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CONSTRUCTION OF DISCRETE DYNAMIC MODEL OF PREDICTION OF PARTICULATE MATTER EMISSION INTO THE AIR

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Abstract: Nowadays due to the negative influence of manufacture on the environment, ecological situation in many regions is dangerous. Thus the prediction of the concentration of harmful emissions into the atmosphere is an actual problem. There is a need to build models of processes occurring in complex ecological systems which can be based on historical data and be aimed to detect the influence of different factors on such systems.

The building of a discrete dynamic model of prediction of particulate matter emission into the air is described in this paper. The discrete dynamic model has been developed using the optimization approach on the basis of historical observation data. The parameters of this model are identified by using Rastrigin's method of a director cone.

The results obtained by applying this model are compared with real results. The error of the developed model of prediction is less than 3%.

Key words: mathematical modeling, dynamic discrete model, prediction of emissions, parametric identification.

1. Introduction

Nowadays, the problem of environmental protection is one of the important scientific tasks, which development is rapidly stimulated by the technical progress in all countries worldwide. Rapid development of industry and significant increase in traffic has lead to a thorny issue of preservation of the ecological systems. Over the past decade ecological systems have experienced significant impact of anthropogenic factors. Therefore, the prediction of changes in characteristics of those systems is an actual problem.

Today the ecological situation becomes dangerous due to the negative influence of manufacturing. In particular, it causes the river basins pollution, air and landscapes pollution, destruction of forests, plants, wild animals and fertile soils, groundwater pollution, acoustic, electromagnetic and electrostatic pollution.

For instance, the air is polluted with gas and aerosol wastes (CO_2, polycyclic aromatic hydrocarbons, CO, NO_x, SO_x, ash, soot, etc.). The combustion of liquid and solid fuel causes the emission of solid particles into the Earth atmosphere, where they mix with air and make an aerosol. Aerosols can be non-toxic (ash) and toxic ($C_{20}H_{20}$ – potent carcinogenic compound). Gas emissions can be toxic (NO_2, SO_2, NO, CO) and non-toxic (CO_2, H_2O) as well. All triatomic gases (gases with three atoms per molecule) are considered to be "greenhouse gases". After being emitted into the atmosphere, these gases have a complex physicochemical and biological influence on living organisms including people. The level of this influence depends on the concentration of gases in the air.

Total influence of gas and aerosol emissions from anthropogenic sources can lead to the appearance of different harmful ecological effects. In particular, it can be critical biosphere conditions, for instance: atmosphere deterioration, downfalls and acid rains, greenhouse effect.

That is why a question of predicting the concentration of harmful emissions into the atmosphere is timely and very important for preventing ecological problems and reacting to them properly.

To detect the influence of different factors on complex ecological systems, there is a need to build models of processes occurring in them. Such models can be based on historical data.

The most effective way to solve this problem is to use modern tools of mathematical modeling that would be convenient for computer implementation.

2. Statement of problem

Using discrete dynamic models that were received using optimization approach [1] is one of the promising approaches to modeling. The main advantage of this approach is its versatility concerning both the class of modeled objects and the mathematical presentation of results. This approach can also be easily automated, so it is suitable to the use of computational methods oriented to modern computing devices.

The method for development of non-autonomous discrete dynamical models of systems with zero initial conditions was proposed in [1–2]. This approach allows building of relatively simple and reasonably accurate mathematical models of linear and nonlinear dynamic systems. Zero initial values of variables in such systems are natural. However, there are many technical and economic objects whose way of operation depends on the initial values of their state variables. The examples of such objects are generators, frequency dividers, electrical grids, etc.

Some features of autonomous systems affect the process of their constructing. They are: absence of input influence and taking into account non-zero terms of initial state. Therefore, autonomous mathematical models can be used to predict the behavior of dynamic systems in time.

The system of differential or difference equations of defined order is synthesized in the autonomous system when modeling of dynamic processes is carried out. The solution of such system allows predicting the behavior of the object in regard to given initial conditions. Information that is necessary to identify the parameters of this model is obtained by analyzing the behavior of the object in the past.

Methods introduced in the classical theory of dynamic systems are the most suitable for this kind of modeling. Usually, dynamic processes in such systems are periodic. In economic and ecological systems such periodicity may be conditioned to seasonality (daily, monthly and yearly). In general, the condition of periodicity is not required while using autonomous models for predicting the behavior of objects. However, predictions are short-term when the periodicity is absent.

Let us consider a generalized mathematical model of a system in the form of discrete state-space equations [3]:

$$\begin{cases} \vec{x}^{(k+1)} = \mathbf{F}\vec{x}^{(k)} + \mathbf{G}\vec{v}^{(k)} + \vec{\Phi}\left(\vec{x}^{(k)}, \vec{v}^{(k)}\right) \\ \vec{y}^{(k+1)} = \mathbf{C}\vec{x}^{(k+1)} + \mathbf{D}\vec{v}^{(k+1)} \end{cases} \quad (1)$$

where $\vec{x}^{(k)}$ is a vector of state variables that characterizes the current state of the object; $\vec{v}^{(k)}$ is a vector of input values; $\vec{y}^{(k)}$ is a vector of output values; F, G, C, D are matrices with unknown coefficients, which have to be found when the model is being built; $\Phi(\vec{x}^{(k)}, \vec{v}^{(k)})$ is some nonlinear vector-function with many variables, whose form and coefficients also have to be found.

The autonomous discrete mathematical model looks as follows:

$$\begin{cases} \vec{x}^{(k+1)} = F\vec{x}^{(k)} + \Phi\left(\vec{x}^{(k)}\right) \\ \vec{y}^{(k+1)} = C\vec{x}^{(k+1)} \end{cases}. \quad (2)$$

This form of the model, that is, the equation of the system (1), is characterized by some set of unknown parameters $\vec{l}$. For a particular model this vector consists of elements of the matrices F, C and coefficients of the vector function $\Phi(\vec{x}^{(k)})$.

The approach to building the mathematical model used in [5–6] provides the optimization which takes the form of minimization of the deviation of model behavior from the behavior of the object, that is, the minimization of some objective function Q. This function may display not only the accuracy of simulation of the system behavior, but it may also consider some characteristics of the model, for example, its complexity. As a rule, the objective function is the standard deviation of the model behavior from the behavior of the object:

$$Q(\vec{l}) = \sum_k |\vec{y} - \vec{y}'|^2,$$

where $\vec{l}$ is a vector of unknown quantities (arguments of the problem of optimization) which characterize the structure and parameters of the macromodel; $\vec{y}$ are transient responses (i.e. output values) which are calculated using the model; $\vec{y}'$ are known characteristics of the object.

In this approach the process of building of the model is reduced to finding the value of the vector $\vec{l}$ at which the function Q is be minimal. Thus, the problem of building of the model is reduced to the search for a minimum of the function which is used as a basis for determining the vector of unknown parameters $\vec{l}$.

This approach can significantly generalize the proposed solution. However, this generalization requires the application of complex optimization procedures, which are difficult to implement even using modern computer technologies.

The problem of finding the minimum of a nonlinear function with many variables that is not described analytically is quite a difficult task. In the process of building the discrete dynamic models, the objective function becomes a “ravine” function with many local minima.

Optimization methods based on Rastrigin’s method of a director cone are considered to be the best for solving those tasks [2, 4]. Purposeful scan of local minima can be done by this approach. It accelerates the process of finding a global minimum of the objective function. However, the considerable computational complexity of this problem should be taken into account. Also, the significant number of a priori data is used for the building of the qualitative model. Therefore, computer time necessary for the implementation of optimization procedures is also significant.

3. Building of discrete dynamic model of prediction of particulate matter emissions

Ecological systems can be characterized by seasonality. The most important tasks which have to be solved during the investigation of seasonality are:

1. detecting the presence of seasonality and obtaining the numerical expression of season oscillations; finding out their strength and character in different phases of the year cycle;
2. determining the factors which cause the season oscillations;

3. estimating the consequences which cause season oscillations;

4. mathematical modeling of seasonality: in order to built the strict model of ecological system the presence of seasonality should be considered. It means that the analysis of data obtained during last weeks, months and years should be done.

In general, the seasonality condition is not obvious regarding the use of autonomous models for the prediction of objects behavior. However, when it is omitted, the forecasts are mostly short-term.

Let us consider the problem of predicting the harmful emissions to illustrate the proposed method of the building of dynamic discrete autonomous models. Particulate matter, also known as particle pollution or PM, is a complex mixture of extremely small particles and liquid droplets. Particle pollution is made up of a number of components, including acids and salts (such as nitrates and sulfates), organic chemicals, metals and soil or dust particles. Those are the particles that generally pass through the throat and nose and enter the lungs. Being inhaled, these particles can affect the heart and lungs and cause serious health effects [5].

The data for our research have been taken from the site [6]. Those are the pollutant concentrations obtained in the system of automatic monitoring stations, including results for the current state of air quality and the results of manual and automated measurements. The data were collected from 18 automated stations in Silesia region (Poland).

Monthly indicators of PM_{10} (particulate matter) emissions into the atmosphere in the city of Katowice (Poland) collected for three years (from January 2009 to December 2011) are known. According to these data, a mathematical model is to be built that would allow predicting monthly emissions of PM_{10} into the air in the future years.

Fig. 1. Location of automated stations which perform ecological monitoring.

To build a linear model the Kozak algorithm [7, 8] is used. At this stage, the main task is to find the matrix **F**. This matrix reflects the qualitative behavior of the model. The procedure of finding this matrix is quite laborious, because, as it is mentioned above, the objecttive function is multiextremal. Rastrigin's method of a director cone with options for adaptation of the search parameters is used for the optimization [7].

The series of models from the first to the ninth order has been built. It is done in order to determine the number of state variables at which the model is the most adequate. The least error of the forecasting has been received with the help of the ninth-order model.

Based on the set of experimental data, the following model has been obtained:

$$\begin{cases} \vec{x}^{(k+1)} = F\vec{x}^{(k)} \\ \vec{y}^{(k+1)} = C\vec{x}^{(k+1)} \end{cases}, \qquad (3)$$

where

$$F = \begin{pmatrix} -0,54 & -0,10 & 0,28 & 0,01 & 0,02 & 0,01 & -0,01 & 0,02 & -0,19 \\ 2,62 & 0,85 & -1,61 & -0,13 & -0,13 & -0,24 & 0,12 & 1,43 & -0,29 \\ -0,26 & 0,10 & -0,11 & 0,01 & 0,21 & -0,02 & -0,01 & 1,89 & 0,05 \\ 14,47 & -0,95 & -3,04 & 0,10 & -268 & -1,13 & -0,03 & 8,53 & -2,88 \\ -0,46 & 0,27 & 0,95 & -0,07 & 0,69 & 0,09 & 0,04 & 4,12 & 0,04 \\ -2,87 & -0,39 & -0,02 & 0,12 & -0,18 & 0,53 & 0,01 & -1,09 & -0,33 \\ -0,72 & 0,36 & -1,55 & 1,02 & 1,59 & -0,52 & 0,07 & 26,12 & 0,02 \\ -0,54 & -0,02 & -0,29 & 0,01 & -0,11 & 0,078 & -0,02 & -0,03 & -0,02 \\ -3,09 & -0,13 & -0,08 & -0,01 & 0,05 & -0,53 & -0,01 & 1,21 & 0,37 \end{pmatrix},$$

$$C = \begin{pmatrix} 0,01 & 3,66 & 0,01 & -1,79 & 9,89 & 0,01 & -4,58 & 0,01 & -6,16 \end{pmatrix},$$

$$k = 0,...,36.$$

Analysis of the system of discrete equations (3) shows that this model does not represent sharp jumps of output value at the initial time.

The next step in building the mathematical model is introducing a nonlinear function $\Phi(\vec{x}^{(k)})$ to the linear model, thus making it a nonlinear one:

$$\vec{\Phi}(\vec{x}^{(k)}) = \begin{cases} a_1 x_1^2 + a_2 x_1^3 \\ a_3 x_2^2 + a_4 x_2^3 \end{cases}.$$

The value $\vec{x}^{(0)}$ for prediction years 2012, 2013, and 2014 is determined by the following approach: nine months of the year 2012 are used for determining $\vec{x}^{(0)}$, because the vector $\vec{x}^{(0)}$ consists of nine components. After solving the system of equations (2), we obtain the values of the initial vector of state variables as follows:

$$\vec{x}^{(0)} = [-105677{,}41 \quad -17811{,}38 \quad 77203{,}99 \quad 6204479{,}03 \quad 251329{,}79 \quad -36408{,}32 \quad 1118247{,}57 \quad -4668{,}03 \quad 244512{,}39]$$

For comparison, the real data on emissions of particulate matter into the air and the data obtained with the use of the developed model are presented in Fig. 2.

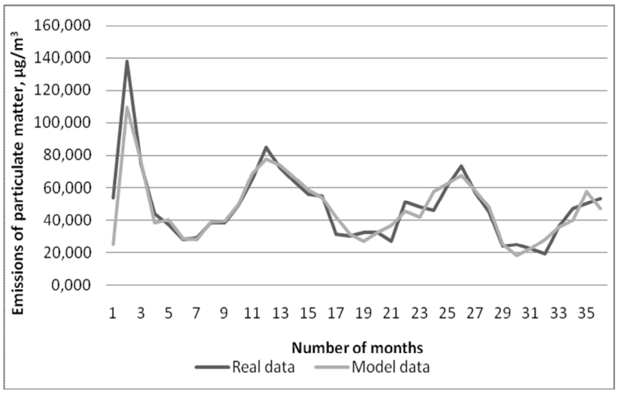

Fig. 2. Real and predicted monthly emissions of particulate matter in Katowice.

The error of the developed model is determined by the formula:

$$e = 1/n \sqrt{\sum_{k=1}^{n} \left((y^{(k)} - y^{*(k)}) / y^{(k)} \right)^2} \cdot 100\ \%,$$

where $y^{(k)}$ is the real value of the k-th discrete of the transient response, $y^{*(k)}$ is the modeled value of the k-th discrete; n is the number of discrete values of the modeled transient response.

The error of the model prediction calculated on the basis of the experimental data is of 2.95 %.

As follows, building of mathematical models with the use of optimization has features associated with the lack or insufficiency of input values, and output variables are functions, whose character is determined only by the initial state of the system. This leads to the necessary changes in the procedure of building the model and algorithm optimization.

Using these features, an autonomous model of emissions of particulate matter in the air in the city of Katowice has been built on the basis of historical observations. The error of the prediction made by the developed model is low. Thus, the optimization approach is suitable for constructing mathematical models of autonomous objects and can be successfully used in practice.

4. Conclusion

The process of the building of the discrete dynamic model for predicting particulate matter in the air is shown in this article. Rastrigin's method of a director cone is used for the optimization of parameters of the autonomous model. The results obtained by using the model are compared with the experimental results.

References

[1] P. Stakhiv and Y. Kozak, "Building of macro-models of electromechanical components using optimization", *Technical electrodynamics*, no. 4. pp. 33–36, Kyiv, Ukraine: Institute of Electrodynamics of Ukraine, 2001. (Ukrainian)

[2] P. Stakhiv, Y. Kozak, and O. Hoholyuk, *Discrete macro modeling in electrical engineering and related fields*. Lviv, Ukraine: Lviv Polytechnic, 2014. (Ukrainian)

[3] L. Zade and Ch. Dezoer, *The theory of linear systems. The method of state space*. Moscow, Russia: Nauka, 1970. (Russian)

[4] L. Rastrigin, *Adaptation of complex systems*. Riga, Latvia: Zinatne, 1981. (Russian)

[5] "Particulate Matter, Air & Radiation", *http://www3.-epa.gov/pm/*

[6] "Śląski Monitoring Powietrza", *http://monitoring.-katowice.wios.gov.pl/* (Polish)

[7] P. Stakhiv, Y. Kozak, and Y. Selepyna, "Improving of the optimization algorithm to identify parameters of macro-models of electromechanical systems", *Bulletin of Lviv Polytechnic National University*, p. 98–102, Lviv, Ukraine, 2010. (Ukrainian)

[8] P. Stakhiv and Y. Kozak, "Modification of the method of Rastryhin's cone", *Selection and Processing of Information*, vol. 92, no. 16, pp. 39–42, 2002.

ПОБУДОВА ДИСКРЕТНОЇ ДИНАМІЧНОЇ МОДЕЛІ ПРОГНОЗУВАННЯ ВИКИДІВ ТВЕРДИХ ЧАСТИНОК У ПОВІТРІ

Ірина Струбицька

Сьогодні через негативний вплив виробництва на довкілля екологічна ситуація у багатьох регіонах є небезпечною. Саме тому передбачення концентрації шкідливих викидів у атмосферу є актуальною проблемою.

Існує потреба у побудові моделей процесів, що виникають у складних екологічних системах, які можуть базуватись на історичних даних та мати за мету визначення впливу різних факторів на такі системи.

У статті описано побудову дискретної динамічної моделі передбачення емісії твердих частинок у повітря. Дискретну динамічну модель було побудовано з використанням методу оптимізації на основі історичних даних. Параметри цієї моделі визначено за допомогою методу скеровуючого конуса Растрігіна.

Результати, отримані за допомогою цієї моделі, порівнюються із реальними результатами. Похибка розробленої моделі є меншою від 3 %.

Iryna Strubytska – Ph.D. in Mathematical Modelling and Computing Methods received from Lviv Polytechnic National University, Lviv, Ukraine (2013). Currently, she is a lecturer of the Computer Science Department at Ternopil National Economic University, Ukraine. Her research interests are focused on mathematical modelling, parametric identification, optimization methods, parallel calculations.