered:

The following input data variation ranges were adopted: $\bar{d}_N$ from 0 to 4.95 in steps of 0.05; $\bar{d}_O$, from 0 to 4.95 in steps of 0.05; α from 0.025 to 2.5 in steps of 0.025; I_t from -13500 to 8800 in steps of 100.

Thus, $2.24 \cdot 10^8$ solutions of the direct problem were performed. This took several hours with a

personal computer with the following parameters Intel Core i5-4590 3.3 GHz, 32 GBt RAM, HDD 2 TBt. For each combination of input data, the CP temperatures were calculated and the oxidiser excess coefficients α were recalculated with respect to the oxidiser and propellant volume flow rates $\dot{V}_{ox}/\dot{V}_f$ Part of the combinations of input data turned out to be incompatible, which was revealed during the solution process. After removing these incompatible combinations, a working data array was generated. When using the text format, it required ~2.7 GBt of memory to accommodate it. After conversion to binary form, the volume decreased to 1.2 GBt.

5 DISCUSSION OF THE RESULTS

In the process of forming a working three-dimensional array for the test problem, 10^8 variants of solutions were calculated, which took several hours. At the same time, the gross formula of the fuel included only three chemical elements: C, H and O. The addition of each next element led to an avalanche-like increase in the number of solutions to the direct problem. Thus, it is necessary to consider the limits of applicability of the proposed solution method.

In most cases, the gases whose composition is determined are organic compounds, and their composition can be determined using six chemical elements. In addition to the three discussed above, nitrogen (N), sulphur (S), phosphorus (P) should be considered. All initial data determining the possible composition of a certain gas are represented as one number of normalised values of the initial data (Figure 1). Therefore, increasing the number of chemical elements taken into account (from three to six) will only double the length of these numbers. The required memory required to store the data will increase to 2.4 GBt if they are represented in binary form.

Accounting for each successive chemical element in the gross fuel formula increases the number of solutions by a factor of 100, which also increases the complexity of the model and the duration of individual solutions. When considering this problem, it should be taken into account:

- phosphorus (P) is rarely found in combustible gases and can be excluded from the calculations;
- the amount of nitrogen (N) and sulphur (S) in the fuel gross formula is significantly less than the amount of other elements taken into account.

The range of their possible variation can be reduced while maintaining the same discretisation step.

The result is an increase in the number of solutions and thus the time spent, but not as catastrophic as originally imagined. The impact of hardware, in particular computing speed, also plays a role. Modern personal computers, even household ones , have high computing power compared to the hardware used in the test task. In addition, the solution of a direct problem may be distributed among several computers. The problem can be solved by using the time of a supercomputer in a network.

It is important to note that the solution of the whole set of direct tasks and formation of the working array is performed once at the preliminary stage without time limits. The work can continue for a week or a month. While the solution of the inverse problem, using the formed array, is performed on an ordinary personal computer and takes only a few seconds.

6 CONCLUSIONS

The paper has accomplished the following:

1) In this paper, a general type of problem, characterised as an inverse incorrectly posed problem, was identified and a narrower class of complex interpretation problems was distinguished. In order to solve this class of problems efficiently, a method based on the use of a library and the matching principle was chosen.
2) A method of structured and compactly placing the results of direct problem solving has been developed to populate the library. In its framework:

- a method for converting the oxidant excess coefficient α as the initial data for the direct problem with respect to the volume flow rates of oxidant and fuel is proposed. The obtained value is used as a measurable technological parameter in solving the inverse problem of fuel composition determination;
- a method of transformation of other initial data of the direct problem (number of atoms of chemical elements in the gross formula and enthalpy of fuel) into one number, which is formed on the basis of the positional principle of recording decimal numbers, is proposed.

3) A method for solving the complex problem of data interpretation based on analysing the generated 3D array was developed. This method involves the application of constraints and sequential selection of areas where the data match. By step-by-step reduction of the amount of magnitude analysis, it was possible to achieve a single result in a limited number of steps that corresponds to the solution sought. An important difference between this method and the previously used method of direct enumeration of library data is its ability to effectively reduce the amount of data analysed, ensuring that the solution sought is found accurately and quickly.

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