Simulation of the gas fractionating unit of depropanization system and development of a computer training software

E A Shulaeva¹, D R Valitov and A I Kubryak

Department “Automated Technology and Information Systems”. Branch of the Ufa State Petroleum Technological University in Sterlitamak. Oktyabrya Av., 2. Sterlitamak, 453118 Bashkortostan Republic. Russia

¹ E-mail:eshulaeva@mail.ru

Abstract. One of the promising and topical directions for improving the quality and safety of control of technological facilities is the use of tools that allow simulating technological processes and control systems on a computer before entering a real production facility. Two main tasks are solved here: personnel training and selection of effective technological modes. This article discusses the creation of a computer simulator complex for the depropanization unit of a gas fractionation plant in Unisim, which in turn should provide practical training for future specialists in the safe conduct of the technological process, thanks to an accurate mathematical model of the depropanization process. It will also help improve skills for quick response and prevention of an emergency. The decision to create a computer training complex arose in connection with the need to train personnel, improve their skills and experience. As a result of the research, a computer training software was developed based on the Unisim Design and Unisim Operations software package for training future operators and industrial operators to consolidate theoretical and practical knowledge.

1. Introduction

At present, the training of working personnel is increasingly attracting the attention of the company's management. The success of any company depends on the quality of training, however, traditional training technologies based on knowledge, skills and abilities are no longer enough, it is necessary to successfully apply the experience gained in solving specific professional problems, including in non-standard situations. In this regard, the enterprises develop and implement all kinds of technologies and personnel training systems using computer training software. They are used both to assess the current level of training and to improve it.

The use of computer simulators for training operators of technological processes is determined in accordance with the Federal norms and rules in the field of industrial safety "General rules of explosion safety for explosion and fire hazardous chemical, petrochemical and oil refining industries" (approved by order of the Federal Service for Environmental, Technological and Nuclear Supervision of March 11, 2013 N 96) clause 2.11 for the acquisition of practical skills for the safe performance of work, prevention of accidents and elimination of their consequences at technological facilities with blocks of I and II categories of explosion, all workers and engineering and technical workers directly involved in the conduct of the technological process and the operation of equipment at these facilities, undergo a
training course using modern technical means of teaching and practicing such skills (computer simulators, training grounds) [1-3].

The introduction of computer simulators, on the one hand, makes it possible to improve the training of operators due to the constant complication of technological processes and the emergence of new control systems in production, as well as to teach better process management of newly arrived workers to prevent emergencies. On the other hand, constantly evolving modern information technologies make it possible to create new systems for training on computer simulators, which are superior in efficiency to known forms of training, including potentially dangerous and not always available training on real facilities. [4].

Now, there are various software and hardware tools for computer modeling of technological objects, selection of technological modes and adjustment of control loops. Such tools include the Unisim Design software package.

Unisim Design software assists engineers in creating stationary and dynamic models for the design and optimization of industrial plants and control systems, emergency and risk analysis, safety assessment, performance monitoring, troubleshooting, performance improvement, business planning and asset management. Process simulation systems can improve design efficiency with workflow management tools and achieve capital cost savings through proper material selection in security design.

### 2. Materials and methods

The process takes place in the propane column K-3. The raw material is the deethanized fraction obtained in the column K-1. Because of rectification, two fractions are separated: propane (propane-butane) fraction from the top of K-3 and butane-pentane fraction from the bottom of the column. The propane (propane-butane) fraction is removed from the unit as a component of domestic liquid gas, and the butane fraction and higher is the feedstock of the K-2 column.

Column K-3 is a column-type apparatus equipped with 60 trays. Deethanized feedstock from column K-1 with a flow rate of 20-110 m³/h and with a temperature of 70-110 °C is fed to the 32, plate of column K-3. The column bottom temperature is 90-125 °C.

The upper product of column K-3 with a temperature of 40-80 °C after cooling in XK-2, XK-3 and water cooler XK-3 enters the reflux tank E-1.

The propane-butane fraction from the tank E-1 is fed to the intake of pumps N-1, N-2, at the outlet of which valves are installed, with the help of which the product is further directed back to the reflux column or to the outlet.

To simulate the technological process of the depropanization unit of the gas fractionation unit was chosen the software package of the Unisim Design simulation environment from Honeywell.

A distinctive feature of Unisim Design from other programs is the presence of rich libraries of technological modules, which was implemented in both static and dynamic modes. These modules have been tested for realistic results and the ability to simulate a variety of emergency situations.

Also, this software package provides support for a full range of models of technological devices, including distillation columns, reactors and heat exchange equipment. Both solids and mixed media are supported. There is also a large selection of logical elements for configuring the control system and the ability to simulate various technological situations. This made it possible to achieve a high level of accuracy in the calculations of the depropanization process of the gas fractionation unit.

Modeling a mathematical model begins with a set of components. The following chemical components were used in the project: methane, ethane, propane, butane, water, hydrogen, carbon monoxide, argon, nitrogen, carbon dioxide, pentane, oxygen [5-6].

Next, 2 input and 5 output streams were created. The following technological equipment was installed: distillation column K-3, tank E-1, pumps P-3 and P-4, air coolers XK-2 and XK-3, water cooler X-3, regulators and sensors. You also need to configure them and set the dynamic parameters.

For the correct model of the technological process in the program, the optimal tuning parameters of the regulators were calculated.
In the regulator setup menu, it was required to set the value of the controlled variable, which is expressed as a percentage of the specified allowable range of its change in accordance with the equation:

$$PV(\%) = \left( \frac{PV - PV_{\text{min}}}{PV_{\text{max}} - PV_{\text{min}}} \right) \cdot 100$$  \tag{1}$$

$$PV(\%) = \left( \frac{52.98 - 0}{100 - 0} \right) \cdot 100 = 52.98$$

where $PV$ (controlled variable) is the measured variable, the value of which is maintained by the controller.

To determine the valve size in the Unisim program, it was required to calculate the $C_v$ factor. The flow rate through the valve is calculated using the following equation:

$$f \left( \frac{lb}{hr} \right) = v_{\text{facfac}} \cdot 3.49 \cdot C_v \cdot \sqrt{\rho \left( \frac{lb}{ft^2} \right) \cdot \sqrt{P_1 - P_2}}$$  \tag{2}$$

$$C_v = \frac{1962}{1 \cdot 3.49 \cdot 0.205 \cdot \sqrt{0.7670} \cdot \sqrt{480 - 400}} = 350$$  \tag{3}$$

Based on the values calculated above, the tuning parameters for the PID controller are set as:

$$\begin{align*}
\text{phase}_{GW} &= (-\pi) + \tan^{-1} \left( \frac{h}{\sqrt{a^2 - h^2}} \right) \\
\varphi &= -\pi + \frac{\phi \pi}{180} - \text{phase}_{GW} \\
T_d &= \frac{\tan(\varphi) + \sqrt{(\tan(\varphi))^2 + \frac{4}{a}}}{2\omega} \\
T_i &= \alpha T_d \\
K_c &= \frac{\beta \cos(\phi)}{a_{GW}}
\end{align*}$$  \tag{4}$$

where $\text{phase}_{GW}$ is the phase frequency;
$\varphi$ - the angular frequency;
$\alpha$ - calculated coefficient specified by the user;
$\beta$ - the gain specified by the user;
$\phi$ - phase angle specified by the user;
h - Hysteresis relay.

$$T_d = \frac{1.73 + \sqrt{1.73^2 + \frac{4}{4.50}}}{2 \cdot 0.05} = 0.61 \text{ minutes}$$
To configure the equipment, the names of the input and output streams were set, as well as dynamic parameters such as volume, height, location relative to other devices, etc.

The Unisim Operation software package was used to create the simulator screens. UniSim Operation implements a computing environment for real-time interaction with mathematical models developed in the UniSim Design software package. This makes it possible to control various technological devices from the depropanization unit in exactly the same way as on an automated workstation (AWP) of a specialist, since the view of the screens can look exactly like on the AWP. As a result of training on such a simulator, the future operator acquires a more improved skill of interacting with the SCADA system [7-8].

3. Results and discussion
To make sure that the developed model works correctly, it is necessary to make sure that the molar fraction of pentane increases its value to no more than 0.36 mol in the final flow, passing through all the simulated technical equipment, relative to the initial one. The initial value of pentane was 0.2333 mol (figure 2), having opened the component composition of the final stream of raw materials, which passed through the entire simulated technological scheme, it is observed that pentane increased its value to 0.2516 mol (figure 2), this confirms the adequacy of the developed model [9].
Figure 2. Concentrations of pentane in the initial and final feed streams.

Figure 3 shows a graph of the concentration of the molar fraction of pentane over the period of time passed after the launch of the mathematical model of the depropanization unit of the gas fractionation unit in the Unisim Design modeling environment and putting it into operation.

Figure 3. Graph of the concentration of pentane over the passed period of time.

Figure 4 shows the developed screen of the computer training software using the Unisim Operations program. A rectification column, technological apparatus of the unit for cooling and condensation of the upper product of the column are installed on the screen.

4. Conclusions
The computer simulator software of the depropanization unit of the gas fractionation plant considered in this article, consisting of a technological model and simulator screens, advises the Federal norms and
rules in the field of industrial safety. This computerized training software allows you to train personnel before launching new automated control systems, to teach the correct and trouble-free operation of the technological process, and is also necessary to maintain qualifications of the existing technological personnel.

![Figure 4. Screen of the propane column K-3 of the computer training complex.](image)

**References**

[1] Shulaeva E A and Pavlov V B 2020 Multi-criteria optimization of the process of electrolytic alkali's evaporation in order to develop a resource-saving chemical-technological system *IOP Conference Series: Materials Science and Engineering* chapter 734(1) pp 1-5

[2] Shulaeva E A, Shulyayev N S and Kovalenko J F 2019 Computer Modelling of Organic and Inorganic Chemistry Processes *Advances in Intelligent Systems Research: 7th Sci. Conf. on Information Technologies for Intelligent Decision Making Support (ITIDS 2019)* chapter 166 pp 230-6

[3] Shulaeva E A, Burdov A E, Valitov D R, Kubryak A I and Yurasov A O 2019 Creation of a training system for operators to improve the reliability and safety of chemical technological systems *Natural and technical sciences* 12 326-8

[4] Dozortsev V M 2009 *Computer simulators for training process operators* (Moscow: SINTEG) p 372

[5] Shultz D S and Krainov A Y 2011 Mathematical modeling of SHS process in heterogeneous reactive powder mixtures *Computer Research and Modeling*, 3 147-53

[6] Vasenin I M, Krainov A Y and Isaychenkov A B 2012 Mathematical modeling of drying of coal particles in the gas stream *Computer Research and Modeling* 4 357-67

[7] Tokarev S M 2013 Mathematic modeling of thermal distillation of water in film flowing under vacuum *Computer Research and Modeling* 5 205-11

[8] Lobasov A S and Minakov A V 2012 Numerical simulation of heat and mass transfer processes in microchannels using CFD-package eFlow *Computer Research and Modeling* 4 781-92

[9] Koteleva N I, Shablonsky I E and Koshkin A V 2011 Computer training simulator for instructionof oil and gas technological processes operators:the analysis of existing decisions and the wayof their improvement *Journal of mining institute* 192 212-5