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Design of Hybrid Model of Fertilizers Production Process for Automatic Control Purpose

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Introduction

Fertilizers are broadly divided into organic fertilizers (composed of enriched organic matter – plant or animal), or inorganic fertilizers (composed of synthetic chemicals and/or minerals). Inorganic fertilizer is often synthesized using the Haber-Bosch process, which produces ammonia as the end product. This ammonia is used as a feedstock for other nitrogen fertilizers, such as anhydrous ammonium nitrate and urea.

Control technologies develope very rapidly, and process automatic control is now ubiquitous within industries. In receant years, modern automatic control technologies are closely related to modelling in chemical industries. For the high quality automatic control purpose one needs to have a reliable process model. Besides, chemical industries save money using models for process control and optimization purposes [1].

With increasing reliance on information technology, systematic decision-making strategies are essential for effective and efficient performance including fertilizers industry systems. To maintain its successes, the industry must be flexible and adaptable to new technologies, external pressures and changing markets. All of these challenges require systematic improvement methodology and advanced technologies for control, optimization and planning. The most commonly used advanced control techniques include such efficiency inferential without analyzer based optimization and modelling, process modeling and system identification (first-principle models and empirical models).

The chemical processes under consideration is characterized by the complex reaction systems [2, 4, and 6]. Hence, it is not possible to describe the process in detail using only first-principle and mechanistic models. To overcome the limitations the hybrid modelling has been used in chemical and biochemical engineering for many years (e. g., [6]). Besides, often it is difficult to describe the chemical processes using only classic methods, which are given in the automatic control theory. Although, using hybrid models improve benefits for modelling and identification of chemical or biochemical procceses. On the other hand, the successful identification of hybrid models using "black box" models is possible having consistent experimental data.

One needs to use suitable hybrid model identification method, which gives good modelling quality and is effective and robust [6]. Besides, hybrid model application for chemical processes requires considering the application of artificial neuron networks.

Moreover, in chemical technology one is most often interested in modelling of specific reaction rates, because they define the behaviour of the conversions in chemical processes. Specific reaction rates have to be determined using feed-forward artificial neural networks where the inputs are the key factors influencing the process dynamics - the concentrations of the reacting components, temperature, pressure, etc.

In the recently published literature, some interesting examples show that hybrid combination of artificial neural networks, mechanistic kinetics and mass balance equations can lead to considerable advantages [2, 6]. On the other hand, many classical identification methods [3] may fail or do not lead to a solution of required precision.

Structure of hybrid model

The general structure of the process reflects several distinct ammonia production levels, i. e. secondary reforming, shift conversion, CO_2 removal, methanation, and ammonia synthesis. The extensive description of the main ammonia production process can be found elsewhere [7]. Also, mass balances equations of main ammonia production process for the components based on chemical equilibriums [7]. Mechanistic model of ammonia production is based on the mass balances equations for the components derived from chemical equilibriums [7]. The dynamic mass balance equation of the following type for each component was created and numerically solved

$$\frac{d(C_N)}{dt} = r_N + (C_{Nin} - C_N)\frac{F}{V}, \quad (1)$$

where r_N – absolute reaction rate. [mol/l/s]; F – flow to the chemical process, [l/s]; V –volume of vessel, [l]; C_N – modeling component concentration, [mol/l]; C_{Nin} – component concentration to process, [mol/l].

Usually, reaction rate of a chemical process is not constant and depends on various factors. Hence, coefficient of proportionality is necessary in order to take into account not only the process temperature, but also the process pressure, activation of catalyst and other important process parameters, which have influence on the reaction rate. For this reason, one needs hybrid model identification that correctly evaluates all the process model parameters.

Instead of mechanistic absolute reaction rates it is of advantage to use artificial neuron networks (ANN) subsystems for modelling ammonia production absolute reaction rates in order to catch the important phenomena hidden in the process data that cannot be used in mechanistic models of the reaction rates. For identification of hybrid model parameters the sensitivity equation technique was applied [6]. A general combination of a mathematical model represented by a set of nonlinear differential equations, mechanistic specific reaction rates expressions and an artificial neural network for ammonia production processes is shown in Fig. 1, where Inputs M are the inputs to the mechanistic model, and Inputs ANN are the inputs of ANN. The main problem arising with such a combination is that the usual training (parameter identification) procedures may not work or their performance is significantly reduced. Hence different training procedures must be used.

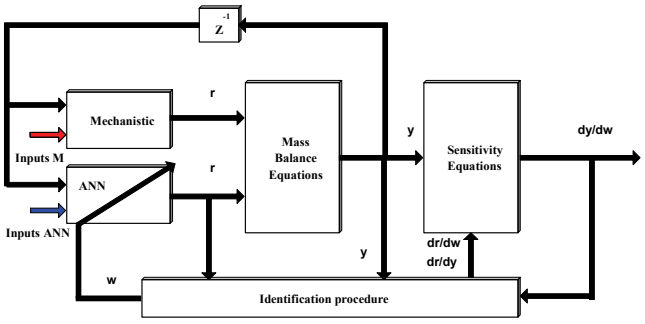

Fig. 1. Identification of ANN parameters using sensitivity equations technique

In order to achieve better extrapolation properties of the ANN, the cross validation technique during the ANN training procedure must be used. The concept of cross validation is that after training using a given sample of data ("training set") the quality of the process representation is evaluated using a different set of data ("validation set"). The root mean square error (RMSE) between predicted and measured outputs in the "validation set" is referred to as the "validation error". Since these modelling and identification procedures are relative simple, they additionally simplify the quick adaptation of the model to changing process conditions. This is why these techniques are so attractive for industrial applications.

Also, different ANN's structures for absolute reactions rates are used. It depends on modelling concentrations numbers and available expermential dates on the plant, which have mostly influence on chemical reaction process. The most used a following structures of ANNs for modelling of absolute reaction rate for ammonia production processes are shown in Fig.2 and Fig.3:

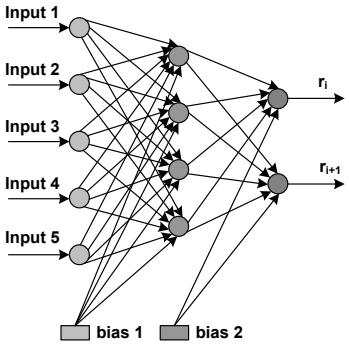

Fig. 2. Tipical structure of ANN for modelling absolute reaction rate

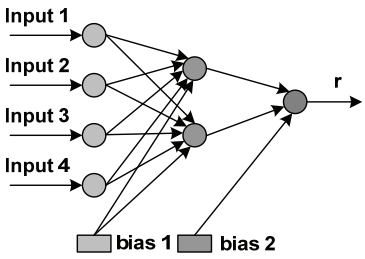

Fig. 3. Tipical structure of ANN for modelling absolute reaction rate

ANN structrure shown in Fig.2 is used for metathanation and second reforming processes in ammonia production. Also, production rates r_i, r_{i+1} are related to the inputs, which usually are most important technological parameters for describing process dynamics, like concentrations and flows (to the processes), processes temperatures. Due to complexity of functional relationship modelling absolute reaction rates it is expressed by a feed forward sigmoid artificial neural network (ANN) containing 5 inputs, 4 nodes in a hidden layer, and 2 outputs (Fig. 2). Taking into account the bias values the ANN results in 34 free tunable model parameters.

In accordance with Fig.3 ANN structure are used for CO conversion, CO_2 conversion and ammonia synthesis procceses in ammonia production. The ANN structure is the same like before mentioned, except (ANN) containing 4 inputs, 2 nodes in a hidden layer, and 1 output (Fig. 3). Taking into account the bias values the ANN results in 13 free tunable model parameters.

There are significant delays in the measured parameters of ammonia production processes, especially regarding flow and temperature signals. As a result, one needs to take into account the delays for ANN in the hybrid model identification procedure. Input data of ANN is of very different range. For example, form methanation process CO concentration is $\sim 10^{-8}$ mol/l, and temperature is ~320 ^{o}C. Besides, one has relatively small variation in some experimental data, for example process temperature varies from 317 ^{o}C to 325 ^{o}C. Hence, a normalization procedure for all input data of ANN is applied in order to deliver better process identification results.

Modelling results

The identification using sensitivity equations technique was performed for the already described ANNs. It was performed using the data from the "training" experiments and it shows good modelling quality. The sufficient modelling quality in both "training" and "validation" experiments sets was reached for main ammonia production processes concentrations.

In accordance with the chemical equilibriums of ammonia production processes [7], some modelling concentrations are very small values in the processes (see Fig. 4 and Fig. 5). Besides this concentrations are some residuals in chemical reaction. For this reason, its gives the worst results of other in modelling. Although, other concentration modelling gives good results, especially CO_2 concentration after CO_2 conversion, CO concentrations after CO low temperetature and CO average temperature converters, ammonia concentration after ammonia synthesis. Generally, in both "training" and "validation" experiments the model shows sufficient modelling quality.

The choice of concentrations of the components that were selected for illustration was based on their importance for the ammonia production processes and on the available measurements in the plant. The model was identified taking into account the experimental data in extreme process operating conditions provided by ammonia plant (SC "Achema"). The measured values are influenced by the disturbances and errors in the control systems and equipment, also by the procedures of the measurement unit conversion (e. g., from [v/v %] to [mol/l]).

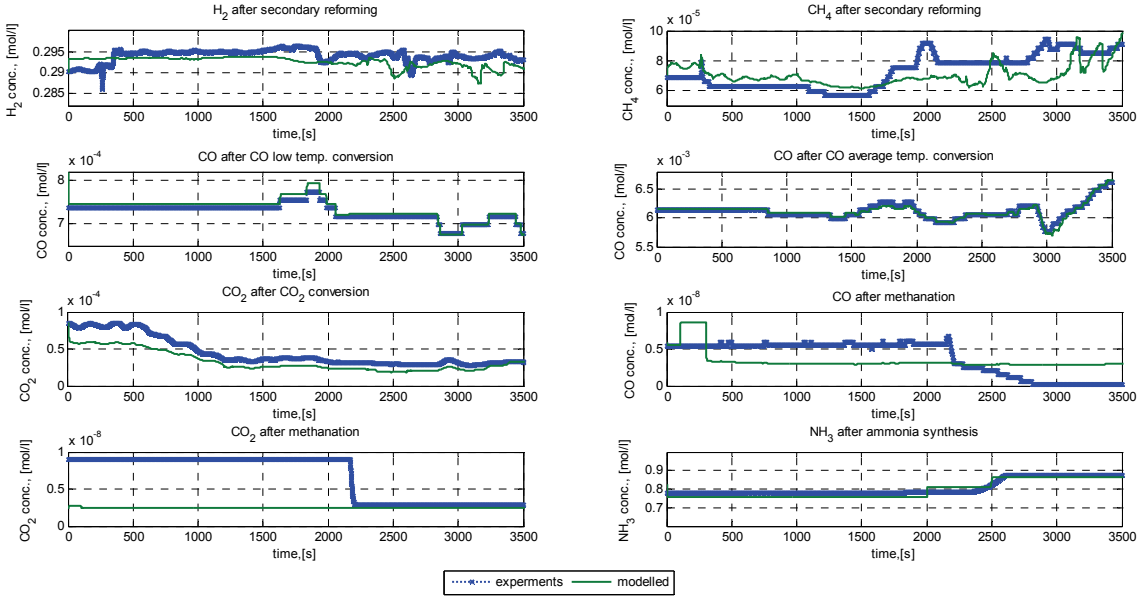

Fig. 4. Hybrid model identification results: training experiments

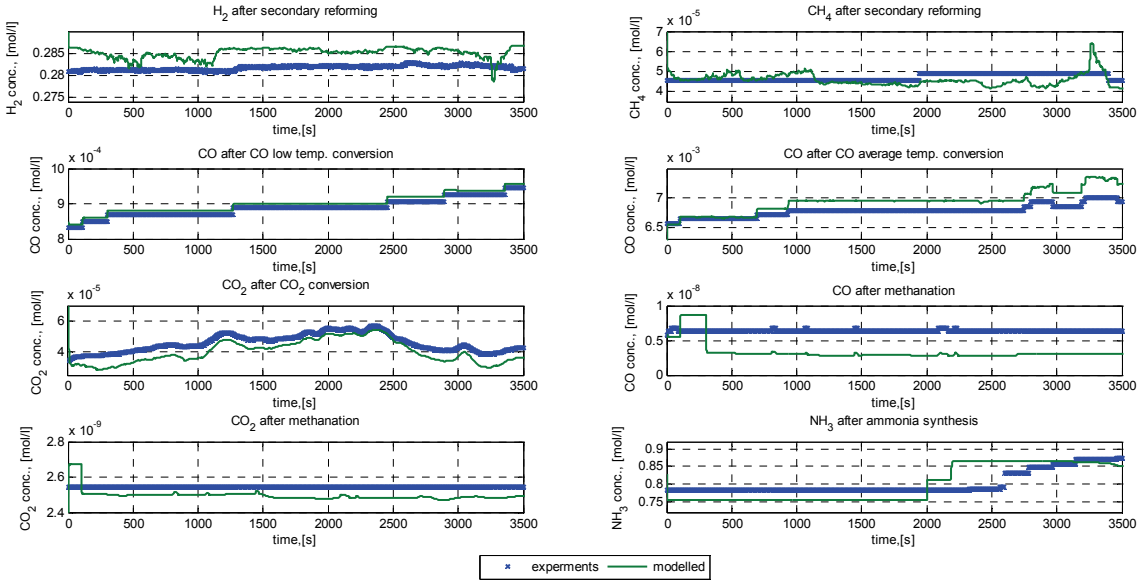

Fig. 5. Hybrid model identification results: validation experiments

Conclusions

Generally, taking into account the complexity of the chemical process the concentrations are modelled with sufficient accuracy as compared to the confidence of experimental values from ammonia production plant. The model is suitable for future application for optimization and automatic control purposes that could save money in ammonia production process.

Taking into account that expermential data from ammonia production plant changes within narrow range, it can cause problems for correct ANN training. In this case, using sensitivity equation method one can expoit its advantages for complex chemical process identification.

Also, the trained hybrid model was tested on training experiments (shown in Fig. 4), and the hybrid model verification of adequacy was performed using data from validation experiments that shows satisfactory modelling quality of the hybrid model (see Fig. 5).

The accuracy and efficiency of the sensitivity equation method depends on the initial ANN weights. The main disadvantage of the sensitivity equation method is that one needs to write down significant number of sensitivity equations as compared with equations number for process model. These sensitivity equations need to be integrated together with the process model. In some analyzed cases, model has 7 mass balance equations and 68 sensitivity equations.

Nevertheless, the further work should involve the application of the other suitable identification methods that potentially provide with better performance of the algorithm with respect to identification time and that lead to better identification quality.

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An improved technique of hybrid modeling of fertilizers production processes for automatic control purpose is described. Design principles of mass balance systems for key components are outlined, and artificial neuron network (ANN) subsystems for modelling of absolute reaction rates are represented for ammonia production processes. The sensitivity equation approach was applied for parameters identification of a hybrid model for ammonia production processes. Possible difficulties and ways of practical implementation of the applied identification method for complex hybrid models for industrial chemical processes are outlined. The hybrid model identification results are presented and discussed. Ill. 5, bibl. 6 (in English; abstracts in English and Lithuanian).

G. Oberauskas, V. Galvanauskas. Trąšų gamybos procesų hibridinio modelio kūrimas automatinio valdymo tikslams // Elektronika ir elektrotechnika. – Kaunas: Technologija, 2011. – Nr. 8(114). – P. 93–96.

Nagrinėjamas hibridinio modeliavimo metodo taikymas trąšų gamybos procesui automatiškai valdyti. Pristatyti amoniako gamybos procesų atskirų cheminių komponentų masės balanso lygčių sistemų kūrimo principai. Taip pat pateikti dirbtinių neuronių tinklų (DNT) kūrimo, modeliuojant absoliučiuosius reakcijų greičius, principai. Amoniako gamybos hibridinio modelio parametrams identifikuoti pritaikytas jautrumo lygčių metodas. Nurodytos galimos praktinio taikymo problemos sudėtingiems pramoninių cheminių procesų hibridiniams modeliams identifikuoti, naudojant jautrumo lygčių metodą. Pateikti ir aptarti hibridinio modelio identifikavimo rezultatai. Il. 5, bibl. 6 (anglų kalba; santraukos anglų ir lietuvių k.).