Multi-objective Dynamical System Parameters and Initial Value Identification Approach in Chemical Disintegration Reaction Modelling

Ivan Ryzhikov, Christina Brester and Eugene Semenkin
Institute of Computer Sciences and Telecommunication, Siberian State Aerospace University, Krasnoyarsk, Russia

Keywords: Multi-output System, Linear Differential Equation, Multi-objective Optimization, Parameters Identification, Initial Value Estimation.

Abstract: A multi-criteria multi-output dynamical system identification problem is considered. The inverse mathematical problem of estimating the parameters of a system of differential equations and its initial point using the measured data is provided for the hexadecane disintegration reaction. The aim of modelling is to approximate the dynamical behaviour of hexadecane and the concentrations of its products, which according to chemical kinetics are determined by a differential equation. Since the dynamical model adequacy is based on the error between its output and the sample data and the output itself depends on the initial point values, the inverse mathematical modelling problem is the simultaneous estimation of the model parameters and the initial point. At the same time, the initial point is unknown and the sample data is noisy, and for this reason, the inverse mathematical modelling problem is reduced to a two-objective optimization problem. The reduced problem is a sample of black-box optimization problems; it is complex, multimodal and requires a reliable technique to solve it. This is why a specific heterogeneous multi-objective genetic algorithm with the island meta-heuristic is used and its efficiency in solving this problem is proved by the investigation results.

1 INTRODUCTION

The inverse mathematical modelling problem for dynamical systems is a problem of current importance. It has many applications in different scientific fields, including chemistry, robotics, mechanics, information science, biology and financial mathematics. There are many different problem statements and most of them are solved by finding the solution of the reduced optimization problem. In general, these optimization problems are so-called black-box optimization problems and, in this case, the model determination using a set of parameters and the extremum seeking algorithm are the most important objects to develop and improve.

In this study, we consider a multi-output system without any control input, but with the vector on the right-hand side for the process of hexadecane disintegration. The proposed approach is applicable to a linear dynamical system with many control inputs, but in this study, the investigated systems have no control inputs and so these inputs were set as unit-step functions. Our aim is to build a mathematical model of the hexadecane and the functions of its disintegration product concentrations, which would give the information about the amount of acids at different time points in the process. Two different process types were considered: diffusion and static, and for each type different disintegration reaction products were considered.

The problem of estimating the parameters of the differential equation using evolutionary, stochastic and other heuristic approaches can be found in many studies. Commonly, evolution-based and nature-inspired algorithms are reliable solvers of reduced optimization problems of different natures. Single-objective and multi-objective optimization problems appear in estimating the parameters of dynamical systems in many different studies. Methods of solving the parameter identification problem with heuristic algorithms of these classes can be found in many different studies.

There is a significant difference between solving one-criterion and multi-objective optimization

Ryzhikov, I., Brester, C. and Semenkin, E.
Multi-objective Dynamical System Parameters and Initial Value Identification Approach in Chemical Disintegration Reaction Modelling.
DOI: 10.5220/0006431504970504
In *Proceedings of the 14th International Conference on Informatics in Control, Automation and Robotics (ICINCO 2017) - Volume 1*, pages 497-504
ISBN: 978-989-758-263-9

problems and a significant difference in the solution of the optimization problem. For the multi-objective optimization problem, an approximation of the Pareto front is required, or, in other words, the set of non-dominated solutions. The reason why we need to reduce the inverse mathematical modelling problem to a multi-objective optimization problem is the impossibility of estimating the system parameters without its initial value for dynamical systems.

The current study is based on the works described in (Ryzhikov and Semenkin, 2017) and (Ryzhikov et al., 2016), where the initial point and the system coefficients were estimated by solving the optimization problem, but for a single criterion. The approach proposed in this study is an extension of previous ones and allows different initial value estimations to be used. Because of the sample size, which is small, the initial value was compared with the first measurements in the sample, but in a general case, it can be compared with some average value, its statistical estimation or some expected value given by an expert, which makes the proposed approach flexible and useful.

It is widely known that each particular problem requires specific problem-oriented optimization algorithm modifications or meta-heuristics, which provide an improvement in the algorithm performance. In this study, we propose a dynamical system and initial value vector determination, and form an unconstrained extremum problem on a real value vector field.

In our consideration of the multi-objective optimization problem, there is a need for a reliable multi-objective optimization tool. The multi-criteria cooperative heterogeneous genetic algorithm with the island meta-heuristic has been chosen, because this algorithm has proved its performance in the solving of many multi-criteria optimization problems of different natures. Experimental results, which are presented in various figures, show that this algorithm is applicable to the considered problem and achieves a very good result.

2 MULTI-OUTPUT DYNAMICAL SYSTEM IDENTIFICATION PROBLEM

In this chapter, we consider the problem statement and related real problem. The hexadecane disintegration reaction consists in the forming of different components: spirits, carbonyl components, lactones and acids for the diffusion reaction and spirits and carbonyl compounds for the static reaction. We assume that the concentrations of products and the hexadecane itself are related and affect one another. The influence of each disintegration reaction component concentration on other component concentrations can be mathematically determined by the addition of some coefficient to the particular equation. The process of how the concentration changes is dynamical and linear, and in this case it is also assumed in chemical kinetics theory that the concentrations can be determined with a linear differential equation of the first order.

Let a set $\{Y_i, t_i\}, i = \overline{1,s}$, be a data sample, where $Y_i \in R^n$ is the dynamical system output measurements at the time point t_i, s is the size of the sample and n is the system output dimension. As was mentioned above, the solution of the inverse mathematical problem is a differential equation and the initial point, so we assume that the real system output $X(t) = (x_1(t) \quad ... \quad x_n(t))$ is determined by the Cauchy problem:

$$\begin{gathered} x_1'(t) = a_{1,1} \cdot x_1(t) + \ldots + a_{1,n} \cdot x_n(t) + b_1, \\ \ldots, \\ x_n'(t) = a_{n,1} \cdot x_1(t) + \ldots + a_{n,n} \cdot x_n(t) + b_n \\ X(0) = (x_1^0 \quad ... \quad x_5^0)^T. \end{gathered} \tag{1}$$

where $a_{i,j}, i = j = \overline{1,n}$ are the system coefficients and $x(0)$ is the initial point. The system parameters and the initial point coordinates, generally, are unknown and to be estimated.

We use the following notation for the concentration functions of the chemical reaction products: hexadecane, spirits, carbonyl compounds, lactones and acids and similar notation for the static chemical reaction.

We also know that the output data $Y_i, i = \overline{1,s}$ is distorted by the additive noise $\xi : E(\xi) = 0, D(\xi) < \infty$:

$$Y_i = X(t_i) + \xi_i, i = \overline{1,s}. \tag{2}$$

where the $X(t)$ function is a solution of the Cauchy problem (1).

Let the model be determined by the given problem: a differential equation in a matrix form and the initial value vector (we know the number of system outputs n)

$$\begin{aligned} &\frac{d\hat{X}}{dt} = \hat{A}\cdot\hat{X}(t)+\hat{B}, \\ &\hat{X}(0) = \left(\hat{x}_1(0) \quad \ldots \quad \hat{x}_n(0)\right), \end{aligned} \tag{3}$$

where $\hat{A}$ is a system matrix, $\hat{B}$ is a vector of coefficients and $\hat{X}(0)$ is an initial point.

It can be seen that the solving of the inverse mathematical modelling problem is related to the parameters and initial point estimation problems on the basis of the sample data, which consists of noisy output measurements. Moreover, the sample size for some particular problems is small and the sample data is flat. These data characteristics make many estimation approaches useless, and require specific tools, which would provide the simultaneous estimation of the parameters and the initial point. Since there is a cross influence between the parameters and the initial point, but at the same time the values of these variables are estimated and based on the sample data, we require not just a criterion, which minimizes the error between the data and the model output, but also a number of criteria.

One of the proposed criteria is the distance between the sample data and the model output

$$C_1 = \sum_{i=1}^{s}\sum_{j=1}^{n}\frac{\left\|(Y_i)_j - \hat{X}_j(t_i)\right\|}{D_j} \to \min_{\hat{A},\hat{B},\hat{X}(0)}, \tag{4}$$

where $\hat{X}(t)$ is the solution of the Cauchy problem (3) for matrix $\hat{A}$, vector $\hat{B}$ and $D_j, j=\overline{1,n}$ is a proposed norming value $D_j = \max_i\left((Y_i)_j\right) - \min_i\left((Y_i)_j\right)$.

The second criterion is the distance between the initial point estimation and the sample

$$C_2 = \left\|Y_0 - \hat{X}(0)\right\| \to \min_{\hat{X}(0)}. \tag{5}$$

The concentrations according to the physical meaning of this term cannot be negative; to achieve this, we add the penalty function into the criterion (4) and criterion (5) with some penalty coefficients. The penalty function is defined by the expression

$$P(z) = \begin{cases} |z|, z<0 \\ 0, z\geq 0 \end{cases}. \tag{6}$$

Finally, we receive the following criteria for the multi-objective optimization problem (4), (5) and (6)

$$\hat{C}_1 = C_1 + c_P^1\cdot\sum_{i=1}^{s}\sum_{j=1}^{n}P\left(\hat{X}_j(t_i)\right) \to \min_{\hat{A},\hat{B},\hat{X}(0)}, \tag{7}$$

$$\hat{C}_2 = C_2 + c_P^2\cdot\sum_{j=1}^{n}P\left(\hat{X}_j(0)\right) \to \min_{\hat{X}(0)}, \tag{8}$$

where $c_P^1, c_P^2 > 0$ are the penalty function coefficients. In the current study, these coefficients were equal to $c_P^1, c_P^2 = 1000$ The current model determination leads to an optimization problem in the $R^{n\times n}\times R^n\times R^n$ field. By determining the problem in this way, the model can be represented with a vector from this field. As can be seen, the problem dimension adds extra complexity to the identification problem.

In this study, the Cauchy problem (3) is solved numerically using the Runge-Kutta integration scheme, which makes the designed approach flexible and useful for nonlinear or nonstationary systems with a known symbolic form but unknown parameters or different input functions.

Now we consider the multi-objective optimization tool, which has been designed to find a solution for complex black-box optimization problems. The proposed algorithm consists of some stochastic and evolution search operators and meta-heuristics. The fitness function is performed on the basis of criteria

$$\begin{aligned} fit_1(a) &= \frac{1}{1+\hat{C}_1\left(a\to\arg\left(\hat{C}_1\right)\right)}, \\ fit_2(a) &= \frac{1}{1+\hat{C}_2\left(a\to\arg\left(\hat{C}_2\right)\right)}, \end{aligned} \tag{9}$$

where $x\to\arg(I)$ is a specific transformation of an alternative x to the arguments of a criterion I. This transformation decodes the individual vector coordinates into matrix coefficients, right-side vector coefficients and into the initial point in the case of the $\hat{C}_1$ criterion. For the $\hat{C}_2$ criterion, it converts the solution vector into the initial point.

3 MULTI-OBJECTIVE COOPERATIVE GENETIC ALGORITHM WITH THE ISLAND META-HEURISTIC

While solving multi-objective optimization problems, we tend to reach a trade-off between competing criteria. The Pareto-dominance idea (Goldberg, 1989) underlies the way we may

compare alternative solutions. As a result, we expect to obtain a set of non-dominated points which cannot be preferred to one another based on all the criteria considered.

Population-based algorithms (in particular, genetic algorithms) operate with a number of candidate-solutions at each generation, and therefore, it was decided to use them as an effective tool to find Pareto set and front approximations. However, there are some open questions researchers usually encounter when they apply multi-objective genetic algorithms (MOGAs) in real problems. Whether choosing one of the existing MOGAs or designing a new one, researches should elaborate three main concepts which are incorporated into the scheme of any MOGA and opt for the most appropriate implementation of each concept for the problem being solved. Firstly, various fitness assignment strategies might be proposed (Zitzler, 2004): the dominance rank (the number of points by which the candidate-solution is dominated), the dominance depth (a population is divided into several fronts or niches and it is determined which front an individual belongs to), or the dominance count (the number of points dominated by the candidate-solution) might be used to assign a fitness function.

Secondly, to keep variety within the Pareto set and front approximations, diversity preservation techniques are applied. In (Silverman, 1986) several variants of these techniques are presented: kernel methods assess the density with a Kernel function which takes the distance to another point as an argument; nearest neighbour techniques are based on estimating the distance between a given point and its *k*-th nearest neighbour; and histograms, using a hypergrid to calculate neighbourhoods, relate to another class of density estimators. In most cases, these approaches calculate the distance between points in the objective space.

Moreover, to avoid the loss of effective individuals during the algorithm execution due to stochastic effects, the idea of elitism has been suggested. There are two basic ways to implement it. The first way is to merge the parent population with the offspring and then to employ environmental selection taking into account the fitness values of individuals from the mating pool. Another variant is based on the usage of an additional set called an archive for copying promising solutions at each generation.

Thinking about these issues, in this study we decided to apply a cooperative MOGA (Brester et al., 2015) which combines three algorithms based on different heuristics. The use of the cooperative MOGA allows us to eliminate the choice of the most effective algorithm and avoid multiple experiments with many different MOGAs. The cooperative MOGA uses an island model (Whitley et al., 1997) and includes NSGA-II (Non-Sorting Genetic Algorithm II) (Deb et al., 2002), PICEA-g (Preference-Inspired Co-Evolutionary Algorithm with goal vectors) (Wang, 2013), and SPEA2 (Strength Pareto Evolutionary Algorithm 2) (Zitzler et al., 2002) as its islands work in a parallel way (Figure 1).

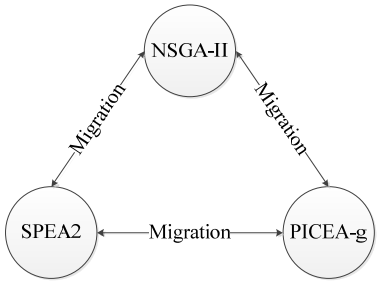

Figure 1: The Island Model Implemented.

The initial number of individuals M is spread across L subpopulations: $M_i=M/L,\ i=1,\ldots,L$ and the same number L of threads is initialized. Thus, the fitness function evaluation for different subpopulations is implemented in parallel threads. At each T-th generation algorithms exchange the best solutions (migration). There are two parameters: migration size, the number of candidates for migration, and migration interval, the number of generations between migrations. Moreover, it is necessary to define the island model topology, in other words, the scheme of migration. The fully connected topology is used, meaning that each algorithm shares its best solutions with all other algorithms included in the island model. The multi-agent model is expected to preserve a higher level of genetic diversity. The benefits of the particular algorithm are advantageous in different stages of optimization.

The cooperative MOGA was investigated on the set of complex benchmark problems CEC 2009 (Zhang, 2008) and proved its effectiveness. It also was applied in a wide range of practical problems: emotion recognition from speech (for feature selection and neural-network design) (Brester et al., 2016), the prediction of cardiovascular diseases (for feature selection) (Brester et al., 2016), and spacecraft control (for the choice of control contour variant by solving an optimization problem) (Semenkina et al., 2016).

4 HEXADECANE DISINTEGRATION REACTION PRODUCT CONCENTRATION MODELLING

To solve the problem we chose the following algorithm resources: 3 different populations with 200 individuals and 500 generations, the migration size was equal to 25, the migration interval was 50. The number 300000 limited the total amount of the fitness function evaluations. After 25 algorithm runs we selected some solutions to be demonstrated. From the whole Pareto front estimation, we selected the model with the highest first criterion value $\hat{X}^{C_1}$, second criterion value $\hat{X}^{C_2}$ and the one model with the values in between $\hat{X}^*$. All the models are presented in the same Figures: the first model is a long dashed curve, the second is a short dashed curve and the last one is a dotted curve. The measurements are marked with grey crosses on the plot.

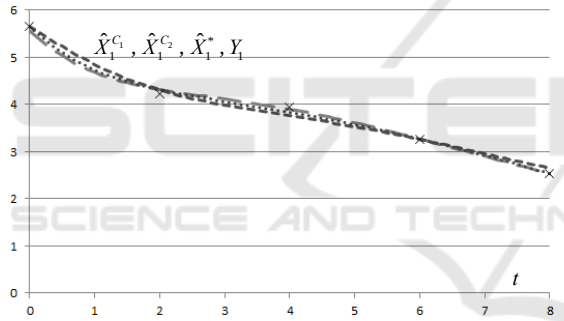

Figure 2: Hexadecane concentration: model outputs and sample measurements.

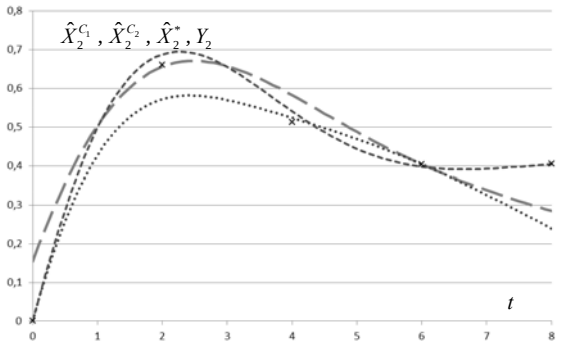

Figure 3: Spirit concentration: model outputs and sample measurements.

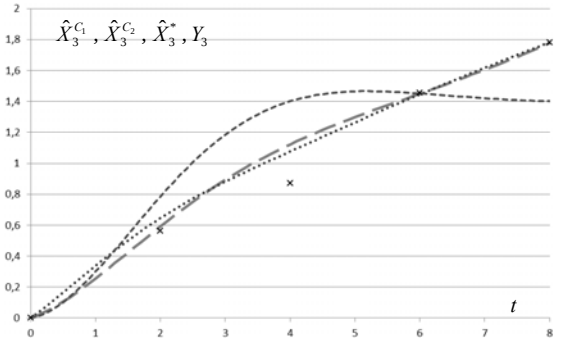

Figure 4: Concentration of carbonyl compounds: model outputs and sample measurements.

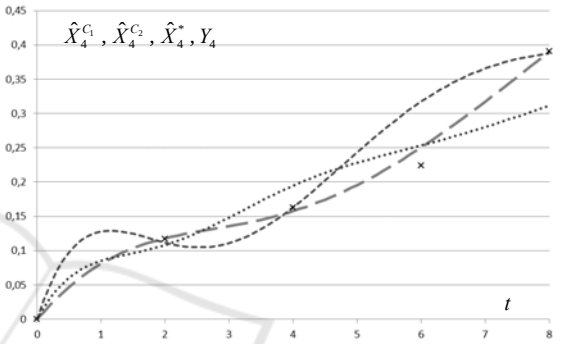

Figure 5: Lactone concentration: model outputs and sample measurements.

In Figure 2, Figure 3, Figure 4, Figure 5 and Figure 6 the hexadecane concentration, spirits, carbonyl compounds, lactones and acids are presented, respectively.

If we compare the initial value and the measured initial value, it can be seen that the model that fits the data sample better has the highest inaccuracy in the initial value. At the same time, the model with the highest value of the second criterion does not fit the sample data as well as other models.

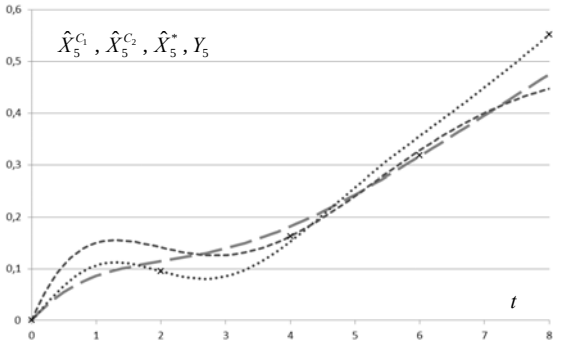

Figure 6: Acid concentration model outputs and their measurements.

In Figure 7 the Pareto front estimation obtained by multiple algorithm runs is given. In the same Figure, the solution found in one algorithm run is marked with grey points.

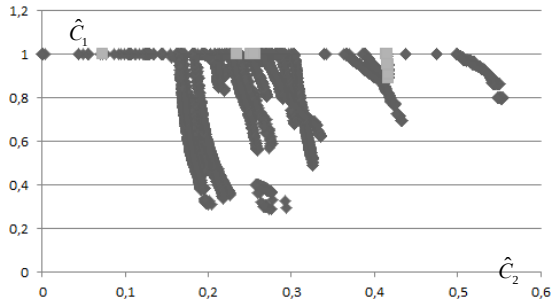

Figure 7: Pareto front estimations for each run (black) and a single run Pareto front estimation (grey).

We see that the Pareto front estimation is a very difficult problem, which is why there is a very complicated relation between the closeness to the initial point estimation and how well it fits the sample data. This means that there is a necessity to solve the inverse mathematical problem as an optimization problem with two criteria.

The same problem was solved for another chemical experiment with different reaction characteristics. In this case it was necessary to build a model for only three outputs: hexadecane concentration, spirit concentration, and carbonyl compound concentration. For this problem we also took three different solutions from the Pareto front estimation in a similar way to how it was performed above.

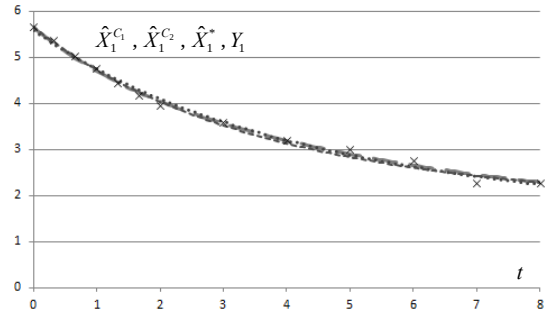

Figure 8: Hexadecane concentration: model outputs and sample measurements.

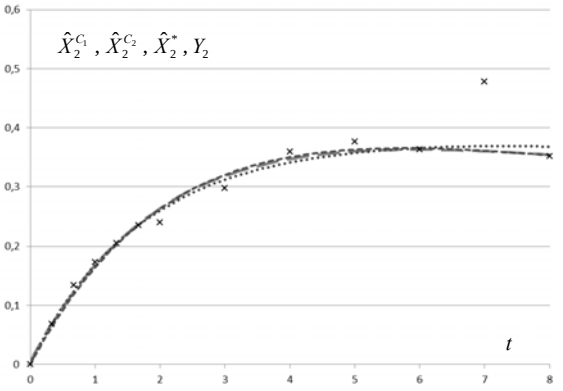

Figure 9: Spirit concentration: model outputs and sample measurements.

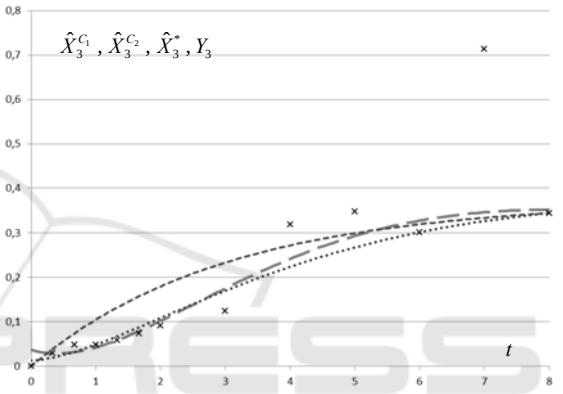

Figure 10: Concentration of carbonyl compounds: model outputs and sample measurements.

As can be seen for the second problem, there is an abnormal measurement. However, the model “ignores” this measurement and fits the sample data. We can conclude that the second problem is easier, since the models do not differ as much as they did in the case above. Also, the Pareto front estimation proves this hypothesis; the estimation is given in Figure 11.

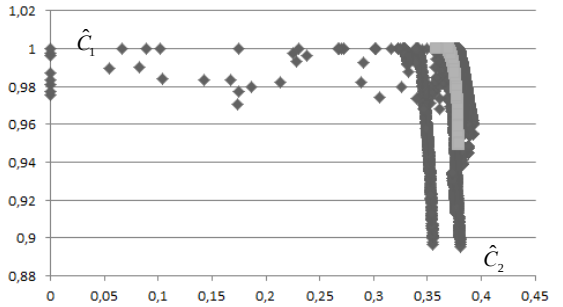

Figure 11: Pareto front estimations for each run (black) and a single run Pareto front estimation (grey).

The last Figure gives us the same information as Figure 7 but for the current problem. It is easier to estimate the Pareto front since many points are localized near the same curve.

4 CONCLUSION

The experimental results of this study prove that the proposed approach is useful in solving inverse mathematical problems for dynamical systems in cases when the initial point and the noisy sample data are unknown. Using this approach, many models of hexadecane disintegration reaction product concentrations were build. It was demonstrated that these models fit the observation data well and behave normally.

In this paper, the multi-output dynamical system identification problem was solved by means of the multi-objective heterogeneous genetic algorithm with the island meta-heuristic. The results prove the high efficiency of the algorithm used and the applicability of the proposed approach, which allows us to solve the inverse mathematical modelling problem in the case of having no information about the initial point value and satisfy the trajectory constraints.

It can be seen that the model output fits the sample data well and represents the physical properties of the process. The multi-objective problem reduction allows us to receive the Pareto front estimation on the basis of estimations of the initial point and system parameters, so the expert can vary the degree of belief in the initial point values and choose the mathematical model that would satisfy his modelling needs. Moreover, the proposed two-criterion approach allows mathematical models to be found, the parameters and initial value characteristics of which can contradict. As can be seen in Figures 7 and 11, different problems have different Pareto fronts, but the criteria have a complex relation and so they cannot be represented as a single one.

The considered sample data has a small size, which makes it impossible to apply statistical methods for the initial value estimation or apply some other identification techniques based on approximating the model output as a static function. This is the reason why the differential equation based models are the most important part of modelling the dynamical processes and so it is important to develop the algorithms for the equation parameter identification.

Further work is related to the inverse mathematical problem solving for multi-output dynamical systems of higher order and control inputs. Another direction is the developing of heuristic optimization tools for the single and multi-criteria problems of dynamical system identification, and designing problem-oriented modifications.

ACKNOWLEDGEMENTS

This research is supported by the Russian Foundation for Basic Research within project No 16-01-00767.

REFERENCES

Brester, C., Kauhanen, J., Tuomainen, T.P., Semenkin, E., Kolehmainen, M., 2016. Comparison of two-criterion evolutionary filtering techniques in cardiovascular predictive modelling. *Proceedings of the 13th International Conference on Informatics in Control, Automation and Robotics (ICINCO'2016)*, Lisbon, Portugal, vol. 1: pp. 140–145.

Brester, C., Semenkin, E., 2015. Cooperative Multiobjective Genetic Algorithm with Parallel Implementation. *Advances in Swarm and Computational Intelligence*, LNCS 9140: pp. 471–478.

Brester, C., Semenkin, E., Sidorov, M., 2016. Multi-objective heuristic feature selection for speech-based multilingual emotion recognition. Journal of Artificial Intelligence and Soft Computing Research, vol. 6, no. 4: pp. 243-253.

Deb, K., Pratap, A., Agarwal, S., Meyarivan, T., 2002. A fast and elitist multiobjective genetic algorithm: NSGA-II. *IEEE Transactions on Evolutionary Computation* 6 (2): pp. 182-197.

Goldberg, D., 1989. Genetic algorithms in search, optimization, and machine learning. *Addison-wesley*.

Ryzhikov, I., Semenkin, E., 2017. Restart Operator Meta-heuristics for a Problem-Oriented Evolutionary Strategies Algorithm in Inverse Mathematical MISO Modelling Problem Solving. *IOP Conference Series: Materials Science and Engineering*, vol. 173.

Ryzhikov, I., Semenkin, E., Panfilov, I., 2016. Evolutionary Optimization Algorithms for Differential Equation Parameters, Initial Value and Order Identification. ICINCO (1) 2016: pp. 168-176.

Semenkina, M., Akhmedova, Sh., Brester, C., Semenkin, E., 2016. Choice of spacecraft control contour variant with self-configuring stochastic algorithms of multi-criteria optimization. *Proceedings of the 13th International Conference on Informatics in Control, Automation and Robotics (ICINCO'2016)*, Lisbon, Portugal, vol. 1: pp. 281–286.

Silverman, B., 1986. Density estimation for statistics and data analysis. *Chapman and Hall*, London.

Wang, R., 2013. Preference-Inspired Co-evolutionary Algorithms. A thesis submitted in partial fulfillment for the degree of the Doctor of Philosophy, University of Sheffield: p. 231.

Whitley, D., Rana, S., and Heckendorn, R., 1997. Island model genetic algorithms and linearly separable problems. *Proceedings of AISB Workshop on Evolutionary Computation*, vol.1305 of LNCS: pp. 109-125.

Zhang, Q., Zhou, A., Zhao, S., Suganthan, P. N., Liu, W., Tiwari, S., 2008. Multi-objective optimization test instances for the CEC 2009 special session and competition. University of Essex and Nanyang Technological University, Tech. Rep. CES–487, 2008.

Zitzler, E., Laumanns, M., Bleuler, S., 2004. A Tutorial on Evolutionary Multiobjective Optimization. In: Gandibleux X., (eds.): *Metaheuristics for Multiobjective Optimisation. Lecture Notes in Economics and Mathematical Systems, Vol. 535*, Springer.

Zitzler, E., Laumanns, M., Thiele, L., 2002. SPEA2: Improving the Strength Pareto Evolutionary Algorithm for Multiobjective Optimization. *Evolutionary Methods for Design Optimisation and Control with Application to Industrial Problems EUROGEN* 2001 3242 (103): pp. 95-100.