

# A Comparative Study of the Modeling and Quality Control of the Propylene-Propane Classical Distillation and Distillation Column with Heat Pump

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**Abstract**—The paper presents the research evolution in the propylene – propane distillation process, especially for the distillation columns equipped with heat pump. The paper is structured in three parts: separation of the propylene-propane mixture, steady state process modeling, and quality control systems. The first part is dedicated to state of art of the two distillation processes. The second part continues the author's researches of the steady state process modeling. There has been elaborated a software simulation instrument that may be used to dynamic simulation of the process and to design the quality control systems. The last part presents the research of the control systems, especially for quality control systems.

**Keywords**—Distillation, absorption, heat pump, Unisim Design.

## I. INTRODUCTION

THE distillation and absorption processes are known as separation process, and they are applied in chemical industry. The study of these processes includes the liquid – vapor equilibrium, constructive problems and control problems. Indifferent to the process particularity, the quality control system does not elaborate without the modeling and simulation chemical process in steady state and dynamic regime. One of the distillation processes is propylene-propane distillation. The classically propylene-propane distillation is very known process. The domains of propylene-propane distillation researches are modeling, design of robust control, and multivariable control systems [7]-[10]. An important research domain is represented by using the heat pumps into distillation or absorption processes [11]-[13]. In these conditions, in the last years, we have studied the propylene-propane classical distillation process and the same distillation process with heat pump [1]-[6]. The focus of this paper is the presentation of the new modeling results and the analysis of the quality control systems for classically distillation column and for column equipped with heat pump.

## II. SEPARATION OF THE PROPYLENE-PROPANE MIXTURE

### A. The Classical Method of Propylene-Propane Mixture Separation

The propylene-propane mixture is a base product of the petrochemical and oil industry that is produced in the catalytic

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cracking and pyrolysis plants. The propane can be used in petrochemical industry as either a raw material in various degrees of purity (concentrations around 90-92%) or as a monomer in polymerization industrial facilities (concentration 99.99%). The propane is used as fuel with a variable degree of concentration. The classical method of separation of the two components of the propylene-propane is the classical distillation, as shown in Fig. 1. The distillation process is a distributed parameter system, and therefore, creating an accurate model with a subsequent set of solutions is a rather difficult task.

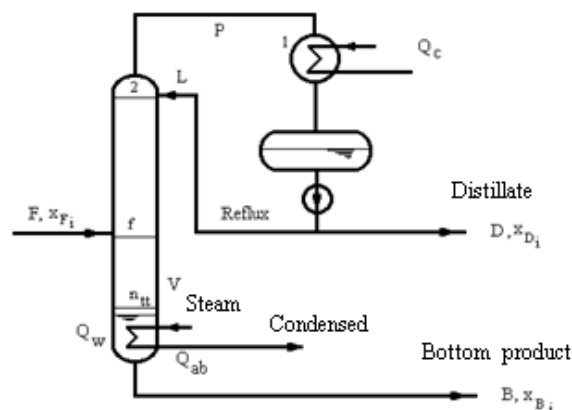


Fig. 1 Classical distillation column

### B. The Heat Pump Based Method of Propylene-Propane Distillation

The alternative method of the separation of the propylene-propane mixture is based on a distillation column with a heat pump. Considering the fact that the difference between the boiling points of the two mixture components is very low, and namely, that the temperature difference between base and top of the distillation column is of about 10 °C, the use of a heat pump thus becomes an interesting technological solution [7]. Fig. 2 presents a principle design of a propylene-propane separation structure [6]. Despite the fact that the main component (the distillation column) of the structure is identical with the one presented in Fig. 1, its principle of operation is completely different. The vapors generated at the top of the distillation column are compressed at a pressure for which their temperature becomes higher than the temperature of the base of the distillation column. This makes possible that the compressed vapors are used as thermal agent for the

distillation column's reboiler. After the thermal transfer takes place, the pressure of the vapor flux can be restored through the use of an expansion valve. Due to the thermal flux exchange and the lowering pressure, the flux is in a partial of total liquid state. An efficient use of such structure should divide the vapor flux in order to introduce flexibility in the operational procedures of the distillation column.

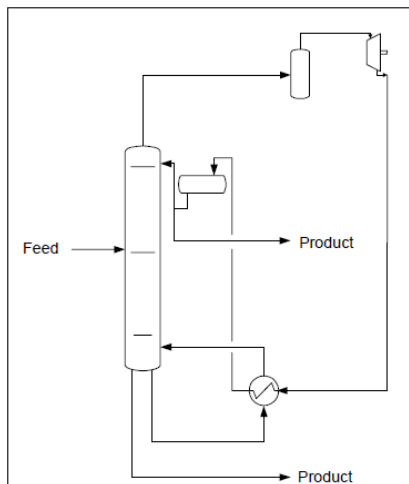


Fig. 2 Distillation column with thermal pump [6]

The main difference between the structure presented in Fig. 2 and the classical structure of a distillation column is marked by the lack of a condenser element. If the vapor flux is divided (a common situation in the industrial operation), the structure must also include a heat exchanger that acts as a condenser, but with a much lower thermal load as the typical condenser associated to the classical structure.

### III. STEADY STATE PROCESS MODELING

The distillation process can be modeled in steady as well as dynamical state of operation. A steady state modeling can be used to determine the statically characteristics of the process, e.g. its sensitivity. Due to the multivariable character of the process, a special use of the steady state simulation is represented by the calculation of the relative gain array, which could allow, in the end, the selection of a robust quality control structure of the separated products.

Based on their previous experience, but also industrial preferences, the authors have selected the Unisim Design<sup>®</sup> software package as the most adequate simulation environment. Real data from the industrial process were used in order to generate inputs for both of the presented solutions of the separation process, as explained in [6].

#### A. Classically Distillation Column Modeling

The Unisim Design<sup>®</sup> simulation environment contains a mathematical model called *Distillation Column*, whose purpose is to model a classical distillation column that is equipped with a condenser and a reboiler. The subsequent

steps are required in order to simulate such a distillation process [6]:

- 1) Selection of the thermodynamic model; namely, the Peng-Robinson model.
- 2) Description of the input flow (generally called *Feed*).
- 3) Running and configuration of the *Distillation Column* mathematical model.
- 4) Running of the simulation software and displaying the results windows.

One of the problems that the modeling and configuration of the distillation process simulators is facing is the adequate selection of the specific parameters needed for a successful completion of solving the mathematical equations of the simulation process. The distillation process requires the proper setup of two specification parameters. Although the model can in principle be run with any combination of parameters, it is recommended that these specification parameters should be closely associated with the automated control systems from the industrial distillation column. Therefore, the *Distillation Column* mathematical model was configured to take into consideration some of the above mentioned industrial particularities, being able to use as input parameters such as reflux and distillate flow rates [6]. Solving the mathematical model of the column leads to the following values of the resulted products: propane concentration in the distillate product is 99.63%, whereas the propane concentration in the base product is about 3.85%. The thermal load of the condenser is  $1.142 \times 10^8$  kJ/h, whereas that of the reboiler is  $1.044 \times 10^8$  kJ/h.

#### B. Thermal Pump Distillation Column Modeling

The removal of the condenser from the distillation column's structure leads to the impossibility of using the *Distillation Column* mathematical model of the Unisim Design<sup>®</sup> simulation environment. In this case, the distillation column can be assimilated to an absorption column with a reboiler attached to it and it can be expected that such modeling assumptions should generate very similar results to the ones obtained through the use of the *Distillation Column* model [6]. Such a requirement leads us to the creation of three simulation models, and each one has a higher degree of complexity than the previous other one.

##### 1. Absorption Column with External Reflux

The proposed simulation diagram contains the *Reboiler Absorber* mathematical model that is normally associated to an absorption column with a reboiler. The module that was used for the absorption column's simulation uses the same data as the ones previously used for the *Distillation Column* module. The simulation diagram contains an additional recirculated flux which had to be corrected by the function called *Recycle*, that transfers the numerical values between fluxes. Among the other advantages, the *Recycle* function balances the propane concentration levels within both fluxes, a result of which can only validate the diagram of the simulation package. More significant results were obtained using the following specifications [6]:

- The reflux that is associated to the *Reboiler Absorber* module is defined by the following: temperature 15.5 °C, pressure 900 kPa, flow 299944 kg/h, and chemical composition 0.9945 molar fractions of propane.
- The *Reboiler Absorber* module has a bottom product flow of 7300 kg/h.
- The condensate flux is characterized by a vaporized fraction (0 being the liquid state), and a temperature of 15.6 °C.
- The reflux is characterized by the flow value of 299944 kg/h.

The obtained mathematical model should simulate the distillation column that is put at test at industrial conditions. The most important perturbation of the process is the column's feed, and therefore, the model was put at test for the variations of such perturbation. We followed the evolution of the following output values: the vapor flow, the thermal load of the reboiler, the propane concentration in the distillate, and the propane concentration at the base of the column.

The numerical tests showed that the differences are due to the variations of the reflux composition that were fed into the model. Thus, in the mathematical model of the distillation column, the reflux composition (identical to the one of the distilled product) is calculated in an iterative way such that, at the end of the calculation, the chemical composition of both fluxes becomes equal. In the absorption column model, the reflux composition is set up during the matter flux configuration stage such that the user does not know the real value. This situation leads to important errors in distillate and bottom product compositions. There were situations in which, for large feed flowrates the calculation was not convergent. Consequently, the simple replacement of *Distillation Column* model with *Reboiler Absorption* model is not sufficient.

## 2. Absorption Column Based on Distillation Column Model

The above mentioned disadvantages of the implementation of the *Absorption Column* model lead the authors to investigate on the possibility that the external reflux composition of the absorption column could be automatically recalculated using a distillation column mathematical model. The compatibility of the two mathematical models was achieved by using a special technique of the Unisim Design® environment. Thus, the *Distillation Column* model has been introduced in the simulation diagram to obtain the same values of the absorption column reflux concentrations in accordance with the values of the distillation column reflux concentrations. The transfer of all the concentrations are passed using *Optimizer Spreadsheet* module's advanced functions [6]. In addition, the transfer of the feed flowrate value from *Distillation Column* to *Reboiler Absorption* was implemented, which simplified the simulation program.

The combination of the *Distillation Column* (DC), *Optimizer Spreadsheet* (OS), and *Reboiler Absorption* (RA) modules resulted into a new model and simulation instrument of the distillation process, which can be confidently used in the simulation of a distillation process that has a thermal pump. In Fig. 3, the variation of the distillate composition

calculated by *Distillation Column* model (DC) and the new model (DC+OS+RA) is presented. The numerical results are identically, that confirms the fact that DC model may be replaced with DC+OS+RA model.

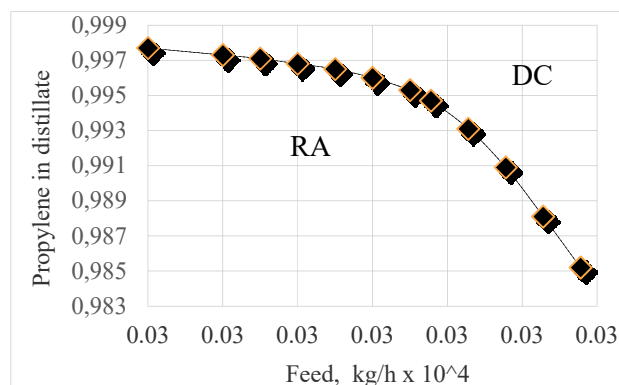


Fig. 3 Propylene in distillate comparison

A very good correlation was obtained also for the propylene in the bottom product as shown in Fig. 4. This comparison confirms the new process model (DC+OS+RA).

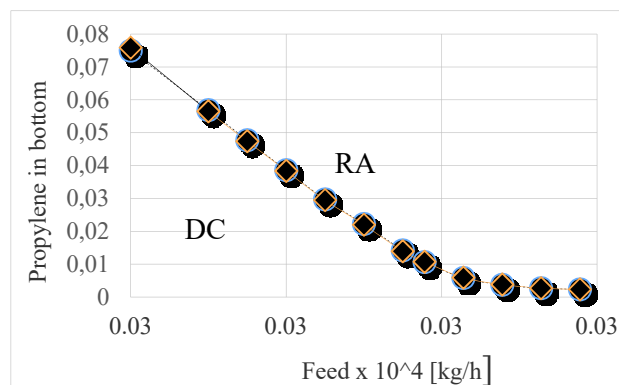


Fig. 4 Propylene in bottom product comparison

Identical results are obtained for reboiler duty. In conclusion, the *Distillation Column* model has been replaced with DC+OS+RA model.

## IV. QUALITY CONTROL SYSTEMS

Principally, the two distillation processes have the same characteristics, and the quality product control is created using different means and technical instruments. For this reason, the authors decided to treat separately the two cases, thus highlighting the common features, as well as underscoring the particularities that characterize their control process.

### A. Quality Control Systems for Classical Distillation Process

We start with a propylene-propane binary mixture and a classical distillation column that, from the point of view of the automated control process of the product quality, is a multivariable 2x2 mathematical system. These features made

possible the study of the quality control systems extensively and from various angles. After a careful reviewing of the literature, the authors of this paper classified the automated systems that control the product quality of the propylene-propane distillation process into multivariable systems (if both products are to be reviewed for quality control) or monovariable (if only the distillate quality control is required).

The multivariable control systems require multivariable regulators or model-based regulators [14]. Regardless of the implemented regulator, these automated systems require chemical composition transducers for both separated products from the distillation column, which can be extremely costly. At the same time, one should consider the fact that the requirements imposed on the distilled quality (rich in propane) are highly restrictive, whereas the base product (rich in propane) quality specification is only defined on a domain of concentrations. All of the above economical restraints make the multivariable control systems quite unpopular choices within the industrial environment. However, the monovariable control systems have several industrial applications such as the feedback control, feedforward control, and optimal control.

In both cases, and for an optimal natural decoupling of the necessary commands used for the quality control processes, a successful calculation of the relative gain array of the multivariable 2x2 system is necessary. There is a large body of research work (authors included) that showed that the most efficient pair of commands whose output generates the lowest effects is the L-B pair [8]-[10].

The control feedback structure is shown in Fig. 5, being tested in both numerical simulations as well as in industrial environments [3], [15]. Considering the fact that the most important perturbation of the process is the feed flow, the numerical simulations put into perspective the robustness of our proposed automated system.

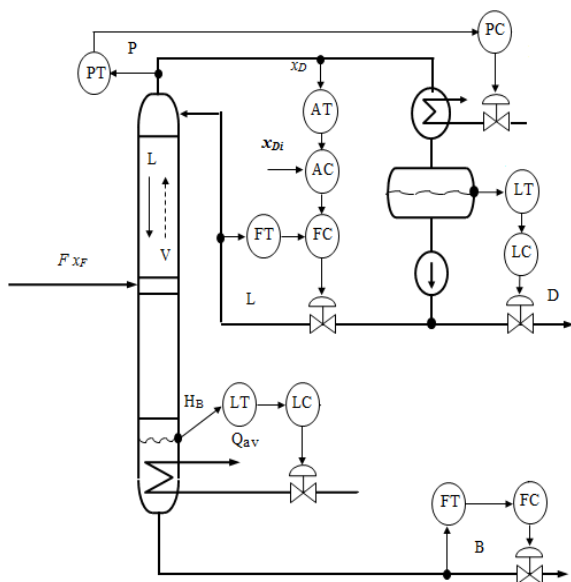


Fig. 5 Feedback control structure of the distillate quality

The feedforward control system was studied extensively in the literature, being a solution that was implemented at an industrial scale in the Romanian industry. Fig. 6 presents such control structure of the distillate quality, which uses the Fenske-Gilliland-Underwood model as the core of the feedforward controller, with the feed flow being the main perturbation to be considered [15].

One version of the system presented in Fig. 6 was implemented in the HC900 distributed system of Honeywell Corporation [16].

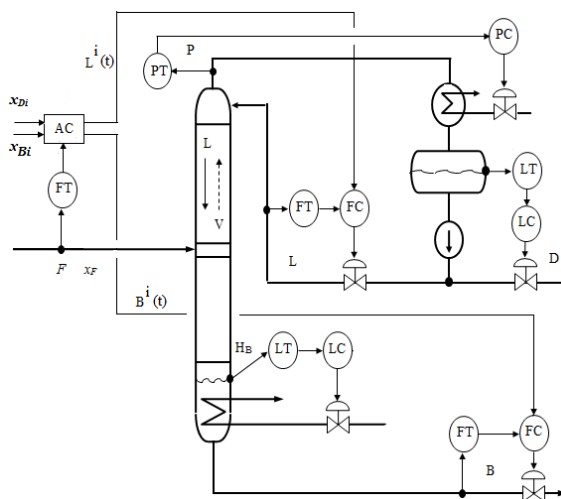


Fig. 6 Feedforward quality control system

### B. Quality Systems for Distillation Column with Heat Pump

The control systems of the distillation columns with heat pumps present certain differences with respect to the control systems of the classical columns. The control systems for this type of process can be classified in the following subsystems [11], [12]:

- Control structures associated to the gas compressor;
- Pressure control structure;
- Quality control structures.

The control systems associated to the gas compressor and the pressure control structure are presented in [11]. In order to design any quality control system, one must conduct studies and simulations of the process in both dynamic and steady state cases.

The previous mentioned works have allowed the authors to propose a new control structure that is presented in Fig. 7. This structure is characterized by the following elements:

- The used commands in the quality control process are the reflux flow  $L$  and the thermal agent flow in the column's reboiler. The thermal agent flow is the command that directly influences the vapor flux  $V$ . In a dynamical regime of operation, the variation of the feed flow values cannot be easily balanced out by the structure. This negative effect can be easily seen at the base of the column where the propane concentration  $x_B$  will suffer from dramatic variations.

- 2) If the thermal agent's flow is relatively constant, the operating pressure would produce minor effects, and the compressor's load will be constant.
- 3) The very high reflux flow values impose important flow variations for maintaining a controlled quality of the distillate, which would, at their turn, produce a negative influence on the pressure inside the distillation column.

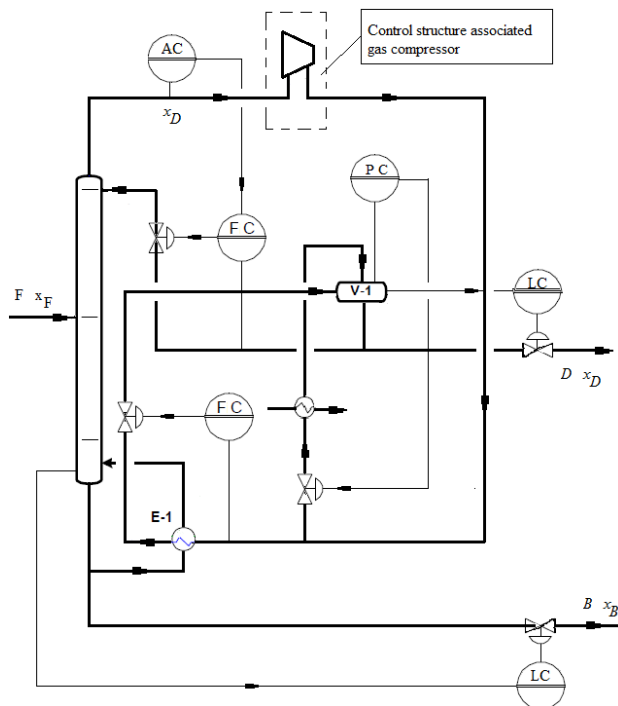


Fig. 7 Feedback quality control structure (1)

The steady state simulations validated the L-B pair of commands also for this type of distillation column, by providing the best decoupling of the commands effects for the 2x2 multivariable system [17]. As a result, such findings allowed the introduction of a new quality control structure, as presented in Fig. 8. The main characteristics of the structure are the following:

- a) The used commands in the quality control process are the reflux flow L and the base product flow B, forming the best pair of commands of the multivariable process. In a dynamical regime, the perturbations of the feed flow can be easily rejected by the structure.
- b) The control system of the column base level could induce considerable variations to the reboiler's thermal load, which, at their turn, could be transmitted to the pressure control system.
- c) The very high reflux flow suggests that its influence in the quality control of the distillate product is rather low.

The selection of either structure is somehow difficult when important information such as structure dynamics and operating restrictions imposed by the statically and dynamical components is not known. The new researches in this domain

will be obtained in future, and the control problem will be resolved.

## V. CONCLUSION

The paper has presented the following problems:

- a) The results obtained for propylene – propane distillation process. This process has been analyzed for two industrial variants: classical distillation column and distillation column with heat pump.
- b) The quality control structure design for both distillation processes.

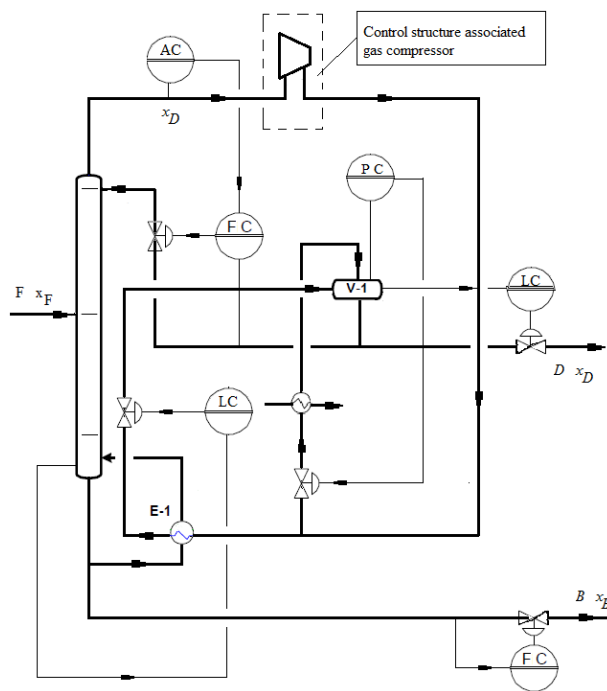


Fig. 8 Feedback quality control structure (2)

The process modeling and simulations are done using Unisim Design® software. The study has been finalized with obtaining of a software instrument of the distillation column with heat pump. This instrument has been validated by comparison between simulation results of the classical distillation column and the distillation column with heat pump.

The process control structures are designed and compared with the structure presented in literature. For the classical distillation column, a robust quality control structure and a feedforward control structure have been designed. For the distillation column with heat pump, two quality control structures have been designed. The selection between these control structures will be realized using the dynamic process simulation.

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