Iterative-connectionist identification of mathematical models of chemical technology processes

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Abstract
There suggested combined iterative-connectionist intellectual method of identification of complex mathematical models of chemical technology processes, which allows to minimize search time for adjusting coefficients using neural network for reduction of number of steps of searching iterative algorithms at different stages of identification. Developed combined algorithm may be used for identification of mathematical models in the systems of optimal control of chemical technology processes.
Key words: CONTROL SYSTEM, MATHEMATICAL MODEL, IDENTIFICATION, ADJUSTING COEFFICIENT, ARTIFICIAL NEURAL NETWORK
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Introduction, problem statement

Continuous improvement of computer equipment and increase of computational capability of microcontrollers allows to use complex mathematical models in modern control systems of chemical technology processes. These models the most accurately describe the process and specificity of its flow. Herein from the one problem hampering advance in this direction, there remains securing of adequacy of mathematical model of control object during rather long period of time [1].

Mathematical models, which are used in the control systems of chemical technology

processes, may be divided into two groups [2]. The first ones are analytical models based on the theoretical analysis of physical and chemical processes occurring in the investigated object and also accounting of apparatus construction and characteristics of processed materials. The second group - empirical models, which consider chemical technology processes as "black box" and build on the base of analysis of input and output data of certain control objects.

Models of the first group because of their complexity require significant span time at the stage of identification. Refinement of all adjusting coefficients of the model takes a lot of time, as while searching with the usage of classic iterative methods during search of each coefficient, one multiply had to calculate mathematical model of the process at each stage of searching algorithm in order to clarify whether search value is achieved (figure 1). In the end, time spent for identification process is difficult to forecast, this does not allow effectively use such models of modern ACS, which realize regimes of real and quasi-real-time at various stages of the system and specify high requirements to the operational efficiency and control quality.

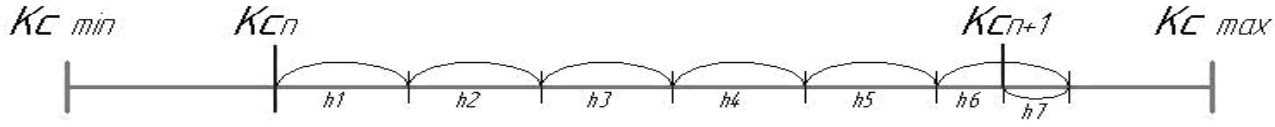

Figure 1. Identification of MM method of stepwise approximations with the change of step and search direction

Kc_{min}, Kc_{max} – range of possible values of adjusting coefficient;

Kc_n – known value of adjusting coefficient;

Kc_{n+1} – search value of adjusting coefficient;

$h_1 \ldots h_7$ – steps of iterative algorithm of search of adjusting coefficient, step size $h_7 = h_6/2$.

Models of the second group differ with low solvability of obtained results and do not consider intricacies occurring in simulated objects of reaction and that is why they rapidly loose adequacy during significant change of input coordinates of the process and require constant current identification.

Application of artificial neural network (NN) on the stage of identification partially solves this problem and allows almost momentary to determine adjusting coefficients due to data approximation about previously found model coefficients [1], but it also have a range of major deficiencies.

NN considering all the parameters, which influence the adequacy of mathematical model, is exuberant complex and requires significant span time for formation and adjustment of adequate learning sample. During significant change of parameters of modeling parameters, such as change of characteristics of feed stock, regeneration or shift catalyst change-out, purge of the apparatus, filters, etc, selection of values, according to which there was fulfilled NN training, stops being actual and calculation of adjusting coefficients according to NN is impossible or is fulfilled with significant error. Preparation of new learning sample and retraining of neural network takes a lot of time. Simplification of NN structure, used for identification, also leads to the loss of accuracy of determination of adjusting coefficients and, as consequence, to the reduction of adequacy of investigated model [3].

The aim of this work is to develop combined intelligent algorithm of identification of mathematical models of chemical technology processes, which combines classic iteration algorithm and neural network for minimization of search time of adjusting coefficients. Herein NN, which have simplified structure and is rather simple in training, is used for determination of approximate value of adjusting coefficient of mathematical model and iterative algorithm – for further search of adjusting coefficient with set accuracy and much lesser number of steps (figure 2).

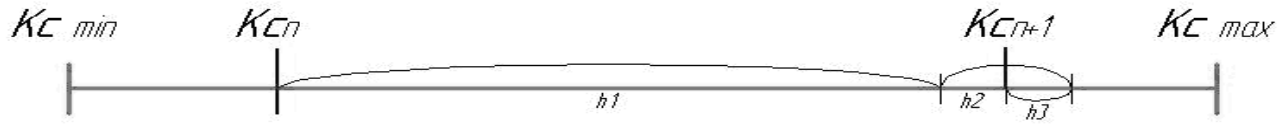

Figure 2. Iterative- connectionist identification of mathematical model

h_1 – distance of search compensated by neural network;

h_2, h_3 – steps fulfilled by iterative algorithm.

In the course of operation of identification algorithm, database containing information about found adjusting coefficients, increase steadily. Correspondingly there steadily increase the amount of examples for study of neural network, and this means also accuracy of determination of adjusting coefficients. If error of determination of adjusting coefficients by neural network is comparable with the error of used iterative algorithms, calculation of adjusting coefficients of mathematical model may be fulfilled only by means of neural network and almost momentary.

Generalized algorithm of iterative-connectionist identification of mathematical models of CTP is represented in the figure 3.

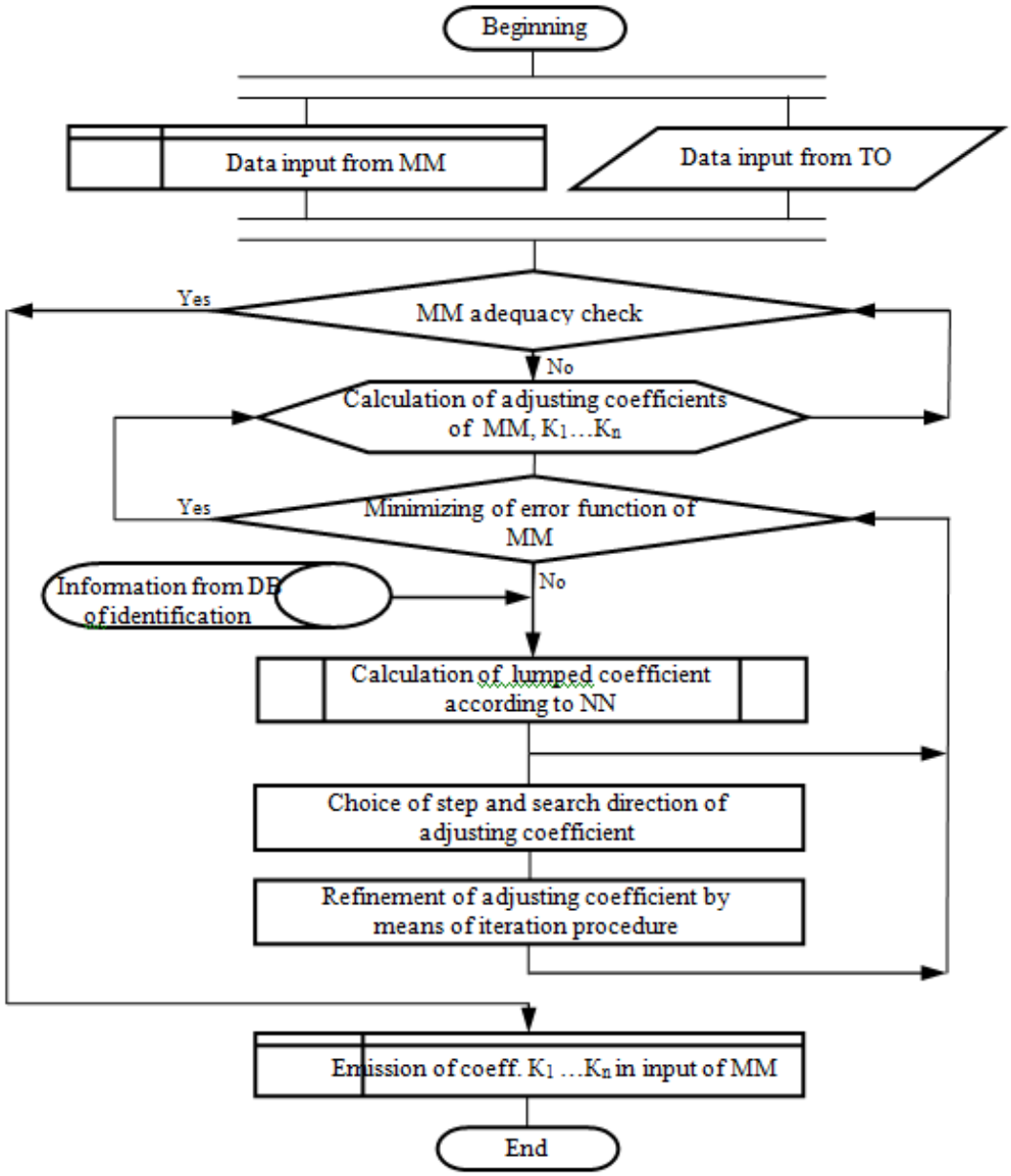

Figure 3. Generalized algorithm of iterative-connectionist identification of mathematical models of CTP

In the input of identification algorithm there come experimental data from technological object and the same data calculated according to mathematical model. Check of model adequacy is fulfilled by means of analysis of function of model errors. If the identification is necessary, there starts cyclic refinement of coefficients K_1 … K_n starting with the last until the condition for minimum of

error function is fulfilled. To minimize the amount of steps of search algorithm, start approximate value of adjusting coefficients is calculated according to NN. Further refinement of the value of adjusting coefficients is fulfilled according to iterative method with the change of step and search direction. Refined adjusting coefficients are transmitted in input of mathematical model.

Efficiency checking of suggested method of iterative-connectionist identification of mathematical models was fulfilled with the help of modified kinetic model of three-reactor block of catalytic reforming unit L35-11/300. Model represents the system from three series-connected kinetic models of separate reactors with three single adjusting coefficients [4].

Connectionist part of identification algorithm was realized on the base of neural network of training according to the principle back propagation of error in the form of three-layer perceptron with one buried layer (figure 4).

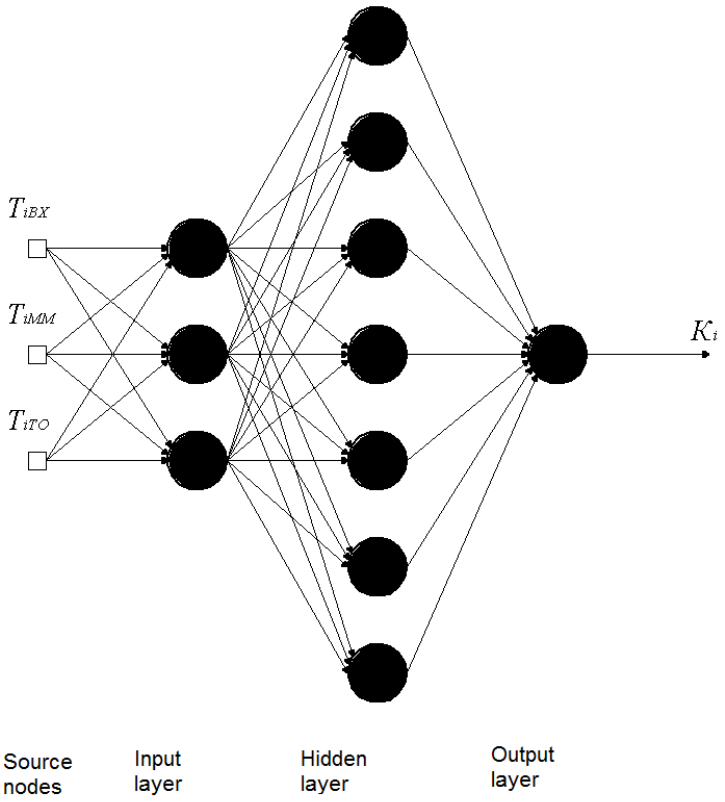

Figure 4. Layout of the neural network, three-layer perceptron

Ki – Adjusting coefficient of separate reactor model;

Ti – Correction factor of the model, temperature difference at the input-output of the reactor.

Optimal amount of neurons in the buried layer was determined experimentally and is equal to seven. Further increase of amount of neurons didn't give noticeable increase of computational accuracy of adjusting coefficient, but increased the volume significantly the initial data necessary for network training.

In the role of neuron activation function there was used sigmoid function:

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

Parameter of sigmoid function was also chosen experimentally and is equal to 0.92. Iteration component of algorithm is realized on the base of the method of bitwise approximation with the change of step and search direction.

Time of work of identification algorithm considerably depends on the instrument and program peculiarities of computer, on which the researches are fulfilled. That is why for quantitative estimation of effectiveness of application of neural network there was used such parameter as total number of iterations, fulfilled by search algorithm during identification of mathematical model of separate reactor of catalytic reforming. This allowed to determine the quantity of steps of search iteration algorithm compensated by neural network, which almost linearly correlates

with the time necessary for identification of mathematical model.

For analysis there was used experimental data obtained from the catalytic reforming unit of "Lukoil-odesa NPZ PAT", which was supplied to the input of two mathematical models. For identification of the first model there was used classic iteration algorithm without NN. For the second one – developed algorithm of iterative – connectionist identification using NN for compensation of steps of search algorithm.

Comparative analysis showed that during usage of NN, total amount of iterations necessary for search of new values of adjusting coefficient of mathematical model will reduce by 17…34% at 300 training examples and by 34…76% at 800 training examples for NN.

Conclusions

Fulfilled experimental check of suggested combined algorithm of iterative – connectionist identification of mathematical models of CTP showed that application of neural network for compensating of steps of searching iteration algorithm allows to reduce time for identification by 30-70% and with increase of training sample for NN, this tendency remains.

References

1. Tsypkin, Ja. Z. Informacionnaja teorija identifikacii [Informative theory of identification]. Moscow, Nauka, 1995, 336 p.
2. Bykov V. I., Zhuravlev V.M. Modelirovanie i optimizacija himiko-tehnologicheskih processov [Modeling and optimization of chemical technology processes]. Krasnojarsk, IPC KGTU, 2002, 298 p.
3. Levchuk I.L. (2012). Identification of mathematical model of catalytic reforming process on the base of connectionist technologies. *Matematichne modeljuvannja*. Dniprodzerzhinsk. No 2, p.p. 77-80.
4. Levchuk I.L. (2012). Development of mathematical model of the catalytic reforming process in reactor columns. *Proceedings of NMU*. No 39, p.p. 122 – 127.