

## Present Chemical Production Simulator Model Validation Method

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The developed new validation method of the simulator model in standard and emergency situations for chemical production management skills training at minimal amount of monitored process variables is presented by the example of fluorine electrochemical production process. The method consists of two stages. At the first stage the validation quality of separate process variables is evaluated. It allows verifying the developed model accuracy and identification of its inputs or indicated the necessity to correct some development phase. At the second stage the model operation and its applicability for training purposes is generally evaluated. The simulation quality of the monitored process variables which enable cause-effect analysis to detect emergency reasons is checked.

### 1. Introduction

The skills and abilities acquired by the operator during training of different situations on the computer simulator (CS), and, consequently, right management decisions in practical work conditions, depend on the correctness of the variables behavior (Dozortsev et al., 2000). At the present day for verification and validation of the simulation model (SM) to use it in the computer simulator a lot of methods have been proposed, which as a rule are used in combination (Sargent, 2013). The choice of appropriate methods and their combination is conditioned by the simulator type and amount of initial data for its development (Yatskiv, 2000).

Suggested approaches in case of unknown input signals amount to the following stages: identification of the input signals using the quantitative criterion, qualitative assessment method development and validity check using this method for making conclusion about the possibility to apply the developed model in the CS. In order to validate the champion simulation model of the actual technological process (TP) it is essential to address the specialists-experts at any stage, depending upon availability of initial information. Very often the main input and output variables for the development production model are not monitored and measures in true-life production as it is rather inconvenient to equip production devices with additional sensors. This in its turn complicates the use of the methods of direct comparison of experimental data with the simulated ones. Industrial data obtained in the course of a passive experiment are difficult to simulate on the model due to indefiniteness of input signals. Active experiment on the simulation of standard and emergency operation modes in real production is practically impossible.

### 2. Background

Thus, the method based on the expert survey approach was developed. The method consists of two main stages. At the first stage the quality of separate process variables is evaluated. It allows verifying the developed model accuracy and identification of its inputs or indicates the necessity to correct any of the development phases. At the second stage the model operation in general and its applicability for the training purposes are evaluated. The simulation quality of the monitored related process variables, which enable cause-effect analysis to detect emergency reasons is checked.

During adequacy evaluation of the SM developed for fluorine electrochemical production process – certain elements of this model were presented in the works model of the electrolyzers series power-supply system (Egorova et al., 2014), and simulation module processes of electrolytic thermal circuit. (Liventsova et al., 2012) there were some difficulties connected with the use of existing approaches, as the input variables are not monitored in real production ahead of every device from the series as presented in Figure 1.

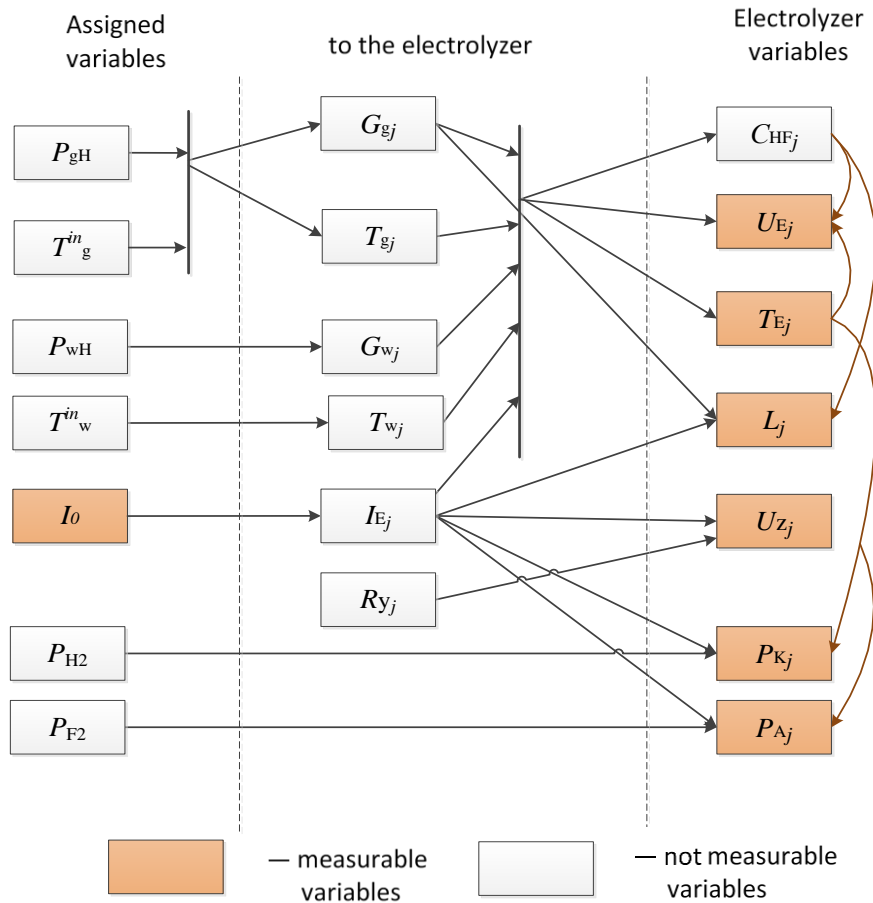


Figure 1: The scheme of the production process main variables

It is considered impossible to carry out an active experiment for simulation of emergency system operation modes. It is very complicated to perform the adequacy evaluation by direct comparison of industrial data with the simulated ones. The process of extraction of sufficient sample size of emergency situations for application of statistical methods as well as reconstruction of complete initial information about the reasons which caused these situations is supposed to be rather impractical.

It can be seen from figure 1 that the input measurable variables which are observed by the operator from the operator panel screen are: temperature ( $T_E$ ) and electrolyte level ( $L$ ), electrolyzer voltage ( $U_E$ ) and cathode-ground ( $U_z$ ), pressure in collectors of anode gas ( $P_A$ ) and cathode gas ( $P_K$ ) of each electrolyzer in the series. Therefore, the model adequacy is evaluated by these variables.

### 3. Approach to the development of SM for the CS

In Figure 2 an approach to the SM development is presented, the main stages and corresponding ways of quality evaluation of the SM intended for computer training purposes and developed for the computer simulator of fluorine electrochemical production process are shown.

At the stage identification verification of the SM in the standard operation mode is carried out by means of comparison of model and industrial data using the weighted root-mean-square deviation. Unknown input signals necessary for the evaluation are identified at the model parameters tuning.

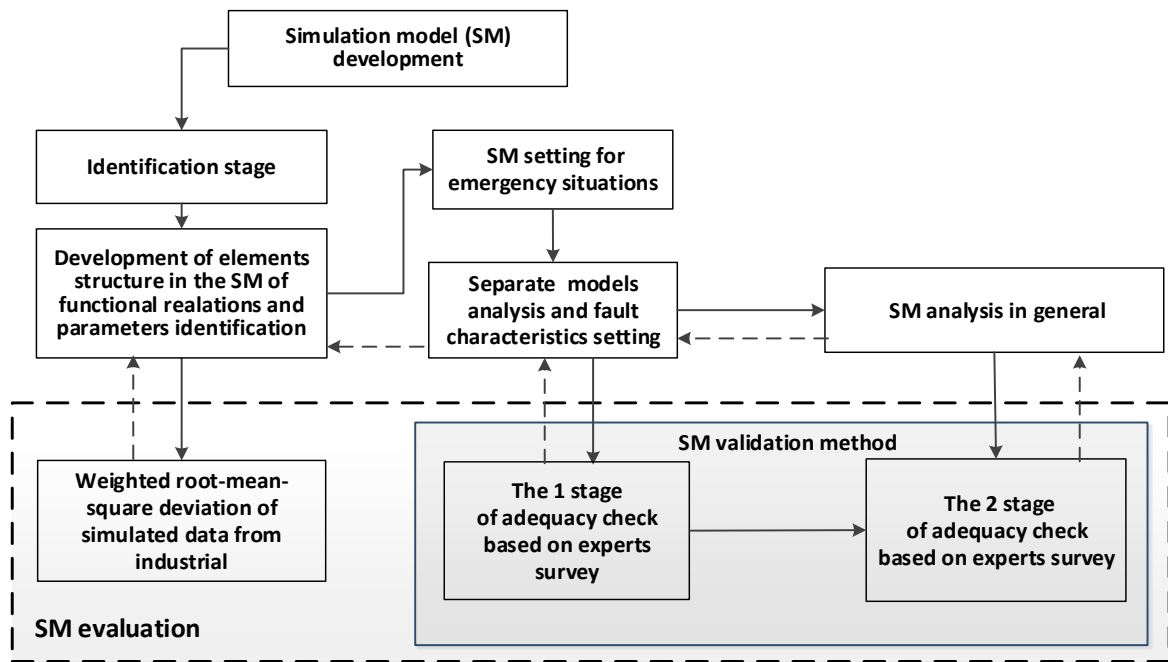


Figure 2: Approach to the development of SM for the CS

Rough setting of the model is performed by adjusting the parameters of separate simulation model parts simulating the variables of the technological process and control system, as shown in Figure 3 for the variables of fluorine electrochemical production process.

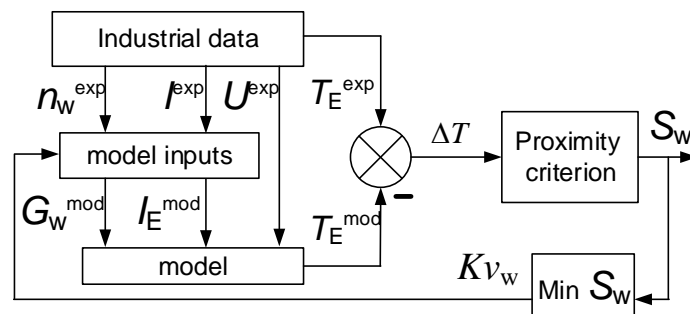


Figure 3: Rough setting of the SM for the CS

The parameters are adjusted in order to minimize the proximity criterion of the model and industrial data obtained during the passive experiment. The variance reduced to the variation range of the compared variable is used as the proximity criterion, as Eq(1).

$$\sigma = \sqrt{\frac{\sum_{j=1}^{k=m} D_j \cdot (n_j - 1)}{\sum_{j=1}^{k=m} (n_j - 1)}} \tag{1}$$

where:  $D_j$ — variance at simulation of the  $j$ -th campaign reduced to the variable variation range, %;  $n_j$ — number of calculated values  $X$ .

Variance at simulation of the  $j$ -th campaign is determined by the formula, as Eq (2).

$$D_j = \frac{100}{(X_u - X_d)} \cdot \frac{\sum_{i=1}^{n_j} (X^{\text{mod}}(i) - X^{\text{exp}}(i))^2}{n_j - 1} \quad (2)$$

where:  $n_j$  — number of calculated values  $X$ ;  $X_u$ ,  $X_d$  — boundaries of the variation range  $X$ .

After the parameters adjustment rough evaluation of the model adequacy in the standard operation mode is performed by calculating the weighted root-mean-square deviation of the model values from the experimental data. It is also possible to use a statistical procedure. Nevertheless the performed evaluation of the model adequacy is not sufficient for making decision about applicability of the model for computer training as it is necessary to evaluate the simulation quality of the SM emergency operation model in a wider range of the variables change, that is, to validate the SM. For this purpose expert evaluation of the SM in both standard and emergency modes is performed. The SM is previously adjusted for the possibility to simulate emergency modes by means of entering defect identifiers into the SM, as shown in model of the electrolyzers series power-supply system (Egorova et al., 2014), and in simulation module processes of electrolytic thermal circuit. (Liventsova et al., 2012)

#### 4. Method description

The SM validation method consisting of 2 stages was developed for the purpose of checking the model efficiency and its applicability for training at the step of setting the SM for emergency situations.

At the first stage the simulation quality of separate process variables is evaluated. It allows verifying the developed model accuracy and identification of its inputs or indicates the necessity to correct any of the SM parts. As a result it becomes possible to perform quantitative evaluation of such qualitative characteristics as the degree of conformity of steady-state and dynamic behavior of separate variables obtained on the model with the behavior of the variables on the operator panel screen.

For the first stage of the SM adequacy check the sequence of all fault characteristics changes preassigned into the SM is implemented according to the list of emergency situations occurrence reasons.

The experts are provided with a range of graphs of each measurable variable behavior obtained by successive value change of the fault characteristics for standard and emergency modes. The number of experiments for 2 modes (standard and emergency) is determined by the number of reasons which caused possible emergency situations, condition of the fault characteristics affecting the behavior of this variable, and is calculated by the formula, as Eq(3).

$$n_{\text{os}} = 2 \cdot n_s \quad (3)$$

where:  $n_s$  — the number of reasons of possible emergency situations for each of the considered measurable variable  $S$ , for the given production.

At the first stage the reproduction adequacy of the following measurable variables  $S$ :  $T_E$ ,  $L$ ,  $U_E$ ,  $P_A$ ,  $P_K$ ,  $U_z$  was checked. The cathode-ground voltage  $U_z$  is not considered at the second stage of the adequacy check, because it depends on the current load and isolation resistance and does not affect other measurable variables notably in standard and emergency operation modes due to alarm generation and defect elimination prior to, for example, electrolyte temperature increase.

At the second stage the model efficiency in general and its applicability for training purposes is evaluated. The simulation quality of interconnected measurable variables of technological processes is evaluated. It allows analyzing the cause-effect relations to determine the reasons of emergency situations occurrence. In particular, the quantitative evaluation of such characteristics as the degree of complex correspondence of steady-state and dynamic behavior of the model interdependent variables with the behavior of interdependent variables on the operator panel screen is determined.

For the second stage of the training model adequacy check the experts are provided with the graphs of interdependent variables behavior in each experiment:  $T_E$ ,  $L$ ,  $U_E$ ,  $P_A$ ,  $P_K$ . The number of experiments is conditioned by the number of nonrepetitive fault characteristics preassigned for the SM. In the experiment the change of the variable in the standard mode, entry to the emergency mode and return to the standard mode is presented in one graph. All graphs of the experiment are presented per equal time period for all variables. This time period is chosen by the most inertial variable.

The results of the behavior adequacy check  $U_z$  obtained at the first stage allow evaluating some mutual influence of the changes of cathode-ground voltages of the electrolyzers series as well as efficiency of the power supply system model, as the expert is provided with the graph presenting the values  $U_z$  of all electrolyzers of the series similar to the graph observed by the operator on the panel screen.

It is suggested that the following four steps should be fulfilled in each of the stages.

#### **4.1 The variables simulated by the model and steady-state and dynamic behavior of which is analyzed by the experts should be chosen from the common set of the variables**

On the basis of analysis of technological process variables and possible technological fault the scheme of information streams reflecting the main measurable and not measurable variables characterizing the process and their mutual influence is drawn, as shown in Figure 1. Hence, a number of variables to be considered at the first and the second stages are determined. At the first stage all measurable variables are considered. At the second stage the variables which do not influence other measurable variables noticeably in standard and emergency modes are not considered (this is discussed with experts), because, for example, alarm is generated and this defect is eliminated prior to any noticeable influence. The simulation adequacy of the variables which are not measured is proved by the simulation adequacy validation of the measurable variables, because all models of the developed modules are interconnected and affect each other.

#### **4.2 A set of chosen variables values changes should be obtained on the model according to the developed program**

During the experiments it is essential to provide the experts with the graphs of the measurable variables behavior with the description of the reasons of their condition change which is required for the adequacy evaluation. Sufficiency of the number of the experiments with corresponding graphs for the SM adequacy evaluation is generally provided by:

–the change of the fault characteristics preassigned into the SM taking into account all possible technological disturbances or emergency situations specified in the regulations and resulting in emergency condition of the simulated variables, that is exceeding the regulation bounds by the variables;

–the time of the variable change in one graph which is equal to time sufficient for indicating and sensing of the most inertial variable in the standard mode, entry into the emergency mode and return to the standard mode;

For the first stage of the SM evaluation the sequence of the change of all fault characteristics preassigned into the SM is executed in accordance with the list of emergency situations reasons. The experts are provided with the range of the behavior graphs of each variable obtained by successive fault characteristics value change for the standard and emergency modes. The number of experiments for 2 modes is determined by the amount of reasons causing possible emergency situations, conditions of fault characteristics influencing the variable behavior, thus, it is determined as the number of reasons of possible emergency situations for each measurable variable multiplied by 2.

For the second stage of the SM evaluation the experts are provided with the behavior graphs of interdependent variables. The number of experiments is determined by the amount of non-repetitive fault characteristics. In the experiment one of the graphs presents the change of the variable in the standard mode, entry to the emergency mode and return to the standard mode. All the experimental graphs cover equal time period.

#### **4.3 Experts survey should be conducted**

Individual polling without giving the reason is used. In case of discordance of the experts opinions validation to find its reason for possible correction of the model and development of input data is performed. The experts are chosen by special competence evaluation study and the significance of the experts is ranked accordingly. If the expert has a work experience more than 20 y in the field of the subject, the competence evaluation study is not necessary and the experts are ranked equally. Then the number of experts is not less than 3 (for example, one manufacturing technician and 2 operators).

In order to carry out the first stage of the adequacy check the expert is provided with n experiments for each simulated measurable variable in the standard mode, consisting of one graph, which should be evaluated numerically (the range of the evaluation is determined in cooperation with the experts). For simplification of the experts' work the range of evaluation is divided into 3 levels: satisfactory, good and excellent. In order to carry out the second stage of the adequacy check the experts are provided with n experiments consisting of k graphs of interdependent variables behavior, which should be also evaluated quantitatively. All poll results of the experts for each experiment are tabulated and processed.

#### **4.4 Tables Obtained results are processed and conclusion about SM applicability for training purposes is made**

At this stage, if required, mathematical description is corrected and additional polling is carried out.

Difference in the experts' opinions is determined. The range of possible difference of opinions is set not more than 5 % and the experts are interviewed to find the reasons of opinion differences (if required, the model is corrected and the polling is repeated).

After checking the range of permissible difference of opinions the survey results are processed: quality evaluation in one experiment is calculated by the average experts' evaluation. Then, the SM variables simulation quality evaluation is performed by the average mean value. Using the suggested approach the number of experiments for each variable is different and results from the scheme of the process information

streams. For example, for critical (measurable) variable it is 2 times bigger than the number of experiments for the controlled variable. Therefore, the weights considered equal at calculations differ and increase for more significant variables (Sheltout, 2007).

Criterion of the variables simulation quality of the SM is fulfillment of the condition of evaluation correspondence to the preassigned value. Numerical evaluation criterion values for the SM and for each variable are set separately. The highest evaluation value should be set for the sensitive (critical) variable. The criteria are set according to international experience with accuracy requirements to the models for the CS and experience of involved in evaluation experts from special production.

Judging by the results of the experts' survey of the fluorine production electrolyzers power system model (Egorova et al., 2014) the evaluation performed using the developed method made it possible to decide upon applicability of the current model.

## 5. Conclusions

The validation method for evaluation of model variables simulation of practical production by the example of fluorine production was presented in general, taking into account its applicability for computer training and conditions of indeterminacy of simulation object input signals. The method consists of two main stages. At the first stage the quality of separate process variables is evaluated. At the second stage the model operation in general and its applicability for the training purposes are evaluated.

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