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Simulation of benzene column distillation for quality control system design

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***Abstract* — The paper presents the research results regarding process simulation and control of benzene separation in an industrial plant. The main purpose of the paper is to design a quality control system for the distillation column. The paper is structured in four parts, the first one being a review of the main simulation process software's and ways of using them. The second part contains an overview of the industrial plant for benzene production. The third part is focused on the process simulation in steady state mode and the sensitivity analysis of the process. The last part is focused on the dynamic simulation of the process and basic control systems. The obtained numerical results had validated the dynamic simulation, creating the premises for designing and developing the automated control system of product quality.**

Keywords—benzene; simulation; Unisim Design; control.

I. Introduction

The petrochemical complex BTX is designed to separate benzene, toluene and light xylenes at the highest purity, to be subsequent use as feedstock for the petrochemical synthesis industry. The separating of benzene, toluene and xylenes is highly energy-intensive process.

The development of an automated system for adjusting product quality for a separation column from the BTX complex requires the following steps to be covered:

- Process simulation of the distillation process in stationary regime, followed by the sensitivity analysis of the process to variations of perturbations and to manipulated variables.
- Dynamic process simulation with conventional control systems.
- Design the structure of product quality control system and design the control algorithms.
- The validation of the proposed control structure through the dynamic simulation

Simulation of chemical processes is the first step in the development of automated systems. In recent years, chemical process simulation tools have stabilized in the PRO II and the HYSYS simulator with the versions Unisim Design and Aspen HYSYS.

The use of the PRO II simulator has been reported in various publications. One such example is the simulation of the Ethylene De-Pentanizer distillation process [1]. The process was elaborated only for the steady state regime and the simulation obtained was used to check the operation of the distillation column and its sensitivity analysis.

A guide for HYSYS software and its simulation of distillation processes is presented in [2]. Although the work can be categorized as teaching material and it only assists for simulations in stationary state.

A complete overview of simulation of the distillation process is presented in [3]. Separation between benzene and cyclohexane had been performed in stationary and dynamic mode. The conventional control structure was used, and the conclusions reflected the performance of the automated control system for quality control [4].

An extensive guide for Unisim Design dynamic simulation of distillation processes is presented in [5]. The main steps necessary to achieve a dynamic simulation of the distillation process are presented. The paper contains a guideline for configurating the Unisim Design process simulator.

A remarkable work is noted in [6]. The paper presents the design, implementation and validation by simulation of an MPC controller for controlling the composition of benzene in the distillate stream. The simulator used for the application: UNISIM R390.1 software.

All these examples had led the authors to analyze the benzene fraction of the BTX complex to design a quality control system. The analysis pursued the following objectives: modeling and simulation of the distillation column in stationary mode; process sensitivity analysis; dynamic simulation of the distillation column associated with an automatic regulation system at the base level.

II. BTX Overview

The benzene, toluene and xylenes can be produced through a series of processes, but most of the production is based on the recovery of aromatic derivatives resulting from the catalytic reforming of a $C_6 – C_{12}$ petroleum fraction. For the extraction of aromatic derivatives, liquid-liquid extraction process is used, which uses furfural ($C_5H_4O_2$) as solvent.

The technological process consists of the following steps:

- Removal of traces of olefins and di-olefins from the raw feed;
- Separation of benzene;
- Separation of toluene;
- Separation of xylenes.

The aromatic hydrocarbons obtained in the petrochemical complex BTX, respectively benzene, toluene, xylenes and ethylbenzene are important raw materials for a large number of intermediate products which are used in the production of synthetic fibers, resins, synthetic rubber, explosives, pesticides, detergents, dyes. The benzene is used in the production of over 250 products, including ethylbenzene (for styrene and polystyrene), cumene (for phenol and acetone), cyclohexane and pesticides. The toluene is used in a very large proportion as an organic solvent, but is also used for production of benzoic acid, chlorinated derivatives, nitro-toluene, etc. The xylene fraction contains four different C_8 isomers, being used to obtain para-xylene, the broadest commercially available isomer used in the production of polyester fibers and resins. Orto-xylene is used for production of phthalic anhydride, commonly used as plasticizer. Meta-xylene is used to produce isophthalic acid which gains wider acceptance in resin mixtures and polyethylene terephthalate (PET).

III. Steady-State Modeling and Simulation of Benzen Didtillation Process

The first distillation column of the BTX petrochemical complex is the benzene separation column. Due to the feed composition, flow variation and the constructional particularities, this column has a particularly important role in the petrochemical complex.

A. Construction and operating data

The benzene separation from the aromatic concentrate is performed in a column with lateral extraction of the concentrated stream in benzene. Figure 1 shows the main column data and structure and Table I describe the column constructive data. The column is equipped with five control systems. They ensure the classic operation of the distillation column, but without ensuring the control of benzene side draw concentration or the advanced recovery of benzene. The structure is operated manually as regarding to the quality of benzene side draw.

TABLE I. Distillation Column Constructive Data

Characteristic	Value
Number of real trays	44
Feed tray	30
Side draw tray	5
Type of trays	Sieve type
Diameter, m	1.65
Height, m	30.0
Construction material	Carbon steel

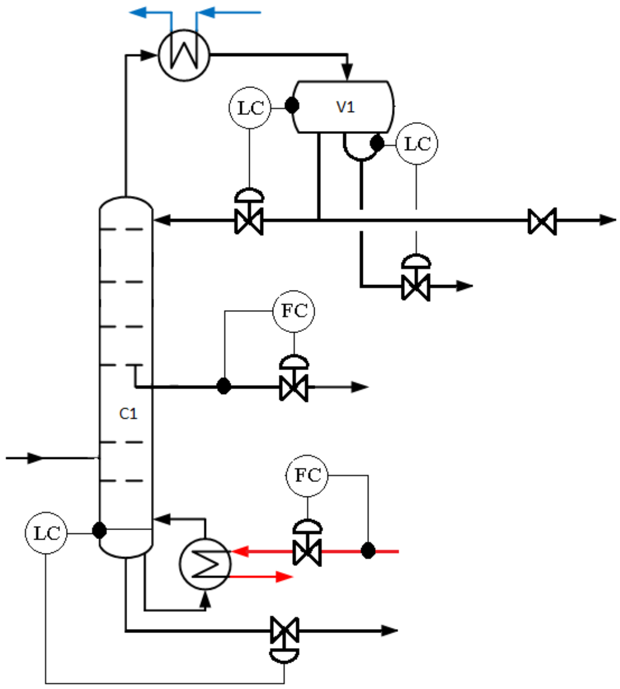

Fig. 1. Industrial distillation column control structure

One of the main operating difficulties of this distillation column is represented by distilled product. This product contains paraffin compounds that require to be removed from the column in order to avoid benzene contamination. The actual control philosophy of the column does not include any control loop for the amount of distillate product and ensure non-contamination of benzene stream.

B. Modeling the distillation process using Unisim Design simulator

The Unisim Design simulator was used to modeling and to simulate the distillation process [7]. Developing the mathematical model of the benzene distillation process is achieved by completing the following steps:

- Define the list of chemical components.
- Defining the feed stream.
- Importing the specific distillation column module and setting it up.
- Specifying the variables required to simulate the distillation column in accord with column control structure.

Considering the chemical structure of the chemical components present in the hydrocarbon system, respectively stable and whit out interactions, Peng-Robinson thermodynamic model was chosen.

The distillation column model configuration requires next specifications:

- Load the Distillation Column module of modules library.

- Connection of feed stream to the column module by making the connection in the Inlet Streams field and define the inlet tray.
- Initialization of the overhead and bottom column stream
- Initialization of the side draw stream by defining it in the Optional Side Draws field
- Filed the column module with the information's regarding the number of theoretical trays in the *Num of Stages* field.
- Setting the condenser and reboiler pressure.

The summary of the specifications used to configure the Distillation Column mathematical model is presented in Table II. Those specifications contain the streams energetical characteristics and the initialization values for flowrate, pressure and temperature profiles.

TABLE II. DISTILLATION COLUMN SPECIFICATIONS

Parameter of Distillation Column module	**Specification**
Column name	T-100
Stages	36
Inlet stream	Flux 9
Inlet stage	25
Condenser	Total
Condenser Energy Stream	Q-cond-T100
Overhead Liquid Outlet	Benzen retur
Reboiler Energy Stream	Q-reb-T100
Bottoms Liquid Outlet	Baza T100
Condenser Pressure	1.02 bar
Condenser Pressure Drop	0 bar
Reboiler Pressure	1.11 bar
Optional Condenser Temperature Estimate	60°C
Optional Top Stage Temperature Estimate	82°C
Optional ReboilerTemperature Estimate	130°C
Liquid rate	4.37 m^3/h
Reflux rate	18.0 m^3/h

An important step of the configuration operation is the selection of variables which will be used to numerically solve the mathematical model of the column. Starting from the mathematical model with three freedom degrees, mathematical model dedicated to separation column with reboiler, condenser and side draw stream, the following variables were selected: reflux rate, distillate rate and side draw rate, Figure 2.

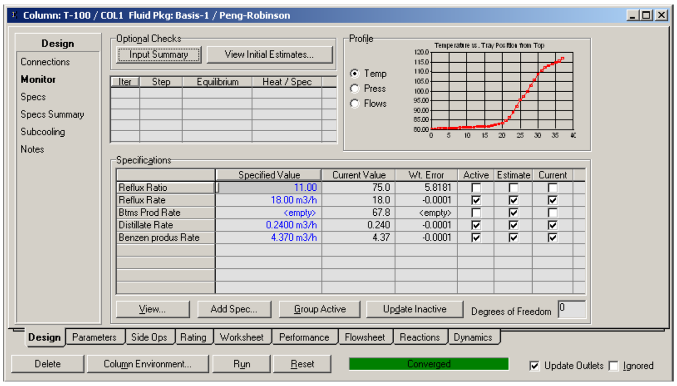

Fig. 2. Variables selected to satisfy the degree of freedom

The steady state distillation column model is presented in Figure 3.

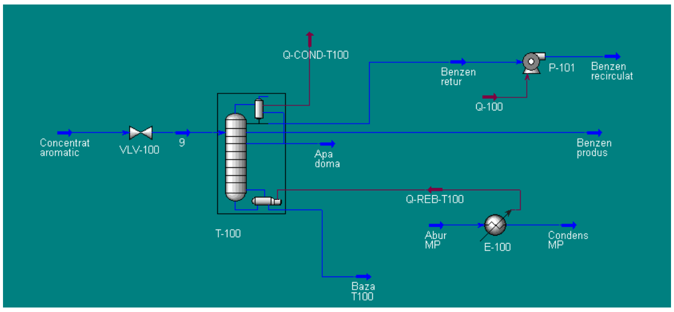

Fig. 3. Benzene distillation column simulation diagram

C. *Simulation of distillation process*

The target of distillation column simulation has been represented by the according the mathematical model to experimental data. The operation was performed using experimental data obtained for 10 days of operation of the industrial plant. Comparative results are exemplified in Figure 4. The results obtained by simulation indicate a similarity with the experimental data. Since the simulation was based on estimation of distillate flow rate, during development the mathematical model has been validated.

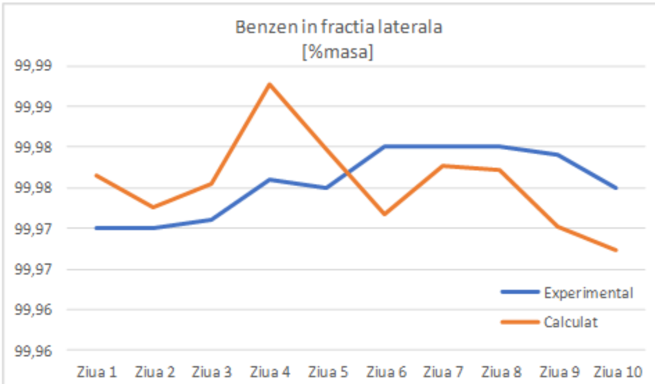

Fig. 4. Concentration of benzene in the side draw stream

Validation of mathematical model for the distillation column is highlighted by analyzing the loss of benzene in the bottom stream of the column. Figure 5 illustrates the comparative evolution of benzene concentration in the bottom product of the column, the results obtained being close to the experimental data.

D. *Sensitivity of the process*

One of the purposes of stationary simulation it's to study the sensitivity of the process and the changes caused by perturbations to the distillation process. The figure 7 illustrates the behavior of the column in case of variation of feed rate and maintaining the rest of operating values. At low feed flowrates, the quality of the benzene side draw is drastically impaired and at high feed flowrates the benzene losses in the bottom product are disastrous.

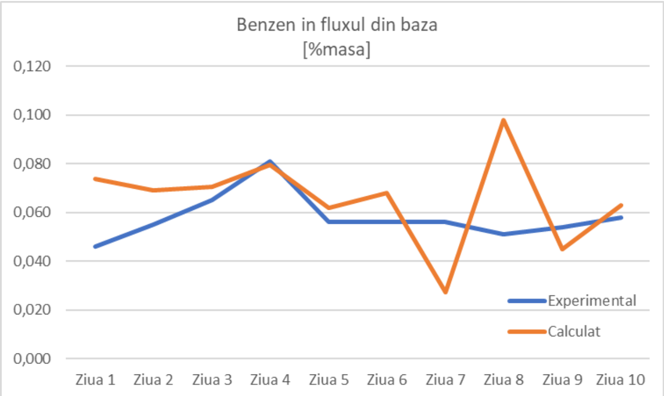

Fig. 5. Loss of benzene in the bottom stream of the column

The conclusion drawn from the analysis is the necessity to correlate the product flowrate with feed flowrates, namely the quality feedfoward control system.

The sensitivity analysis of the process also followed the influence of the reflux flow rate to the quality of the products separated in the distillation column, figure 6. Increasing the reflux flow rate in the range of 15...18m^3/h generates the increase the concentration of benzene in the side draw fraction. Exceeding the upper limit of the mentioned range no longer produces significant variations in benzene concentration. It can be appreciated that the reflux rate is a command with a linear influence on a certain range of variation, exceeding this area only leads to an increase the energy consumption of the process. Consequently, only the existence of a control system with action after perturbation of benzene concentration in side draw won’t be sufficient.

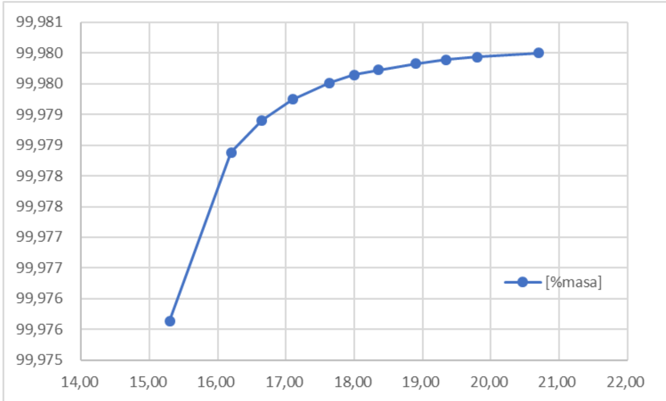

Fig. 6. Influence of reflux flow rate on benzene side draw stream quality

Although the distillate flow rate is low, the influence on product quality is very important. Increasing the distillate flow rate over a certain threshold, in a non-correlation with the feed rate, leads to a decrease the benzene concentration in the benzene side draw, figure 8-a, but the loss of benzene in the bottom product decreases, figure 8-b. It can be appreciated that the distillate flow is a fine control action for the quality of separated products.

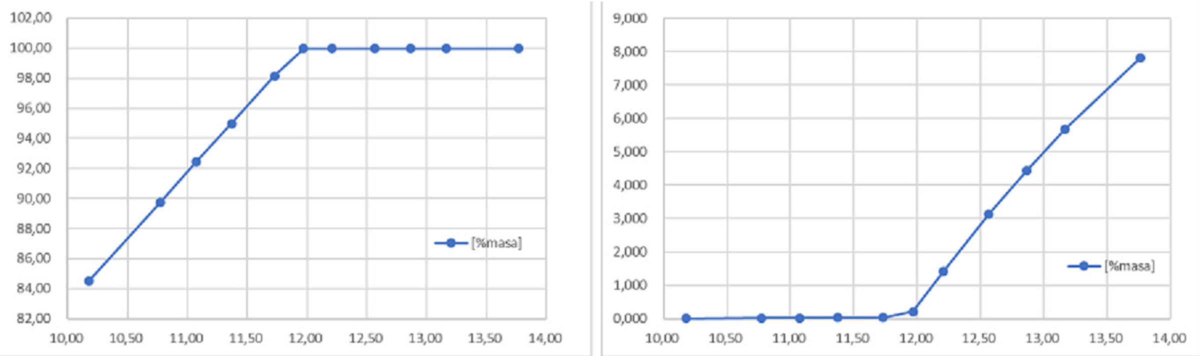

Fig. 7. Sensitivity analysis in relation to feed flowrate: a) benzebe in of the benzene side draw; b) benzene in bottom product

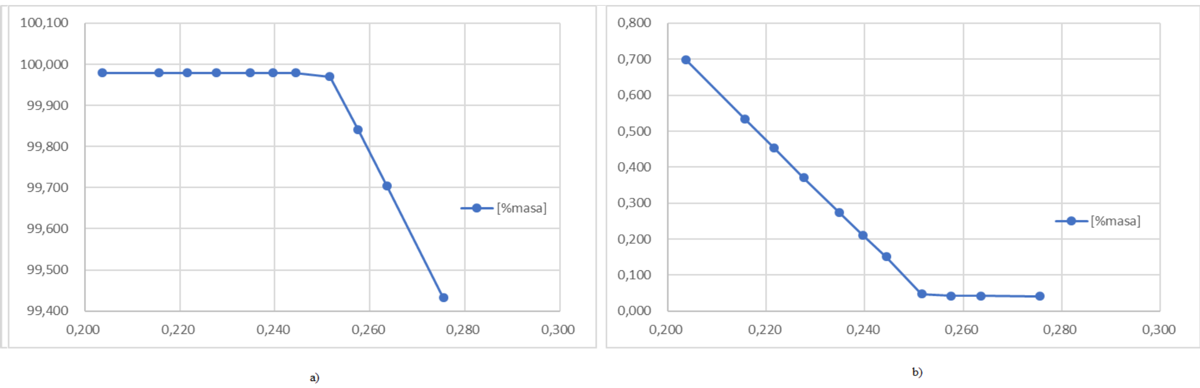

Fig. 8. The benzene content in the side draw stream at the variation of distillate product rate: a) benzene concentration in the benzene side draw; b) benzene in the bottom product

The conclusions generated by the process sensitivity analysis can be synthesized as follows:

a) The feed rate is an important disturbance of the distillation process. It's influence on the quality of the separated products is particularly important, requiring the design of an feedfoward quality control system to maintain the quality of both products (side draw – benzene and bottom stream)

b) The reflux flowrate has a relatively low influence on the quality of the side draw – benzene. It's noted the nonlinear character of the quality-flow characteristic, the reflux flow increases leading to capping the quality of the benzene side draw. Consequently, around the average operating point, the reflux rate has no influence on the quality of the products separated in the fractionation column.

c) The distillate flow rate has a reverse influence on the quality of the products. The influence is especially felt on the bottom product where the variation in benzene concentration is significant. The characteristic generated by the distillate flow rate indicate first the necessity for flow control and second the correlation required with the feed flowrate.

d) The flowrate of the side draw has an inverse influence on the quality of the two obtained products. Extreme flow rates only influence the quality of the side draw product. Under these circumstances, the best control system will have to include this parameter in its structure to ensure command in case of disturbance in the quality of both products.

IV. PROCESS DYNAMIC SIMULATION

The principles of dynamic simulation of the distillation process have ben extensively presented by the authors [5]. According to this reference, the steps necessary to achieve the mathematical model of the dynamic process are as follows:

a) Steady state modeling of distillation process.

b) Selection of the dynamic specifications of the material streams and ensures the continuity of pressure flows.

c) Implementation of the flow control systems and the level control systems of the fluid accumulation points.

d) Dynamic integrator settings configuration

A. Steady state modeling

The modeling of the distillation process in stationary mode is presented in detail in the part III of the paper.

B. Configuration of dynamic attributes asociated with product streams

To solve the differential equations associated with stream flow, the mathematical models of the material streams must contain initial conditions that allow determination of the solution. For this purpose, mathematical models associated with material streams must be configured with the Dynamic Specifications / Pressure = Active option, Figure 9.

C. Control systems implementation

Dynamic process simulation using the Unisim Design environment involves the implementation of the control systems. For the distillation process shown above, five automated control systems were required. All of them are required by the Dynamic Assistance control. Three of them are associated with process input / output flow rates, while two are associated with two liquid storage points (the reflux / condenser vessel and the base of the column). Figure 10 shows a dynamic simulation diagram of the process with all associated automated control systems.

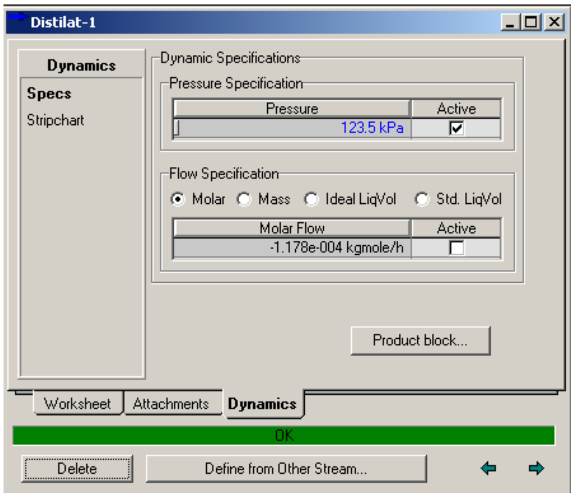

Fig. 9. Dynamic configuration of stream material flow

TABLE III. CONTROLLER'S SPECIFICATIONS

Tag	PV		OP	
	Object	***Variable***	***Object***	***Variable***
FC-100	Concentrat aromatic	Liq Vol Flow @Std Cond	VLV-100	Actuator desired position
IC-110	Distilat	Std Ideal Liq Vol Flow	VLV-Distilat	Actuator desired position
FC-120	Benzen produs	Liq Vol Flow @Std Cond	VLV-101	Actuator desired position
FC-160	Q-REB-T100 @COL1	Heat Flow	Q-REB-T100	Control Valve
LC-130	Condenser @COL1	Liquid Percent Level	Reflux @COL1	Control Valve (controls flows)
LC-140	Reboiler @COL1	Vessel Liq Prercent Level	VLV-Baza T100	Actuator desired position

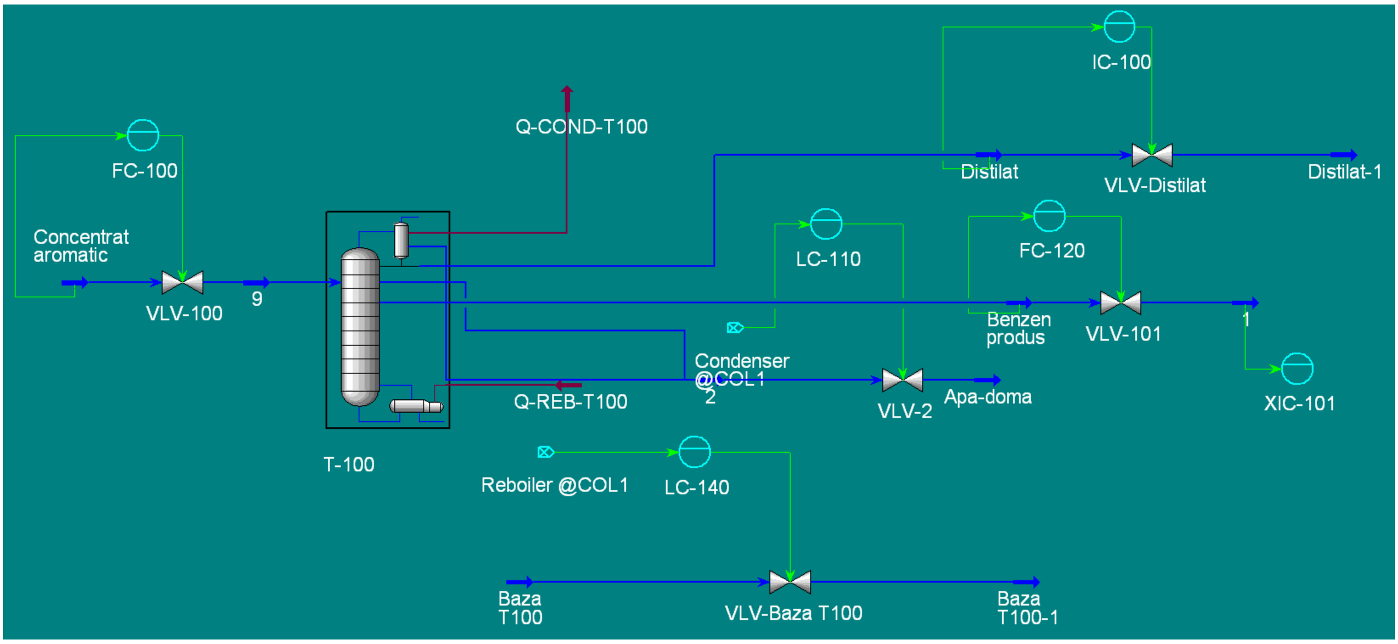

Fig. 10. Dynamic process simulation diagram

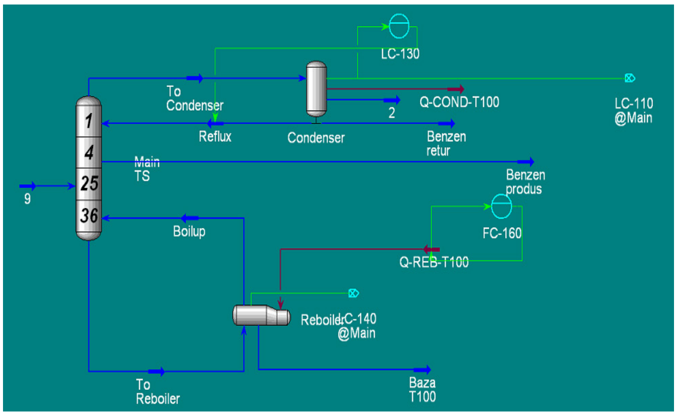

Fig. 11. Internal column dynamic simulation detail chart

The process diagram contains control systems for column feed rate (FC-100), distillate product (IC-100), benzene side draw (FC-120) and the level in reboyler / bottom of the column (LC-140). To access the rest of control systems, it is necessary to activate the column object (T-100). Figure 11 shows the internal column dynamic details. According to the figure, automatic level controller for level in the condenser (LC-130) and the water brine level (LC-110) are implemented for top of the column control.

Configuration of each automated control system requires defining the process variable and the associated command variable [8]. In table III are presented the elements necessary for configuring all the six automated control systems, respectively the process values PV and process outputs OP values.

The desired performance of the process simulation can be achieved by fine tuning of the implemented control systems [9]. The operation involves two categories of actions. First requires a try and error approach - simulation at different values of the controller's parameters, the best K_p and T_i pair is considered the optimum parameters of the controllers, Table IV.

A raised problem during developing the dynamic simulation was the correct dimensions of the control valves. Although the simulator has the size function, in some cases the adjusting valve is oversized, leading to the instability of the automated control system. The authors experience in this field was decisive and some errors induced by the sizing function by the simulator were corrected [10].

TABLE IV. CONTROLLER CALIBRATION

Controller	Tag	K_p	Ti [min]
Feed rate controller	FC-100	0.2	4
Overhead water brine level controller	LC-110	0.5	3
Side draw rate controller	FC-120	0.1	0.5
Reflux rate controller	LC-130	0.4	5
Bottom stream level controller	LC-140	0.2	3

D. Dynamic simulation results

Following the steps described in paragraphs B and C, the simulation program of the distillation column and the basic control system (Figure 1) were obtained. All controllers have been tuned and they are operated in automatic mode. Running the dynamic simulation for infinite time of integration generates several types of results. In the first phase, the results lead to a numerically accepted stationary state. By reaching in dynamic mode the stability of the stationary state showed the stability of the automated control system. For this reason, the sizing and tuning of the control valves is an important component of the simulation. If this stage is successfully completed, the stability of the control system is reached. The most important controller faceplate is shown in the Figure 12.

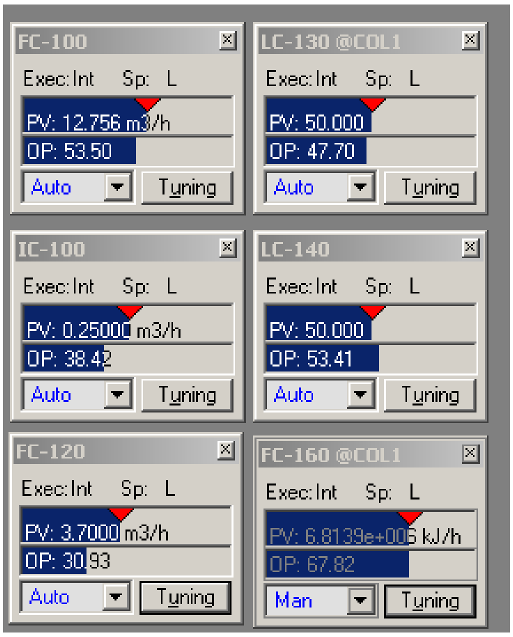

Fig. 12. Controller faceplates in dynamic mode

Due to the integrator component of the controllers, all of them are stable with very low dynamic errors. Under these conditions the dynamic simulation of the benzene distillation column is validated and can be used. The current stage of the research included also few tests, one of them involves modification of the benzene side draw flowrate from 3.7 to 3.9m^3/h. The dynamic response of the concentration of the benzene component in the benzene side draw is shown in the Figure 13. The concentration of benzene decreases over time and the dynamic response is similar and corresponds to a second order dynamic element.

The obtained numerical result validates the dynamic mathematical model of the process and, implicitly, the dynamic simulation as an informatic instrument designed to analyze the dynamics of the distillation column and the future quality control system structure.

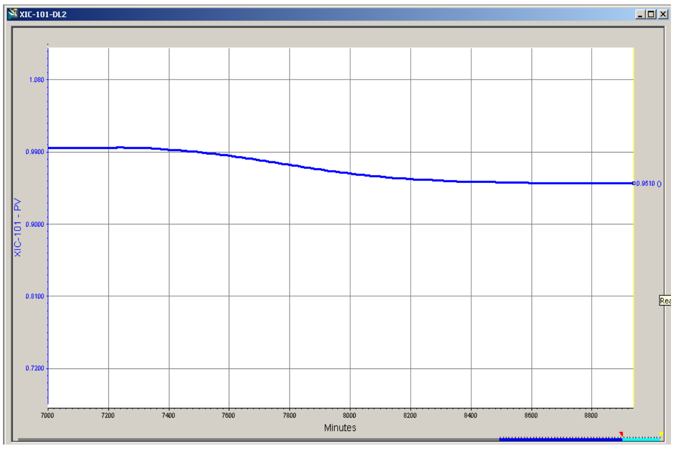

Fig. 13. The dynamic response of the benzene concentration into the benzene side draw.

V. Conclusions

The paper presents the authors researched in the field of control system of the benzene distillation process from an industrial plant. From all the necessary stages required to design the automated quality control system, the modeling and simulation of the distillation column have been solved.

Simulation of the process in stationary regime was used for process sensitivity analysis. The analysis had led to the following conclusions:

a) The feed flow is an important process perturbation, which requires a control feed structure for control product quality.

b) At high values, the reflux flow rate has a low influence, which is why this variable will not be included in the quality control structure. However, reducing operating costs requires minimizing the reflux flow rate, especially in context of maintaining product concentration at specified values.

c) The benzene side draw is the most powerful command for the future automated control system.

The dynamic regime of the simulation has been calibrated to ensure the stability and control for further tests and for design of the automated quality control system.

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