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### Modelling of Displacing Complex Chromatography Automated System by KT-NIMFA Software

# Alexandr I. Gozhimov<sup>a,\*</sup>, Sergey N. Liventsov<sup>a</sup>, Alexandr O. Pletnev<sup>a</sup>, Olga V. Schmidt<sup>b</sup>

<sup>a</sup>National Research Tomsk Polytechnic University, Institute of Physics and Technology, Department of Electronics and Automation of Nuclear Plants, Tomsk 634050, Russian Federation

<sup>b</sup>Bochvar Research Institute of Inorganic Materials, 123060, Moscow, Rogova st., 5a, Russian Federation aig3@tpu.ru

Modelling of technological processes and its controls systems is one of the important stage in production design cycle. Adequate mathematical models of the control object or control system allow to find optimal process control algorithm, which allows to achieve required performance, to calculate required amount of source products and to estimate amount and quality of a produced product. In addition, by using models it is possible to analyze the behaviour of the system in various accidents.

At the moment there is a large number of software packages that help to mathematical models developing. This paper shows modelling of the control system of the separation process by displacing complex-forming chromatography in the simulation software "KT-NIMFA".

#### 1. Introduction

In Russian Federation, there is a modern nuclear project, which called "Proryv" ("Breakthrough"). In this project it is planned a creation of new generation nuclear energy technologies which are based on fast neutrons nuclear reactors and on closed nuclear fuel cycle (CNFC). The current state of the "Proryv" project development is represented by Adamov and Rachkov (2017).

Creation of closed nuclear fuel cycle requires accurate analysis of each nuclear fuel recycling and preparation stages. Some of the existing technological lines of recycling and preparation of a spent nuclear fuel (SNF) have to be redesigned, and some new technological lines must be designed for CNFC technology. In order to technological lines performance analysis, mathematical models of technological processes and their control systems should be developed.

Another important task in the "Proryv" ("Breakthrough") project is the implementation of training simulator systems for training personnel in the control of processes for reprocessing SNF.

Simulation software "KT-NIMFA" was developed for analysis of control systems efficiency and performance and for training systems. "KT-NIMFA"-training system is based on adequate mathematical models of technological lines and it works by principle which is described by Patle et al. (2014).

#### 2. Simulation software "KT-NIMFA"

Simulation software "KT-NIMFA" is is used for designing and modelling technological lines of recycling and preparation of nuclear fuel stages in a closed nuclear fuel cycle. "KT-NIMFA" consists of two main modules: visual module and calculation module. Visual module tasks are technological line configuration from the set of technological objects and visualization a calculation data. Calculation module tasks are calculation of the technological line model and sending the calculation data to visual module and training simulation module. Technological object in the "KT-NIMFA" software is presented as graphic block in visual module and as

Technological object in the "KT-NIMFA" software is presented as graphic block in visual module and as mathematical model in calculation module. Setting the object's parameters occurs by entering values in the appropriate input fields.

#### 3. Assembling of technological process simulation model

Assembling of technological process imitational model is carried out by the next way. Required technological objects are carried over to workspace from the library. Needed parameters are setting for each object, for example, P-, I-, D-values for an analogue PID-controller, geometrical parameters for buffer tank, initial values of temperature, elements concentrations for technological plants etc.

Further, links between objects are installed by ports connection: output object ports are have connected with input ports. There are different types of ports in the "KT-NIMFA" software: informational and material. Material lines are flows of substances; these lines transmit data about solution flowrate, solution temperature, elements concentrations. Informational lines transmit data about control signals, measured values by sensors etc.

The final stage is setting of data collection points. For this, special objects as "Indicator" and "Chart" are placed on the workspace and their input ports are connected to those lines in which it is necessary to record data. "Indicator" shows data values at the current calculation time, "Chart" shows changing calculation data at time. A file forms from the collected scheme of the simulation model and it is transmitted to calculation module.

## 4. Model of the displacing ion-exchanging complex-forming chromatographic column in "KT-NIMFA" software

At previous work (Chursin et. al., 2016) mathematical model of the chromatographic column was developed. This model describes separation process by displacing ion-exchanging complex-forming chromatography method. Chromatographic column model was implemented at simulation software "KT-NIMFA". Column parameters are column height, column diameter, number of elementary cells.

According technological scheme (Figure 1) simulation model of chromatographic columns cascade control system was collected (Figure 2).



Figure 1: A generalized scheme of the columns cascade

Each element in simulation model (Figure 2) has own computer model which is located in corresponding dynamic link library (DLL).

Similar objects, like chromatographic columns use one computer model, but they have different values of model parameters, such as height, volume etc. Calculation process of simulation model is carried out by the next way: each element takes input values from connected elements output values, calculates model step by corresponding computer model and forms its output values.

This "KT-NIMFA" model of columns cascade control system contains seven computer models: tank, pump, valve, concentration meter, flowmeter, ion-exchanging chromatographic column and control block. Elements "Indicator" and "Chart" doesn't have computer model, they collect calculation data only.

Setting values of flowrates at which the greatest performance of separation in columns cascade were based on previous work (Chursin et. al, 2017).



Figure 2: KT-NIMFA model of the columns cascade control system

Next charts are recorded while modelling: flowrates of initial solution and eluent (Figure 3), elements concentration at outlet of the first, third and fifth columns (Figures 4, 5, 6).



Figure 3: Solution and eluent flowrates







Figure 5: Output of the 3<sup>rd</sup> column



Figure 6: Output of the 5th column

#### 5. Using "KT-NIMFA" software as training system

In the future, it is planned to use adequate mathematical models of technological processes and control systems implemented in the simulation software "KT-NIMFA", to create a training system for training technical personnel. Such models should simulate those technological parameters that the operator controls in the workplace and must be calculated in real time.

The structure of the training system based on the "KT-NIMFA" software is proposed as follows. Most SCADAsystems work with OPC / DDE-servers, which are directly connected to the technological object, as shown in Figure 7.



Figure 7: Typical structure of the automated control system

To implement the simulator system, it is proposed to replace the controlled parameters of the technological object with calculated values, which are calculated in "KT-NIMFA" software (Figure 8). For this, connection module is implemented, which communicates with OPC / DDE-server and receives tags of parameters that are transmitted to SCADA-system. Conformity between tags and model variables is established in calculation model. The same way it is necessary to establish control variables for controlling calculation model.



Figure 8: Structure of the training system based on "KT-NIMFA" software

Thus, the operator in the workplace monitors and controls the process model, as well as if he controlled the real object. If process model is developed with availability to simulate different accidents, then with the help of this it is possible to train the personnel in actions to prevent an accident and stabilize the state of the process.

#### 6. Discussion

Simplified models of additional objects (pumps, tanks, valves) were used to model the cascade of chromatographic columns. Complicating the models of these objects will slightly increase the accuracy of the calculation, because the separation process takes place directly in the columns, but will also increase the calculation time, that can be critical for the implementation of the training system, because the training system requires the calculation of the model in real time.

In the future, it may be necessary to complicate the model of the chromatographic columns control system, if additional sensors will be added to the actual installation.

In addition to the presented model, the following models are implemented in "KT-NIMFA" software: evaporator control system (Efremov et. al., 2017), linear crystallizer control system (Ochoa Bique et. al, 2016), control system for cascade of centrifugal extractors (Zelenetskaya et. al., 2016).

#### 7. Conclusion

Adequate mathematical models of the technological processes implemented in the simulation software "KT-NIMFA" can be used to optimize control modes, to correct algorithms, and to train the plant operators in working with it in various modes, such as start, stop, parameters controlling and emergencies.

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