Specific Problems of Using Unisim Design® in the Dynamic Simulation of the Propylene-Propane Distillation Column

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The paper analyzes the principles and particularities of using Unisim Design® environment in the dynamic modelling and simulation of chemical processes. The paper presents the four stages of configuration and simulation of the distillation process: steady-state modelling and simulation of the process, particularities of dynamic model configuration for propylene-propane distillation column, configuration of control structure for separated products quality, and dynamic simulation of propylene-propane distillation column. There are also presented the results of dynamic simulation of propylene-propane separation process with L-B structure for separated products quality control. The obtained results validate Unisim Design® as a powerful tool in dynamic simulation of distillation processes control systems.

Keywords: distillation, dynamic modelling, simulation, quality control systems

In order to design control systems for distillation processes the knowledge of the process mathematical model is required as a form of expression of its functional characteristics. Thus, both the design and simulation of the control systems involve two types of models: steady-state simulation model and dynamic simulation model. Dynamic mathematical models present high complexity compared with steady-state models, therefore the aspects related to the correlation of model dimensions with the solving time become of special importance. The design, configuration and solving these models was and is dependent on the programming environment, simplifying hypothesis etc. Over time, there were developed and used many types of dynamic models for distillation processes.

Analysis of some published works in the field of dynamic modeling and simulation of chemical processes, especially the fractionation processes, highlighted several approaches to this problem. Thus, four types of approaches have been identified:

-analytical modelling and development of simulation programs using classic programming environments;

-analytical modelling and model programming using dedicated dynamic simulation environments;

-analytical modelling and/or adaptation of models based on transfer functions and programmed in MATLAB® or SIMULINK®;

-configuration of simulators for chemical processes dynamic.

In the following are presented briefly some particularities of chemical processes modelling and simulation based on the four types of approaches.

Analytical modelling and development of simulation programs using classic programming languages were approached in [1] for the dynamic simulation of optimal control system for an industrial furnace.

The paper [2] treats the problem of dynamic modelling and simulation of an atmospheric distillation process. Mathematical modeling was addressed structural, meaning that the distillation process was decomposed into sub-processes (column, strippers, pumparounds, condenser-reflux drum), for each of these sub-processes being developed dynamic mathematical models. Dynamic simulation was based on a steady-state determined with PRO/II® simulator. The structural approach of the process imposed for the dynamic simulation the use of a versatile and powerful simulator, DIVA [3], designed for simulation of complex industrial plants.

An original approach of dynamic modelling and simulation of a reactive distillation process was presented in [4]. This approach is based on the detection of existence of potential phase splitting in reactive distillation columns, the simulations leading to much more precise results compared to the classical approach in terms of dynamic behaviour of the process.

Other approach [5] in the field of dynamic modelling and simulation is based on the dynamic model proposed by Skogestad [6, 7] which is associated to a binary distillation column. This model is based on the use of overall material balance and component balance, equilibrium equations and hydraulic delays associated with the transport phenomena of vapor and liquid flows. The model adapted in [5] takes part of a dynamic simulation structure associated with the main control systems for a distillation column, the simulation being performed in SIMULINK®.

Important elements regarding the dynamic simulation of a distillation column using DYNSIM® environment are presented in [8]. The paper investigates the dynamic behaviour of the column to changes in set points of the composition control systems, and also to changes of disturbances, feed flow rate and composition.

The purpose of dynamic simulation presented in [9, 10] for the propylene-propane distillation column was the investigation of the column dynamic behaviour and use of the obtained data for the development of simplified dynamic model for the process used further for analysis and synthesis of the control system for this column. Process simulation was performed in HYSYS®, while the control system was implemented in MATLAB®, the connection between the two environments being carried out through a specific communication system.

Dynamic simulation has been addressed for other chemical processes, an example being the catalytic

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Table 1
GEOMETRICAL CHARACTERISTICS OF THE DISTILLATION COLUMN

Parameter	Value [mm]
Column diameter	2440
The arrow at the side weir	365
Distance between central weir chords	292
Distance between trays	457

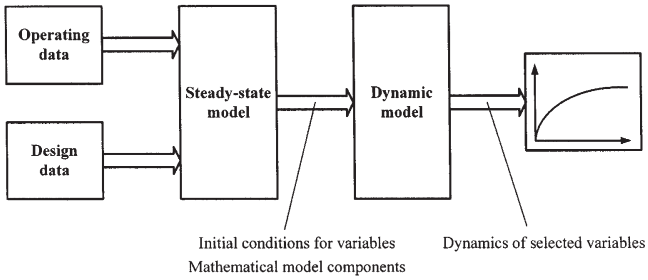

Fig. 1. Structure of operations associated to dynamic simulation

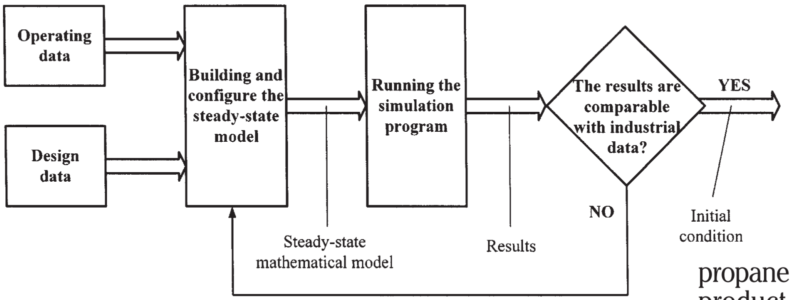

Fig. 2. Detailing the development of steady - state model

cracking process. The dynamic mathematical model for this process, presented in [11, 12] treats its sub-processes as lumped parameter systems. The model consists of first order dynamic equations and was implemented using SIMULINK®.

Another example of the use of dynamic modeling and simulation is from waste water treatment field [13]. The dynamic model of the process and the controllers were implemented in SIMULINK® environment.

In the article there are investigated the specific problems of using Unisim Design® in the dynamic modeling and simulation of the propylene-propane distillation column.

Propylene-propane separation process

Distillation is the most common process for separating mixtures of chemical components, being used in most chemical and oil processing plants. This separation technology is especially recommended for high purity separations since any degree of separation can be achieved in case of a constant energy consumption by increasing the number of theoretical equilibriums.

The propylene-propane separation process is part of the pyrolysis plant and the catalytic cracking unit, which are currently the systems that produce large amounts of propylene. The importance of this distillation process, and hence the column in which the process takes place, is given by the uses of propylene. The resulted propylene is used in polymerization and in a series of chemical synthesis, such as the obtainment of isopropyl-benzene by alkylation, of alcohols by oxosynthesis, of propylene oxide by chlorine hydration, of isopropyl alcohol by hydration. For this reason, the propylene from the propylene-propane separation column requires purities such as 92-94 % volume for the propylene used in chemical treatment, and 99.5 - 99.8 % volume for the propylene used in polymerization. The propane resulted from separation is far from being a residual product, being used as LPG fuel.

The studied industrial propylene-propane column is part of GASCON unit from the catalytic cracking platform. The distillation column has 90 Glitsch trays, each of these having two side weirs and a central weir. Some design data of the column are presented in table 1.

Principles of Unisim Design® use in dynamic simulation of chemical processes

Unisim Design® simulation environment is intended for both steady-state and dynamic simulation of chemical processes. In order to use the Unisim Design® to simulate the dynamic mode, the user must follow the steps shown in the diagram from figure 1. The input data necessary for simulation are the operating data of the chemical process and design data associated with static and dynamic equipment present in the chemical plant. In the first stage is designed and simulated the process in steady-state and after validating the model the second step is addressed, the dynamic modeling of the chemical plant.

Figure 2 presents the development stages of the steady-state model. Using the initial data and the predefined models for each type of chemical process the steady-state model for the plant is built. At this point the user must configure each predefined model according to the operating and design data. Because Unisim Design® is always in RUN mode, debugging the model is easily accomplished. Upon completion of the development and simulation of steady-state model, the user has to validate the developed model by comparing numerical results with industrial data. If there are significant differences, some predefined models require reconfiguration aiming to reduce these errors. At the end of this phase the initial condition for the dynamic model is obtained.

The development of the dynamic model is different from the steady-state model building. The starting point is represented by the model and results obtained from steady-state simulation. The next step is defined by the dynamic model building and configuration, figure 3. This stage

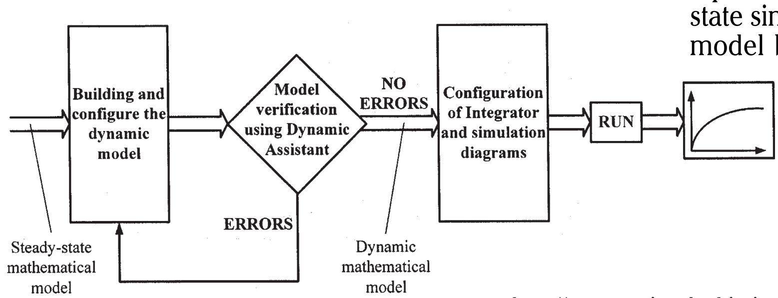

Fig. 3. Detailing the development of dynamic model

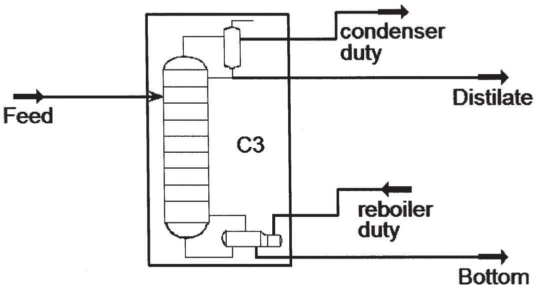

Fig. 4. Steady-state simulation diagram for propylene-propane distillation column

Table 2
REBOILER AND CONDENSER DIMENSIONS

	Reboiler	Condenser
Diameter [mm]	755	1041
Height [mm]	2767	7410

requires data regarding geometric and functional characteristics of plant equipment and also an appropriate configuration of the models associated with these equipment. To verify the correctness of design and configuration of the dynamic model Unisim Design® provides a verification tool called Dynamic Assistant. This tool detects possible errors, signals their presence and directs user action to eliminate them. After eliminating all errors the dynamic model of the chemical plant is obtained. For the dynamic simulation, the user must configure the module for numerical integration, configuration which refers to the integration time and the variables for which the dynamic characteristics are wanted for display.

Steady-state modelling and simulation of distillation process

The need for steady-state simulation of a process is motivated by the determination of the initial conditions of all the variables that describe that process. The use of Unisim Design® in steady-state modelling and simulation of the distillation process implies the following sequential steps [14]:

a) define the list of chemical components and thermodynamic model selection;

b) create the simulation diagram and configure the distillation column model;

c) process simulation.

Define the list of chemical components and thermodynamic model selection

Distillation column feed consist of propylene, 70 mole %, and propane, 30 mole %. Taking into account the fact that the chemical structure of the components present in the system, which are hydrocarbons characterized by absence of interactions, the Soave - Redlich – Kwong (SRK) thermodynamic model is selected.

Create the simulation diagram and configure the modules

The simulation diagram represents one of the main elements of process simulation in Unisim Design®. In order to simulate the propylene-propane distillation process the following stages have to be performed:

a) definition of feed;

b) loading and configuring the distillation column module;

c) configuration of results windows.

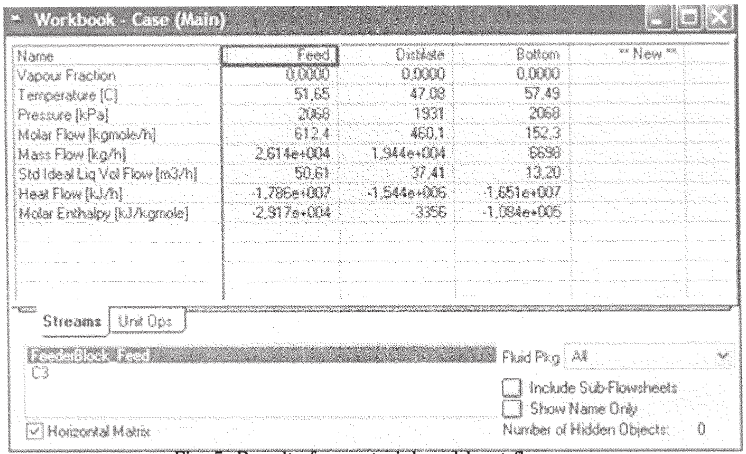

Fig. 5. Results for material and heat flows

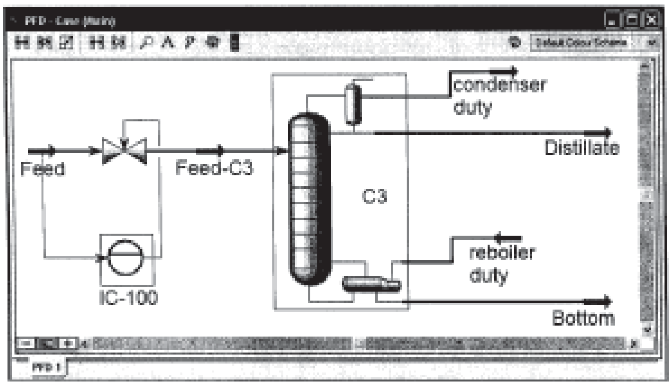

Fig. 6. Intermediary phase of dynamic simulation diagram

The feed, implemented by a *Stream* module, contains industrial specifications of the feed flow: vapour fraction = 0; pressure = 20.68 bar; flowrate = 612.4 kmol/h.

Loading and configuring the distillation column module is the focal point of the simulation diagram. The *Distillation Column* module (fig. 4) is configured based on the technical specifications of the real column. The distillation process model is particularly complex, the numerical solving being iterative, by improving an initial solution. This solution can be estimated only if two additional variables are specified, operation performed by the group of commands Design – Specs. The selection of the two additional variables must be done in accordance with the structure of the process control system.

After this sequence of configuration operations, by activating *Run*, the mathematical model can be solved.

The configuration of results windows is necessary because Unisim Design® is always in Run mode and any change of input data is immediately processed and the output data are recalculated. Figure 5 presents a typical image of input data, and material and heat balance for the distillation column.

The results obtained in steady-state simulation of the propylene-propane separation process, regarding compositions, are $x_D = 0.9127$ mole fr. and $x_B = 0.0873$ mole fr., these being similar with the industrial data. This comparison represents the validation of the steady-state model for the propylene-propane separation process.

Particularities of dynamic model configuration for propylene-propane distillation column

In Unisim Design® the dynamic models of chemical processes are hosted in the same modules as the steady-state models. The specific elements for dynamics have to be activated or created respecting the environment-specific modeling concepts presented in the section on steady-state modeling and simulation of distillation

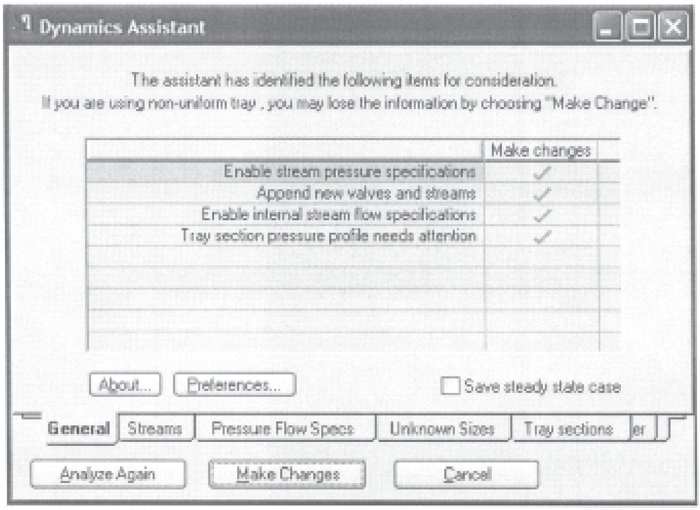

Fig.7. Errors generated by Dynamic Assistant

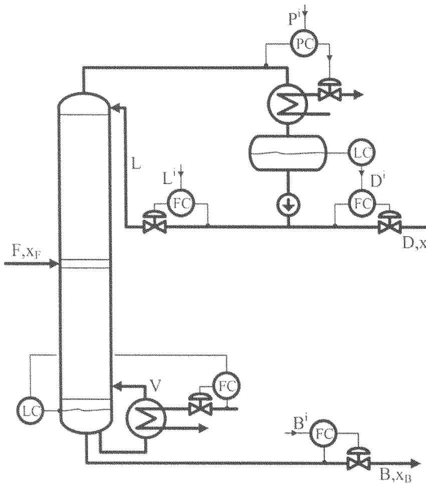

Fig. 8. L-B control structure

process. In order to create and configure the dynamic model of the propylene-propane distillation column the following steps must be performed:

a) feed stream configuration;

b) holdup configuration for the distillation column;

c) dynamic model verification using Dynamic Assistant.

Feed stream configuration

The column feed is modeled according to steady-state model concepts. First change to the steady-state model is the introduction of dynamic elements in the model of this stream. The change is the implementation of control systems for the feed flow rate. Starting from the steady-state model the steps bellow must be covered:

a) disconnect the feed from the distillation column, insert and configure a control valve on this stream. The following parameters are set: a pressure drop of 5 bar (similar to industry values), a linear inherent characteristic, 50 % opening;

b) reconfigure pressure value and connect the new feed stream to the distillation column. Because the control valve introduced an additional pressure drop, which was not considered in steady-state, the reconfiguration of feed pressure is required so that the control valve upstream pressure to be equal to feed tray of the column, pfed = 19.81 + 5 = 24.81 bar;

c) configure the feed flow rate controller. Dynamic simulator operation requires to control the feed flow rate. Therefore the user must implement a flow rate control system using PID – Controller module from Unisim library. Initial controller configuration consists of specifying: the process variable (defined as internal variable Std Ideal Liq Vol Flow), the actuator (the internal variable Actuator desired Position), and the controller parameters (acting mode, Action=Reverse; operating mode, Mode=Man; controlled variable range, [0…80] m^3/h; initial value of control signal, 50%; gain, Kp=1).

Configuring holdup for the distillation column

The distillation column is characterized by two holdup points which were not considered in steady-state, namely the reboiler and the condenser. Industrial dimensions of these elements are presented in table 2 and Unisim calculates the equipment volumes and initializes the liquid holdup used in the dynamic equations. After these two configuration steps the simulation diagram looks like in figure 6.

Dynamic model verification using Dynamic Assistant

To debug the dynamic model, the user has available Dynamic Assistant function that investigates modelling elements, initial conditions and how the dynamic models are configured. After completing the two stages described above, Dynamic Assistant led to four sources of error for dynamic models, figure 7.

The first error, Enable stream pressure specifications, is generated by the lack of pressure specification for the stream Feed. To solve this error, in Dynamic – Specs option for stream Feed, Pressure Specification is set active. In this way, Unisim introduces holdup dynamic model for Feed module.

The second error, Append new valves and streams, is generated by the lack of (control) valves for distillate and bottom streams. One of the particularities of Unisim dynamic modelling is the need for valves or flow rate or pressure control systems on the output streams. Accordingly, for streams Distillate and Bottom (control) valves must be inserted, as suggested by Dynamic Assistant in option Streams, Stream Spec – Insert Valves. For stream Distillate is inserted a valve configured with a 0.5 bar pressure drop (50kPa), linear inherent characteristic, and valve opening 50%. To eliminate the error Append new valves and streams, a pressure specification has to be activated for the new stream Distillate2 inserted after the valve. Similar action is made for stream Bottom. After these configuration operations, the error Append new valves and streams is completely eliminated.

The third error, Enable internal stream flow specification, is generated because the column reflux is not included in the dynamic model. Using the command Make changes from Dynamics Assistant, option Stream Spec-Int. Flow Spec is activated and the variable Reflux@COL1 is included in the model.

The error Tray section pressure profile needs attention shows the fact that the column trays pressures calculated in steady-state are not the same with the ones associated with the dynamic regime. After activating the dynamic specification for column reflux the column pressure drop is 73.96 kPa and the reboiler pressure is 2005 kPa. In these circumstances, the dynamic pressure drop is 108.3 kPa which differs with 35 kPa from steady-state pressure. This situation leads the user to modify the reboiler pressure to 2040 kPa. Because the reboiler pressure has changed, so are the trays (including feed tray) pressures.

After this operation, Dynamic Assistant has a single error, Stream pressure differ from attached stages which is generated by the difference of 10 kPa between feed tray pressure and feed stream pressure. To correct this

Table 3
CONFIGURATION PARAMETERS OF PID – CONTROLLER AND CONTROL VALVE FOR LEVEL CONTROL SYSTEM FROM COLUMN BOTTOM

	Module	
	PID – Controller	***Virtual Valve***
Flowsheet	C3	C3
Object	Main TS	Reboiler duty
Variable	80_MainTs (last tray)	Total Liquid Volume Percent
Variable Specifics		80_Main TS

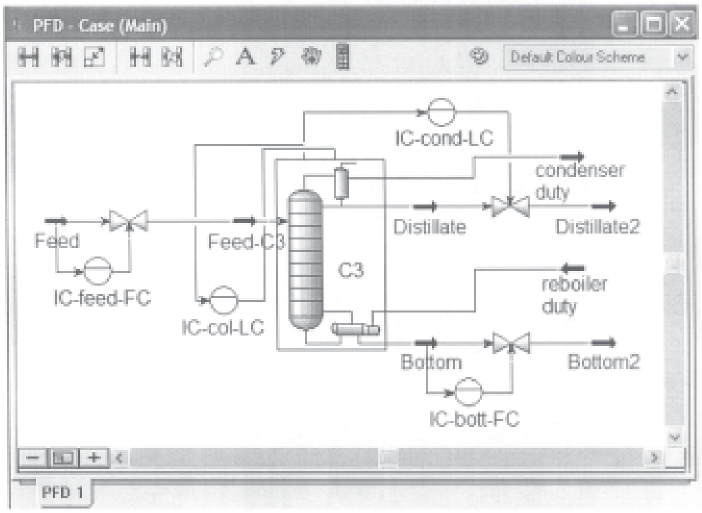

Fig. 9. Dynamic simulation diagram of the distillation column

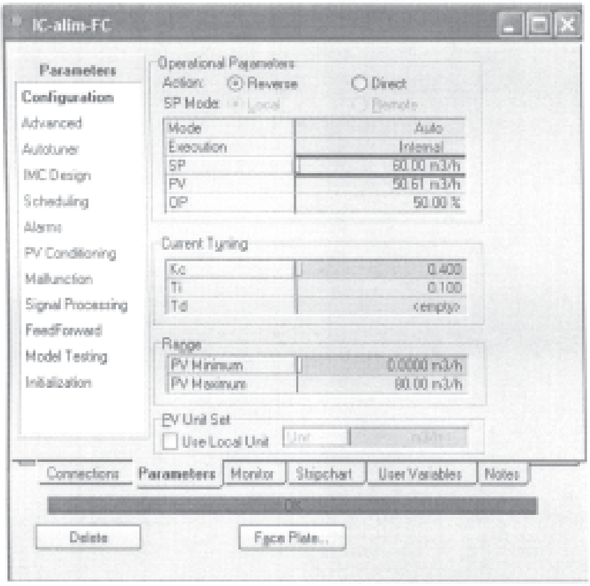

Fig. 10. Change of set point for feed flow rate control system

difference, the pressure of stream Feed is modified to 2071 kPa. In this way, all the conditions for dynamic simulation are satisfied.

Configuration of product quality control structure using L-B control agents

The dynamic model to this step does not contain the main control systems associated to a distillation column. For the propylene-propane distillation column was chosen L-B control structure, figure 8 [16, 17]. This structure contains five control systems for the following parameters: reflux flow rate (for distillate quality control), bottom flow rate (for bottom product quality control), column top pressure, reflux drum level, and column bottom level.

For dynamic simulation of the distillation column equipped with the five control systems described above is necessary to create and configure these systems in Unisim Design®. In the following are presented the most important aspects of these configurations.

Bottom flow rate control system. In order to control stream Bottom flow rate a PID – Controller and a Control Valve are used. The controlled variable measurement range is set so that the measured flow rate is 50% of that range. From steady-state data, Bottom flow rate is 13.01 m^3/h and, consequently, the measurement range of the sensor will be [0…26] m^3/h.

Reflux drum level control system. For the implementation of this control system are used a PID – Controller and a Control Valve, and the level measurement range is [0…100] %.

Column bottom level control system. According to figure 8, column bottom level is controlled by modifying the reboiler thermal load. In this case, the level controller will act on a virtual valve which has as variable Reboiler Duty. The configuration parameters for the controller and the control valve are presented in table 3. The controller set point is $7.172 \cdot 10^7$ kJ/h and therefore the upper limit of the measurement range is set to $1.4344 \cdot 10^8$ kJ/h.

A.Reflux flow rate control system. This system is configured in the Column Environment flow sheet. In this case the actuator will be a virtual one, and the measurement range of the flow rate is set to [0…894] m^3/h.

With this operation, the dynamic simulation diagram of the propylene-propane distillation column, with the L-B structure, will have the form shown in figure 9.

Dynamic simulation of the propylene-propane distillation column

Runtime configurations

In this last stage, the user must configure both numerical integrator and selection of variables whose dynamics will be monitored.

Numerical integrator configuration consists of setting up the integration interval [0…t_{max}], without this option being considered an integration on an infinite period of time.

In order to monitor the results, Stripchart option is used. First, is opened the window of the controller whose variables are to be monitored and are selected the desired variables under the Variable Set option. It is recommended that, after this action, the user to save the application into a file considered starting point for any subsequent change.

After completing this step the simulator can be switched in dynamic mode and the integrator activated. When the integration time reaches t_{max}, graphic trends are obtained for the selected variables dynamics.

System simulation to feed flow rate change

The dynamic simulation of the propylene-propane distillation column is performed to a change from 50 to 60 m^3/h in feed flowrate, which is a disturbance for this system. This change can be done by modifying the setpoint of the feed flowrate control system, figure 10.

Figures 11 and 12 present the dynamic trend for propylene concentration in distillate and in the bottom product, respectively. After a 13 h dynamic, propylene concentration in distillate has reached a steady-state at 0.9241 mole fr. and propylene concentration in bottom product has reached a steady-state at 0.0582 mole fr.

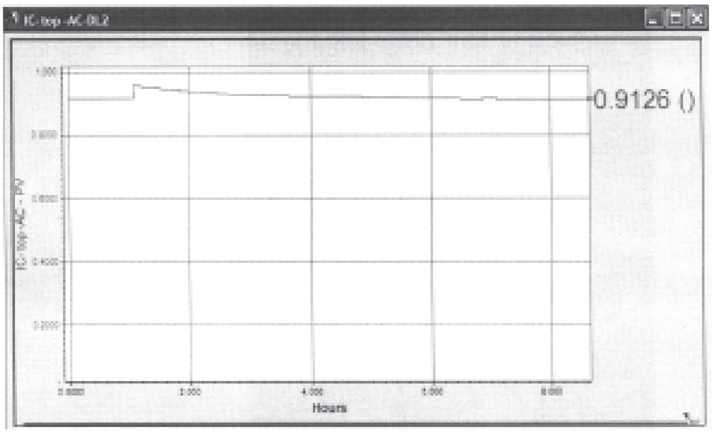

Fig. 11. Dymanics of x_D composition

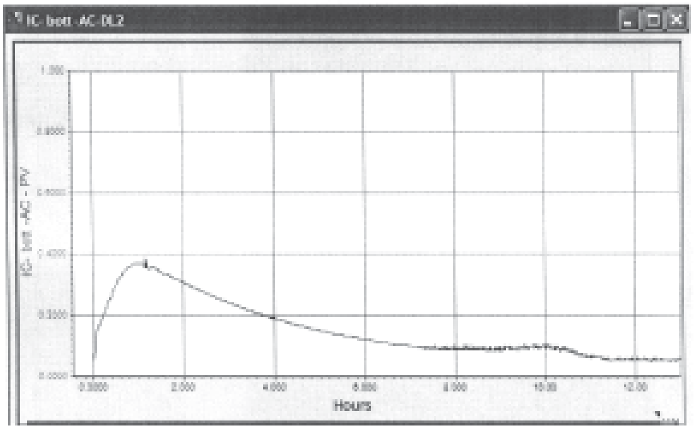

Fig. 12. Dymanics of x_B composition

Conclusions

The paper treated the issue of using Unisim Design® environment in dynamic simulation of propylene-propane distillation column. There were identified the principles of Unisim Design® use in dynamic simulation of chemical processes: steady-state modelling and simulation, dynamic modelling, dynamic simulation. The steady-state simulation results were validated by comparison with industrial data. There were identified the particularities of dynamic modelling and configuration of propylene-propane distillation column: feed stream configuration, holdup configuration for the distillation column and dynamic model verification**.** The obtained dynamic model was used for simulation of a control structure for separated products quality.

References

1.PATRASCIOIU C., MARINOIU V., Proceeding of the 5th IFAC Symposium on Dynamics and Control of Process Systems, 1998, p. 490-495.
2.RĂDULESCU, G., PETRE, D., Bul. Univ. Petrol-Gaze din Ploieşti, Tech. Series,**LV**, No. 2/2003, p. 94-101.
3.KRÖNER, A., HOLL, P., MARQUARDT, W., GILLES, E.D., Computers & Chemical Engineering, **14**, Is. 11, 1990, p. 1289-1295.
4.RĂDULESCU, G., PARASCHIV, N., MIHALACHE, S.,Rev. Chim. (Bucharest), **64**, no. 9, 2013, p. 1043
5.MIHALACHE, S.F., POPESCU, M., Proceedings of the 11th WSEAS Int. Conf. on Circuits, Systems, Communications and Computers, 2007, p. 75-80.
6.SKOGESTAD S., MORARI M., Ind. Eng. Chem. Res., **27**, 10, 1988, p. 1848-1862.
7.SKOGESTAD, S., POSTLETHWAITE, I., Multivariable Feedback Control, 2nd Edition, John Wiley & Sons, 2007.
8.POPESCU, M., FRÂNCU, S., Bul. Univ. Petrol-Gaze din Ploieşti, Tech. Series, **LVIII**, No. 1/2006, p. 160-164.
9.BĂIEŞU A., Control Engineering and Applied Informatics, **10**, No. 3, 2008, p. 46-52.
10.BĂIEŞU A., Control Engineering and Applied Informatics, **13**, No. 1, 2011, p. 49-53.
11.POPA C., PĂTRĂŞCIOIU C., Rev. Chim. (Bucharest), **61**, no.4, 2010, p. 419
12.POPA C., PĂTRĂŞCIOIU C., Proceedings of the 6th WSEAS International Conference on Dynamical Systems and Control, 2010, p. 95-100.
13.OSTACE G.S., CRISTEA V. M., AGACHI P. S., Environmental Engineering and Management Journal, **11** (1), 2012, p. 147-164.
14.*** Process Modelling using UniSim Design, Student Guide 4526, Honeywell, 2009.
15.*** Dynamic Modelling using UniSim Design, Student Guide 4528, Honeywell, 2010.
16. MARINOIU, V., PARASCHIV, N., Automatizarea proceselor chimice, Ed. Tehnică, Bucureşti, 1992.
17.SKOGESTAD S., LUNDSTRÖM P., JACOBSEN E.W., AIChE Journal, **36**, No. 5, 1990, p. 753

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