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**Basell  
Poliolefinas Ibérica**

# **Optimization and dynamics of a propene-propane splitter with vapor recompression**

**Master thesis presented by Anna Esteve**  
to obtain the Master degree in Chemical Engineering  
from the Universitat Rovira i Virgili

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**NOMENCLATURE**

<b>Acronym</b>	<b>Meaning</b>
LYB	Lyondellbasell
EDR	Aspen Exchanger Design & Rating
MPC	Multivariable Predictive Controller
PDH	Propane Dehydrigeneration
PPII	LyondellBasell Novolen plant II
PPIII	LyondellBasell Novolen plant III
VRC	Vapor Recompression Column
<b>Symbol</b>	<b>Description</b>
A	Heat transfer area
B	Bottom of heater (%)
C	Initial value of the controller
$C_v$	Effective flow coefficient
$dp$	Pressure difference
$\Delta T_{LM}$	log mean temperature difference
$E(t)$	Controller error
f	Overall mass flow
F	Molar flow rate
$F_p$	Piping geometry
$F_t$	LMTD correction factor
H	Enthalpy
$K_c$	Controller gain
L	Liquid percent level(%)
M	Fluid flow rate
MW	The molecular weight of the gas
$OP(t)$	Controller output
P	Pressure
$P_d$	Absolute pressure at downstream location
$P_u$	Absolute pressure at upstream location
Q	Duty
$\rho$	Density
$\rho_l$	Liquid mass density
$\rho_v$	Vapor mass density
T	Temperature
T	Top of heater (%)
$T_{amb}$	Ambient temperature
$T_d$	Derivative time constant
$T_i$	Integral time
U	Overall heat transfer coefficient
V	Volume
vpfrac	Adjusted vapor mass fraction
W	Work
x	Pressure drop ratio
Y	Gas expansion factor

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## SUMMARY

Distillation is an important unit operation in polypropylene production. It is common for separation of liquid mixtures, and is an energy intensive operation, accounting for about 10% of industrial energy consumption. Energy consumption can be reduced through more efficient designs, and through optimum operation of existing equipment.

In this thesis, a steady-state and a dynamic model describing the propane-propene distillation column with vapor recompression has been simulated. A VRC distillation column is used to reduce costs and energy consumption because it avoids the heat loss.

Another way to reduce utilities cost and enhance distillation separation is performing an analysis of the system through an accurate plant simulation. To reach a model similar to the plant, process variables and design equations have been considered and assumed. Also, model development involves fundamental chemical engineering principles and the Aspen HYSYS simulation tool.

To start the analysis, both simulations confirmed to predict similar values as the ones displayed in reality. The average accuracies for the steady-state and dynamic simulation are 89.2% and 88.1%, respectively. Given these results, simulation is assumed to be consistent and thus subsequent case studies are developed.

As the Aspen simulation recommended parameters are different to the plant used ones, it is recommended to perform step by step an upgrade in the tuning parameters of each controller of the column.

The simulation engine has been used to study the dynamic response of process in the variation of feed flow rate, feed compositions, and reflux flow rate. The resulting graphs for each scenario are discussed and compared.

Having concluded that the reboiler heat flow is not dependent on feed composition, the main difference is when the reflux rate increases the heat flow required is larger. Furthermore, it is proved that for --%Wt propene purity feed concentration is better using a ----- of ----- kg/h. Similarly, given a same flowrate, for a --%Wt propene purity is better using ---- ---- flowrate, -----kg/h.

Given the same purity for a ----- feed flow rate, a larger reflux is recommended.

One of the purposes of the dynamic simulation is to study changes caused by perturbations to the distillation process. In this study, several streams and equipment process parameters such as temperature, flowrate, the feed tray, etc. have been evaluated. However, the plots shown and analyzed in detail are the reboiler heat flow, the distillate purity, and the splitter top pressure.

Furthermore, a comparative study of the consequences of the last process hazard analysis (using HAZOP methodology) with the simulation results has been explored, proving that most of the identified consequences are confirmed by the simulated ones.

Finally, after simulating different scenarios and being more familiar with the process some recommendation are given. Additionally, further proposals are suggested such as implementing a multivariable model predictive control to reduce energy consumption, reduce emissions, and minimize pollution.

## 1. INTRODUCTION

Propylene is one of the most important products in the petrochemical industry, which is used as raw material for a wide variety of products.

One of the products is polypropylene (PP) which is made from the polymerization of propylene in the presence of a catalyst system usually Ziegler-Natta or metallocene catalyst. PP market size in 2020 was estimated at over 80 million tons. (*Polypropylene Market | 2022 - 27 / Industry Size, Growth - Mordor Intelligence, 2021*)

### 1.1. Distillation

In the petroleum refining industry, propylene is mixed with other gases such as hydrogen, ethylene, ethane, propane, etc., but gases lighter than propylene are typically separated earlier, therefore, propylene is separated from propane in most cases. This separation is typically executed via distillation. As propylene is essential in the production of PP distillation is an important unit operation in PP production.

Moreover, propene and propane have very close boiling points, so it is difficult to separate this combination. The number of trays required for the distillation column is a large number of theoretical plates (>100) and a high reflux ratio due to the low relative volatility (the relative volatility of propylene and propane is close to the unit) and high product purity (>99.5 wt % purity). So the distillation is a capital and energy intensive process.

For separation of chemical components, distillation is the most common technology which is responsible for 3% of the world's energy consumption and 10% of industrial energy consumption. (Kazemi *et al.*, 2016)

To reduce high capital costs and high energy consumption, a distillation column with vapor recompression (VRC) can be used. The amount of energy that can be saved has made this technique highly popular in many industrial settings. (Kiss, 2013)

The basic idea of using distillation with vapor recompression is to avoid the heat loss to surroundings at the column's condenser by improving the quality of this heat and using it as the source to provide the heat required for the column's boil up. (Kazemi *et al.*, 2016)

In Figure 1. 1 is shown a process flow diagram of a conventional distillation column and a vapor recompression column. Conventional distillation columns are composed of stripping and rectifying sections. Generally, as stripping section it is used a reboiler which provides a thermal energy gain in the column and as rectifying section it is used a condenser to reject thermal energy of the column.

Vapor recompression column can reduce energy consumption by using the energy from the column overhead stream, which is compressed in a compressor and then it is used as an internal source of energy in liquid reboiling. An external refrigerant is used to facilitate the energy transfer between the top vapor stream and the bottom liquid stream. (Kazemi, Mehrabani-Zeinabad and Beheshti, 2018)

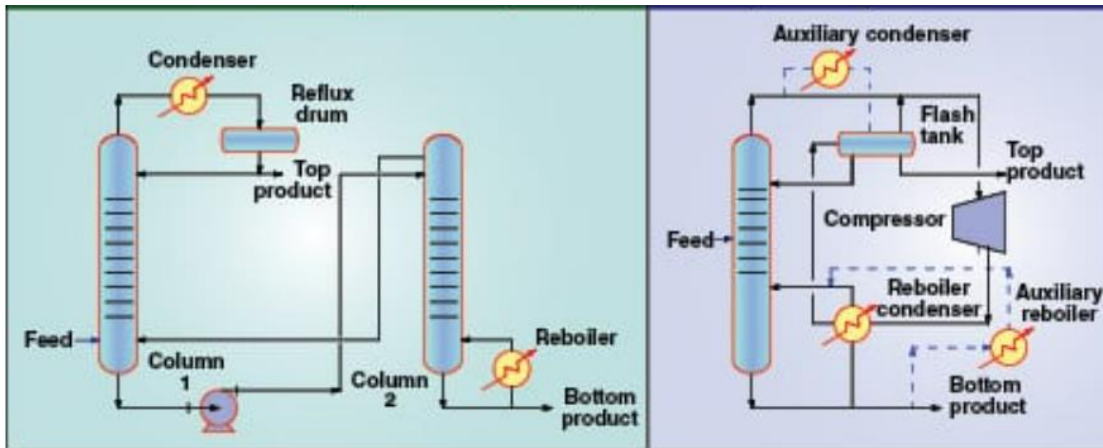


Figure 1. 1. Schematic of a conventional distillation column (two column system) on the left and a vapor recompression column on the right. (Distillation Optimization By Vapor Recompression - Chemical Engineering)

So the main difference between both columns is that the conventional distillation column has a separate condenser and reboiler, each with its own heat transfer fluid such as cooling water and steam, conversely, the VRC has a combined condenser-reboiler with no external heat transfer fluids.

Vapor recompression systems have additional advantages if it is compared to the conventional distillation column. The main advantage, as explained, is the energy saving due to the great amount of heat moved between the condenser and reboiler. Because of how mechanical vapor compression works, the technique is ideal for systems that are meant to operate on a relatively low temperature difference.

Better efficiency will result producing fewer greenhouse gas emissions and hence environmental advantages. Another benefit is that the column height and the reflux flowrate can be reduced.

The analysis, design, operation, control, and optimization of distillation columns have been extensively studied for almost a century. From 1950, either analog or digital computer simulations started to solve many engineering problems. The analysis of distillation consists of iterative vapor-liquid phase equilibrium estimations and tray-to-tray component balances. Nowadays distillation columns can be simulated to optimize the process. (Luyben, 2013)

## **1.2.Simulation**

Chemical process simulation has been widely used by chemical process engineers to design, evaluate, understand, optimize, and integrate process plants. Simulations try to shape real processes as accurately as possible using models. These models consist of several mathematical equations. Basic simulations are in a steady state, as the models do not depend on time.

However, chemical plants are never steady-state so dynamic simulation helps to do a better design, optimization, and operation of a chemical process or refining plant. Environmental changes, heat exchanger fouling, and catalytic degradation constantly disturb the conditions of a running process. Thanks to dynamic simulation can be used for a variety of purposes, some typical examples are:

- Process optimization: through simulation can find ways to move the plant operation to similar and safe but more profitable conditions.

- Modification of process and control system design: determination of parameters as controller tuning parameters, analysis of controllability, depressurizing, feed differentiation effects, etc.
- Safety and environmental issues: testing of plant procedures and detection of unfavorable conditions, verification of distributed control system, depressurizing procedures, etc.
- Investigation of operational issues: simulators can help to find the problems of some process behaviors, assess alternative solutions to what-if scenarios, achieve optimal plant conditions after any change, investigate for future prevention, etc.
- Startup/Shutdown of the process: creating, testing, and verifying procedures for the safe start-up and shutdown of the process or for the minimization of time that plant equipment stays out of operation.

To achieve it can be used a dynamic simulation through Aspen HYSYS. (AspenTech Documentation, 2006)

HYSYS Dynamics constructed a very complex simulation that requires multiple steps and scripts in a very extensive design and analysis technique. Using basic and engineering relationships such as mass and energy balance, phase and chemical equilibrium can be easily predicted any process behavior. One of the best utilities of a process simulation is to run different cases, to analyze, to do the sensitivity analysis and optimization runs. Doing several runs of an existing plant can be designed optimized plants as well as improve the effectiveness. (Taqvi, Tufa and Muhadizir, 2016)

### **1.3. Controllers**

To obtain a dynamic simulation controllers are a fundamental part, as happens in real plants. The choice of control structures for distillation columns is important to get the desired product. Each column has a different structure of controllers, so it is fundamental to find the structure for each process. Moreover, the effective operation of a distillation column is determined by the control of many variables.

The control theory aims to build a model or algorithm to drive the system to the desired state while reducing any delay, overshoot, or steady-state error and guaranteeing control stability, and normally intending to optimize the system.

One control mechanism is PID controllers. PID is a control loop mechanism that has been widely adopted in the chemical process industry since the 1940s. This control system tries to estimate the values of the manipulated variables that allow the controlled variable to reach the setpoint. The feedback system computes the error between this setpoint and the value of the controlled variable measured in the process. (Shin, Smith and Hwang, 2020)

Involves three separate parameters: the proportional, the integral, and derivative values, denoted P, I, and D. Basic structure of PID is shown in Figure 1. 2:

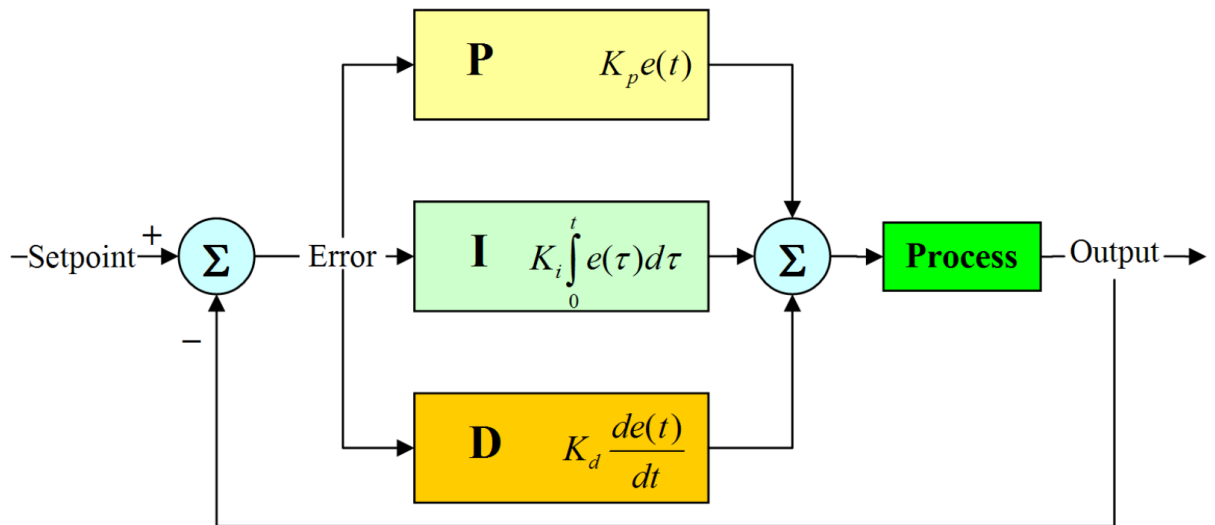


Figure 1. 2. The basic structure of PID. (*The ABC's of PID's – The Society of Aerial Cinematography*, 2015)

To obtain the output of the process PID controller adjust the control input minimizing the error and also correlates the controller output, the integral of the error, and the derivative of the error. The output of the PID controller can be calculated using this equation:

$$OP(t) = k_c E(t) + \frac{k_c}{T_i} \int E(t) dt + k_c T_d \frac{dE(t)}{dt} + C \quad (1.1)$$

#### **1.4. Model predictive control**

One of the more advanced control methods is model predictive control (MPC), which is very effective and has been extensively executed in plants since the late 1970s. (Adánez, Al-Hadithi and Jiménez, 2018)

MPC systems can use both feedforward and feedback functions. Thanks to the feedforward controller, it can balance disturbances before they have any effect on the system. MPC is used to predict the responses of the process and find its optimal operating condition because it can capture static and dynamic interactions and simultaneously can consider several constraints.

This model can be differentiated from regular control methods, for example, the PID controllers, which do not directly utilize the process model. Many researchers have investigated the efficiency of MPC, comparing it with conventional PID controllers. Several investigations showed that the performance of MPC had superiority over the PID controllers. (Nurul Nadia Mohammad, 2018)

The first step in the industrial implementation of an MPC is the process modeling, in which usually it is necessary to invest up to 90% of the total cost and time of the commissioning. Furthermore, must be considered that the initial process modeling cannot be expected to be useful during the whole process lifetime because processes degrade over time. (Larsson *et al.*, 2015)

### **1.5. Process hazard analysis**

Process hazard analysis (PHA) is a method of technical risk assessment. It reviews chemical and manufacturing plant operating procedures step-by-step to identify hazardous situations and assess their potential impact if improperly managed.

The most common PHA methods used in the process industry are the Checklist, What-If, What-If Checklist, and HAZOP Study.

Hazard and operability analysis (HAZOP) is the most commonly used PHA method, specially in the petroleum industry. HAZOP methodology is a practice procedure for identifying and controlling process safety hazard scenarios. Predicting and preventing chemical process hazards is an essential part of the chemical engineer's job.

Hazardous scenarios are identified by an experienced team of multi-discipline engineers and operations personnel. The effectiveness of the team depends on the creativity and knowledge of the participants in discovering effects that could trigger a major accident. This is no easy task as the team works with final design documents and their experience, and they have to identify errors in the design.

The technique is based on breaking the overall design of the process into simpler sections called "nodes" which are then individually examined. HAZOP consists of looking for inadequacies in the design, which may trigger serious accidents. Formal HAZOP review uses a list of guide words, as can be seen in Table 1. 1, to examine each part of a facility, to determine the possible deviations and consequences of each mode of failure. Each consequence is evaluated against frequency and severity. Finally, for each undesirable consequence, corrective actions are evaluated. (Eizenberg, Shacham and Brauner, 2006)

Table 1. 1. HAZOP table.

<b>Guide Word</b>	<b>Deviation</b>	<b>Causes</b>	<b>Consequences</b>	<b>Action required</b>
No, less, more, other, etc.	Flow, pressure, temperature, level, etc.			

Combining HAZOP with dynamic simulation can help to investigate those consequences. Dynamic simulation allows quick analysis results of the strategies in preventing the failure into major accidents. These simulations reduce the subjectivity involved in the determination of dangerous event severities and possibilities. Moreover, the simulation allows combining mathematical modelling with process simulation that can further reduce the subjectivity involved. (Isimite and Rubini, 2016)

## **2. SCOPE OF THE PROJECT AND SPECIFIC OBJECTIVES**

Distillation is a common unit operation for the separation of liquid mixtures, and is an energy intensive operation, accounting for about 10% of industrial energy consumption. Energy consumption can be reduced through more efficient designs and optimum operation of existing equipment.

Distillation with Vapor Recompression (VRC) is a commonly used design to reduce energy requirements in applications with very similar boiling points, such as propene-propane splitters.

There are several ways to reduce energy consumption and optimize the process through dynamic simulation, so the development and success of this work require the achievement of several objectives:

- To do a literature review about Dynamic simulations, multivariable control theory, and review the available information of P&IDs, control narratives, operations manuals, etc.
- To develop a steady-state simulation that properly represents the distillation column with Vapor Recompression.
- To simulate a dynamics model of the system, which includes the physical dynamics of the system coupled to the basic controller already implemented for the safe operation of the system.
- To propose different operation ways to optimize energy efficiency through perturbations and sensitivity analysis.
- To explore and understand not only the behavior but also the actions to prevent possible accidents through the verification of a HAZOP analysis.
- To recommend PID controllers for optimal operation in different operational modes.

To sum up, the principal objective of the project is to optimize and obtain the dynamic simulation that properly represents the propane-propene splitter with vapor recompression through Aspen HYSYS.

### 3. STUDENT’S ROLE IN COMPANY

Through this section is described the company, its goal, and products, as well as an overview of the activities carried out by the student during the internship.

#### 3.1.LyondellBasell

LyondellBasell is one of the largest plastics, chemicals, and refining companies in the world. As shown in Figure 3.1, it has manufacturing sites, technology centers, joint ventures, and administrative offices distributed in 24 countries. Moreover, the products are sold in more than 100 countries.

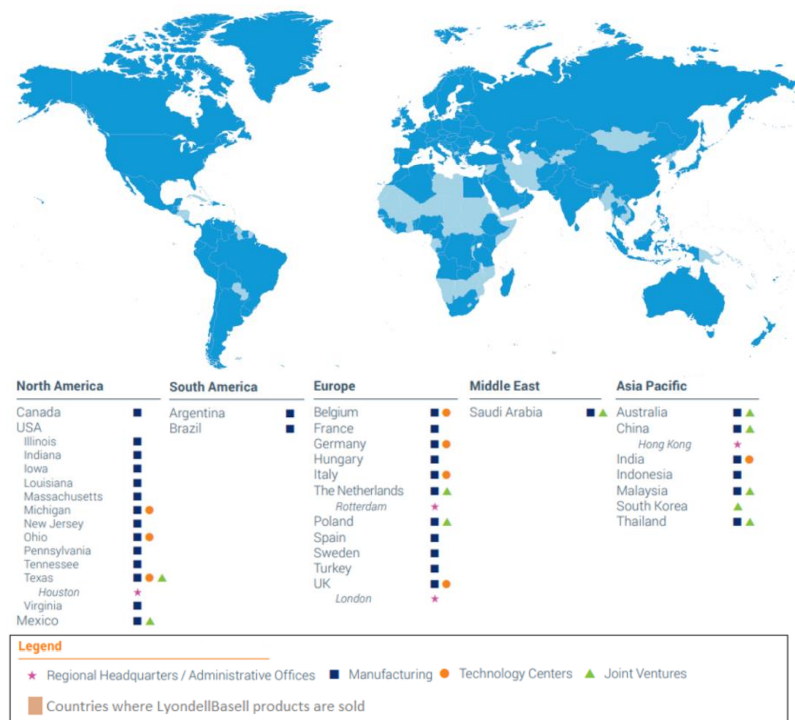


Figure 3. 1. Worldwide distribution of LyondellBasell (LyondellBasell Industries webpage)

The company, as can be seen in Figure 3.2., participates in the full petrochemical value chain, from refining to specialized end uses of petrochemical products. Is the world's largest producer of polypropene compounds, being one of the main products along with polyethylene. Furthermore, LYB produces large quantities of ethylene, propene, polyolefin, oxyfuels, etc.

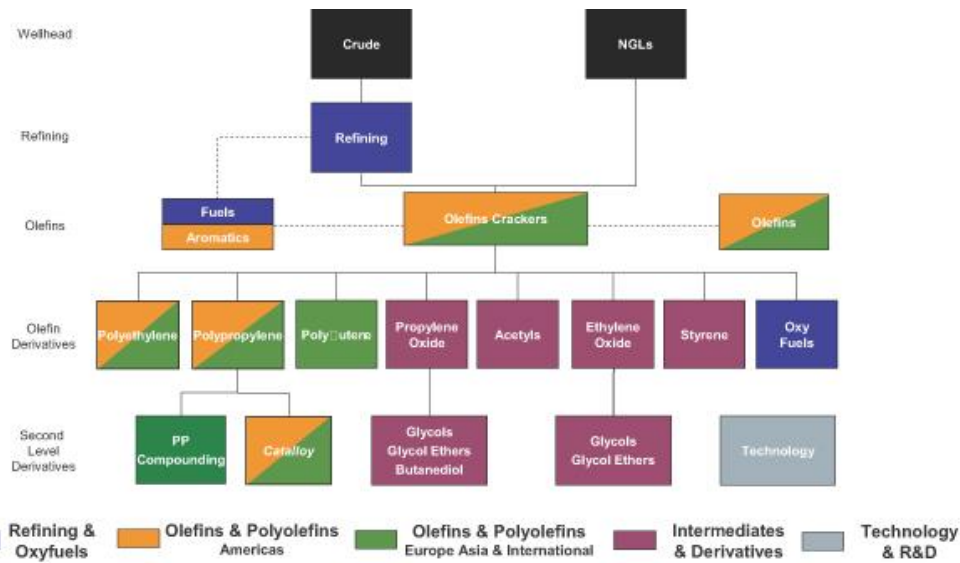


Figure 3. 2. World scale diversified vertically integrated portfolio structure. (Securities and exchange commission)

Its range of applications includes quotidian products such as personal care, packaging for the food industry, detergents, non-carbonated drinks, high resistant construction materials, automobile industry, electro appliances, biofuels, medical applications, etc.

Their mission is to consistently deliver industry-leading performance by:

- Safely and reliably delivering high-quality products to customers
- Being the company of choice for employees and shareholders
- Being a responsible, good neighbor in the communities where we operate (LyondellBasell website)

The internship has been carried out in the Lyondellbasell site of Tarragona, Spain. This site is divided into two areas: Tarragona East and Tarragona West. The project is focused on Tarragona East which is located within a complex owned by BASF.

The West area of LYB has eight extrusion lines while the east has the entire process of production like polymerization with two production lines, PPII and PPIII.

The propene supplier is the Propane Dehydrogenation (PDH) plant owned by a joint venture between BASF and Sonatrach. Depending on the type of polypropene made, PPII produces between - and - kt/year, and the production of PPIII is between - and - kt/year. The main difference between them is the capacity plant.

Both PP plants produce three different products:

- Polypropene homopolymer: It is the most common product. It has a high heat resistance and good rigidity, for use in a vast range of applications. Can be improved with additives in the compounding plant.
- Polypropene heterophasic copolymer: It is produced with the incorporation of different co-monomers (in this plant, propene, and ethylene). It is a highly resilient material that appears to be opaque.
- Polypropene random copolymer: It is produced by introducing ethylene links into the polypropene chain. It has improved optical properties so it's used for packaging applications where transparency is required.
- Homopolymers and random copolymers can be polymerized in a single reactor, otherwise, random copolymer requires two reactors connected in series.

PPII and PPIII plants are responsible for producing polypropene from propene using stirred-bed reactors. This process can be divided into three parts: polymerization, extrusion, and distillation.

In the polymerization process, the propene gas reacts on a gas phase stirred-bed reactors, under certain pressure and temperature conditions with the catalyst system, producing powder of polypropene. That powder is discharged in a big cyclone to separate the powder from propene/ethylene gas, which is recovered and re-feed to the reactors once the propane has been removed.

On the other hand, the polypropene powder is transferred to another vessel to be stripped with nitrogen and deactivated with demineralized water and isopropyl alcohol. The deactivated powder is sent to the powder storage silos, to be either granulated or exported as the powder itself. The granulated is deodorized with steam and sent to the logistics area for blending and distribution as bulk or bags.

This project is focused on propene gas recovery of PPIII, for that it is used a distillation column with vapor recompression (VRC). The concerning section follows this flowsheet:

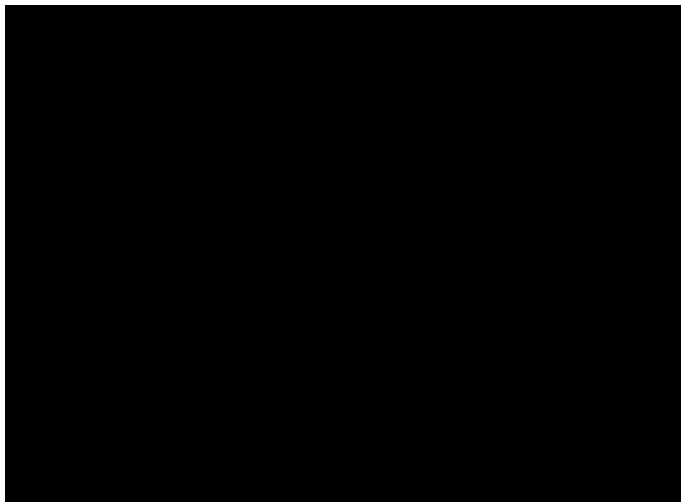


Figure 3. 3. Flowsheet scheme of PPIII plant. (LyondellBasell)

### **3.2. Activities carried out**

The different tasks carried out during the internship are:

- Conduct a critical literature review about propane-propene splitters, Dynamic simulation, and review the available information of P&IDs, control narratives, operations manuals, etc.
- Get familiar with Aspen HYSYS and model the steady-state of PPII propene gas recovery.
- Simulate properly the heat exchanger of this process node using Aspen EDR.
- Obtain the dynamic simulation from the HYSYS steady-state model previously designed.
- Propose some recommendations after the simulation of different scenarios.
- Compare the consequences of the HAZOP analyzed in 2017.

Therefore, the first activity done was to study and review the literature about Dynamic simulations, control theory, and review the available plant information: P&IDs, control narratives, operations manuals, etc. of the focused plant node. This activity is of great

importance before starting the thesis, because it allows us to understand the process and the overall project.

Secondly, the steady-state simulation was carried out in the Aspen HYSYS program. To achieve it the values of the process flow diagram and the design datasheet for the equipment have been used. Moreover, for the heat exchanger simulation was used The Aspen Exchanger Design and Rating (EDR). One of the most difficult parts was to converge the column sub-flowsheet. Having the steady-state model allowed continuing with the dynamic simulation development.

A simple model with the actual operating data for the dynamics of the system was developed, which includes the physical dynamics of the system coupled to the basic controller dynamics already implemented for safe operation of the system. Getting an accurate dynamic simulation has been the hardest part because the simulation had several errors and the variables such as pressure, temperature, flowrate, etc. took a long time to get stabilized.

Once the dynamic model was proved, numerous perturbations and sensitivities analyses of the system were done. Additionally, a comparative study of the HAZOP consequences analyzed in 2017 by the plant engineers with the simulation consequences was explored.

Consequently, after simulating different scenarios and being more familiar with the process some recommendations to be applied are proposed.

#### 4. MODELING AND SIMULATION

The diagram of the PPIII distillation that is required to simulate is shown in Figure 4. 1. This section describes some of the equations, parameters, methodologies, and assumptions related to the model development.



Figure 4. 1. Flowsheet scheme of the PPIII plant distillation. (LyondellBasell)

The design of the distillation column is performed using the simulator HYSYS, first the steady-state simulation and then the dynamic one. Appendix A collects more indications, parameters, and values.

Note that it is important to specify as many values as possible to get better accuracy. However, to obtain the convergence is better if the first calculation contains just the required information, and then step by step more values can be introduced.

##### **4.1. Steady-state process modeling and simulation**

First of all, it is necessary to introduce the relevant components for that it is decided to create two components list because in this node there are two different pipes systems. The water for cooling in the heat exchanger and the methane, ethane, propane, and propene for the other system.

Note that other components as hydrogen, nitrogen, and ethylene are neglected because they do not interact with each other and this make easier the convergence of the simulation.

The fluid package must be chosen depending on the interaction parameters required between the components. In this case, is used Peng-Robinson (PR) question state as it has been proved the adequacy for propene-propane mixtures and their deviation from ideal mixtures. (Zabaloy *et al.*, 1993)

##### **Column K-860 and reboiler W-860A**

Once the property part is completed, the distillation column is designed. As the column distillation is with vapor recompression and does not have a condenser like the conventional,

the column subflowsheet must be modified as it shows in Figure 4. 2. Streams data and the specification of the unit's operation are provided by the company.

The reboiler is connected to the bottom stage in the column with the streams to reboiler and boil up. The liquid from the bottom stage of the column is the reboiler's feed, and the boil up from the reboiler is returned to the bottom stage of the column. The Reboiler is used to vaporize liquid feed streams.

The reboiler energy balance is:

$$H_{To\ reboiler} + Duty_{Q1} = H_{Boil\ up} + H_{890-a} \quad (4.1)$$

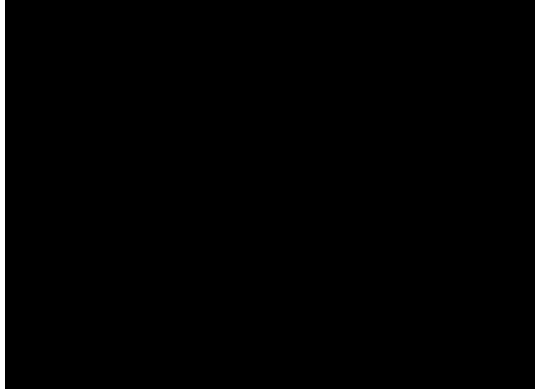


Figure 4. 2. Subflowsheet column in Aspen HYSYS.

The column is designed as the specification sheet, the main variables are collected in Table 4. 1. The column is divided into two sections, the upper part from stage 1 to 53 and the lower part from stage 54 to 120.

Table 4. 1. Column variables. (LyondellBasell)

Number of trays	-
Diameter (mm)	-
Feed stage	
Height skirt (mm)	
Internal type	
Tray type	
Reboiler geometry	

To solve the sub-flowsheet a solving method is required. The HYSIM Inside-Out method is compatible because there is no reaction between the components and the reboiler and the distillation column are included in their equations.

For petrochemical columns including C2= and C3= splitters, the Damping factor is 1.

Figure 4. 3. shows the process simulation diagram. It contains the streams, the unit operations, the valves, and the feed conditions described in the process flow diagram. (LyondellBasell)



Figure 4. 3. Steady-state flowsheet propane-propene splitter with vapor recompression in Aspen HYSYS.

The valves are used to control the system, so it is used in the dynamics simulation, for the steady-state is just required to introduce the pressure drop.

### Compressor V-860

This compressor is responsible for compressing the column head gas to obtain an optimal separation and provide the required heat to boil up the column bottoms. The purpose of the design is to set the power of the compressor, the rotational speed, the efficiency, etc. The main design variables are collected in the next Figure 4. 3.

Table 4. 2. Compressor operation data. (LyondellBasell)

Speed (1/s)	-
Shaft power required (kW)	
Isentropic exponent average	
Pressure ratio	

The compressor operates as centrifugal and Schultz is the method compiled and follows the next equation (Aspentech, 2020):

$$W = \int VdP \tag{4.2}$$

### Heat exchanger W-862

The heat exchanger's function is to reach the dew point to improve the heat transfer in the reboiler and exchanger W860 (to use only latent heat instead of sensible heat plus latent heat), so the inlet and outlet propene stream must be totally vapor.

The design of the shell and tube heat exchanger has been performed using Aspen Exchanger Design & Rating an Aspen interface because using the Aspen HYSYS heat exchanger the calculated values differ from the specification sheet ones. Furthermore, using the EDR heat exchanger the transfer coefficient is recalculated while changing the initial values, getting closer to the real one.

The procedure is similar to the column design. First, the components and the fluid package must be chosen and after that, the configuration and the size are shown in Figure 4. 4.

Table 4. 3. Heat exchanger W-862 values. (LyondellBasell)

TEMA type	-
Position	
Tube OD / pitch (mm)	
Shell ID / OD (mm)	
Tube length (mm)	
Number of tubes / Tubes passes	
Shell side	
Tube side	
Water inlet / outlet temperature (K)	
Water inlet pressure (bar)	

For steady-state simulation hot fluid (the distillate) supplies the Heat Exchanger duty to the cold fluid, the cooling water. The general relation is the following:

$$Balance\ error = (M_{cold}[H_{out} - H_{in}]_{cold} - Q_{leak}) - (M_{hot}[H_{in} - H_{out}]_{hot} - Q_{loss}) \quad (4.3)$$

The total heat transferred between the tube and shell sides can be described in terms of the overall heat transfer coefficient, the area available for heat exchange, and the log mean temperature difference:

$$Q = UA\Delta T_{LM}F_t \quad (4.4)$$

Once the parameters are entered, the program is run and the calculation results are compared with the specification sheet values not specified, to ensure that the heat exchanger is well designed.

### Reboiler and exchanger W-860

In the PPIII plant, the reboiler and the exchanger are the same unit operation, but in the simulation, it is necessary to split it. A way to relate them is to link the heat streams with a spreadsheet. The exchanger's purpose is to condensate all the flow and use this heat flow to perform the reboiler.

The inlet stream (865) of the heat exchanger is cooled, and the energy stream absorbs the enthalpy difference between the two streams. So, the heat balance of the cooler is:

$$H_{865} - Duty_{Q2} = H_{866} \quad (4.5)$$

This Q2 energy stream is the inlet reboiler's heat flow. Therefore, the total energy balance of W-860, using equations 4.1 and 4.5, is:

$$H_{865} + H_{To\ reboiler} = H_{Boil\ up} + H_{890-a} + H_{866} \quad (4.6)$$

### Tee B-860

This equipment is designed to split the stream with the same conditions and composition as the feed stream. This splitter is in charge of dividing one stream into the reflux and the pump inlet stream.

In the plant, the reflux flow is a parameter that must be introduced depending on the product, the feed flow, etc. so the splitter will divide the streams to fulfill the reflux value entered.

**Pump P-860**

The pump is used to transfer the distillate product to the next process step. The measured results at - rpm rotating speed are shown in Figure 4. 4. The efficiency at the inlet flow is approximately -%. (LyondellBasell)



Figure 4. 4. Measured pump curves. (LyondellBasell)

In the design data sheet the characteristic curves are missing so the energy required can be calculated as the following:

$$Power\ required = \frac{(P_{out}-P_{in}) \cdot Flow\ rate}{Liquid\ density \cdot Efficiency} \tag{4.7}$$

Once the steady-state is simulated the stream values of the process flow diagram and the simulation are compared to see if it is properly simulated.

**4.2. Dynamic process modeling and simulation**

The dynamic simulation allows knowing the process behavior towards possible disturbances and changes in the operating variables over time. So for the controllers’ study is fundamental to simulate the dynamic simulation.

For the steady-state simulation, the stream values used are from the process flow diagram because it collects all the variables for each stream, and using it is easier to do an accurate design. However, for the dynamic simulation is used the plant values because the main objective is to obtain the simulation of the current pant.

The values changed are:

- the feed stream
- the reflux flow
- the bottom flow
- the column pressure
- the cooling water stream

The dynamic simulation requires more input data as block sizing, controllers, tuning parameters, etc. For the dynamic simulation, it is important to define the base elevation relative to the ground Elevation of each unit operation, Table 4. 4.

Table 4. 4. Base elevation relative to the ground for each unit operation. (LyondellBasell)

<b>Unit Operation</b>	<b>Base Elevation (m)</b>
FVK-F86018	-
V-860	
B-860	
P-860A	
W-860	
FVK-F86121	
K-860	
W-862	
PVK-P86100	
FVK-F86100	
FVK-F86101	

### **Column K-860**

For the dynamic simulation of the distillation column, the K-value is required for vapor pressure correlations and it can be calculated using the tower diameter method, the equation is:

$$K = 0.1 \cdot \text{tray diameter}^2 \cdot \sqrt{\text{vapor molecular weight}} \quad (4.8)$$

### **Reboiler and exchanger W-860**

For dynamic simulation, the duty applied to the vessel depends on the liquid level in the tank, the level of the bottom, and the top of the heater. These values are used to scale the amount of duty that is applied to the vessel contents.

$$\begin{aligned} Q &= 0 & (L < B) \\ Q &= \frac{L-B}{T-B} Q_{Total} & (B \leq L \leq T) \\ Q &= Q_{Total} & (L > T) \end{aligned} \quad (4.9)$$

In the simulation, the energy stream of the reboiler and the cooler is connected, so the dynamic specification of the cooler is product temperature specification. Furthermore, the purpose of the cooler is to condensate and the reboiler duty is going to vary to satisfy the column specifications.

The exchanger as the following equation shows will cool and change the temperature outlet depending on the reboiler heat flow.

$$\text{Heat Flow} = UA(T_{amb} - T) \quad (4.10)$$

The cooler follows the next equation in the dynamic operation:

$$M(H_{in} - H_{out}) - Q_{cooler} = \rho \frac{d(VH_{out})}{dt} \quad (4.11)$$

### **Compressor V-860**

As the information curves are not available, fixing two specifications HYSYS let the compressor run in Dynamic mode. In this case, it has been chosen the duty and the efficiency.

The power in a dynamic compressor can be calculated from:

$$W = F_1 \cdot MW \cdot \frac{n}{n-1} \cdot CF \cdot \frac{P_1}{\rho_1} \cdot \left( \left( \frac{P_2}{P_1} \right)^{\frac{n-1}{n}} - 1 \right) \quad n = \frac{\ln\left(\frac{P_2}{P_1}\right)}{\ln\left(\frac{\rho_2}{\rho_1}\right)} \quad (4.12)$$

The Schultz method for centrifugal compressors is based on the assumption that the gas compression follows a simple polytropic path, as shown below:

$$PV^n = C \quad (4.13)$$

This equation is combined with the definition of polytropic head:

$$H = \frac{n}{n-1} \cdot (P_2V_2 - P_1V_1) \quad (4.14)$$

And the polytropic efficiency:

$$H = e \cdot (h_2 - h_1) \quad (4.15)$$

### **Heat exchanger W-862**

The following general relation applies to the shell side, the distillate, of the Heat Exchanger when it is simulating in Dynamics.

$$M_{shell}[H_{in} - H_{out}]_{shell} - Q_{loss} + Q = \rho \frac{d(VH_{out})_{shell}}{dt} \quad (4.16)$$

For the cooling water that is the tube side:

$$M_{tube}[H_{in} - H_{out}]_{tube} - Q = \rho \frac{d(VH_{out})_{tube}}{dt} \quad (4.17)$$

For the dynamic mode is specified the overall heat transfer coefficient is calculated by the Aspen Exchanger Design & Rating and for the specification section. The k value used to relate the frictional pressure loss and flow through the heat exchanger is calculated automatically by the program.

### **Pump P-860**

To set the dynamics the pump requires two specifications, in this case, it is selected the efficiency and the power, the dynamic simulation follows these equations:

$$\eta = \frac{W}{F(MW)(h_2 - h_1)} \quad (4.18)$$

$$\begin{aligned} \text{Duty} = & \text{Power supplied to the fluid} + \\ & \text{Power required to change the rotational speed of the shaft} + \\ & \text{Power lost due to mechanical friction loss} \end{aligned} \quad (4.19)$$

### **Valves**

The sizing of the control valves consists of calculating the flow coefficient necessary to be able to select a nominal size of the valve. The flow coefficient, in this case, is expressed as Cv.

The design of the control valve for the simulation has been calculated with the Linear valve operation characteristic, it has a directly proportional flow to the valve percentage opening.

$$\%Cv = \%ValveOpening \quad (4.20)$$

The sizing method of the valve used is the ANSI/ISA, the equation used is the following:

$$f = (1 - vfrac)63.338F_p C_v \sqrt{\rho_l(P_u - P_d)} + vfrac63.338F_p C_v Y \sqrt{\rho_v x P_u} \quad (4.21)$$

$$x = \frac{P_u - P_d}{P_u} \quad \text{and} \quad Y = 1 - \frac{x}{3F_k X_T} \quad (4.22)$$

The control valves are listed below:

Table 4. 5. Valve control list.

Valve	Position	Cv (USGPM(60F,1psi))	Phase	Type
FVK-F86100	Colum Feed	-	Gas	Globe valve
FVK-F86101	Reflux		Liquid	Globe valve
FVK-F86018	Column Bottom		Liquid	Globe valve
PVK-P86100	Cooling Water		Liquid	Globe valve
FVK-F86121	Pump Outlet		Liquid	Globe valve

### 4.3. Controllers

The distillation column is the main element of this study process. In order to hold the operating conditions as close as the steady-state design, the controllers are essential. In the following flowsheet, Figure 4. 5, it is shown the controllers to establish the dynamic simulation.



Figure 4. 5. Dynamic simulation flowsheet of a propane-propene splitter with vapor recompression in Aspen HYSYS.

These are the principal controllers of the current plant, which follow the general equation 1.1. The input to the feedback controller, called error, is the difference between the output process variable and the setpoint. This error is defined depending on whether the process acts directly or reversely. For a process with a positive steady-state gain the error should be set as reverse acting:

$$E(t) = SP(t) - PV(t) \quad (4.23)$$

For a process with a negative steady-state gain, the error should be defined as direct-acting:

$$E(t) = -SP(t) + PV(t) \tag{4.24}$$

-----

The following table, Table 4. 6, is a visual summary in accordance with the above.

Table 4. 6. Variables and parameters established in the controllers.

<b>Controller</b>	<b>Process variable</b>	<b>Manipulated Variable</b>	<b>Setpoint</b>	<b>Action</b>	<b>Gain</b>	<b>Integral time(min)</b>
-						

## 5. RESULTS

This chapter presents the results of the distillation with vapor recompression simulation. The validation of the steady-state and dynamic simulation, a sensitivity analysis, some proposals, and finally a HAZOP study.

### 5.1. Simulation results

Simulation results are divided in two different sections: steady-state and dynamic.

#### 5.1.1. Steady-state results

The simulation results should be as accurate to the real values as possible to obtain reliable results. After achieving the Aspen HYSYS steady-state simulation the results are compared with the process flow diagram files provided by the company. In the next table the stream variables are compared:

Table 5.1. Data streams of the process flow diagram, the simulation and the accuracy.

	Feed			Splitter reflux			Splitter bottoms		
	PFD	Sim	Acc%	PFD	Sim	Acc%	PFD	Sim	Acc%
Ethane (kg/h)	-								
Propene(kg/h)									
Propane(kg/h)									
Methane(kg/h)									
Massflow (kg/h)									
Wt%Propene									
Temp (°C)									
P(bar)									

Table 5. 1. Data streams of the process flow diagram, the simulation and the accuracy. (Cont.)

	Between exchangers			Splitter overhead		
	PFD	Sim	Acc%	PFD	Sim	Acc%
Ethane (kg/h)	-					
Propene(kg/h)						
Propane(kg/h)						
Methane(kg/h)						
Massflow (kg/h)						
Wt%Propene						
Temp (°C)						
P(bar)						

Table 5.1. Data streams of the process flow diagram, the simulation and the accuracy. (Cont.)

	Overhead after comp			After exchangers		
	PFD	Sim	Acc%	PFD	Sim	Acc%
Ethane (kg/h)	-					
Propene(kg/h)						
Propane(kg/h)						
Methane(kg/h)						
Massflow (kg/h)						
Wt%Propene						
Temp (°C)						
P(bar)						

Almost all the stream values are very close to the diagram data, the accuracy mean obtained is 89.2%. However, there are temperature differences in the splitter overhead and after compressor stream, as the process flow diagram is performed using more components, hydrogen for example, the temperature at the same pressure may change. Furthermore, both streams are the only ones that are in a gaseous state.

Another difference shown is the propane and propene compositions after the distillation. Converted in weight fraction percentage the principal difference is in the bottom stream, the propene fraction in the simulation is -% below the diagram which means that the current simulation is more efficient. Being the only difference the model simulated is validated.

**Sensitivity analysis**

From the distillation column is taken the hydraulic plot. Each distillation column stage has its hydraulic plot. The plot varies depending on the hydraulic internal column analysis. The status of the hydraulic plot indicates healthy because the operating point is inside the limits. One of the representative internal column hydraulic plot is shown below, Figure 5. 1, in this case, the plot is of the first stage.

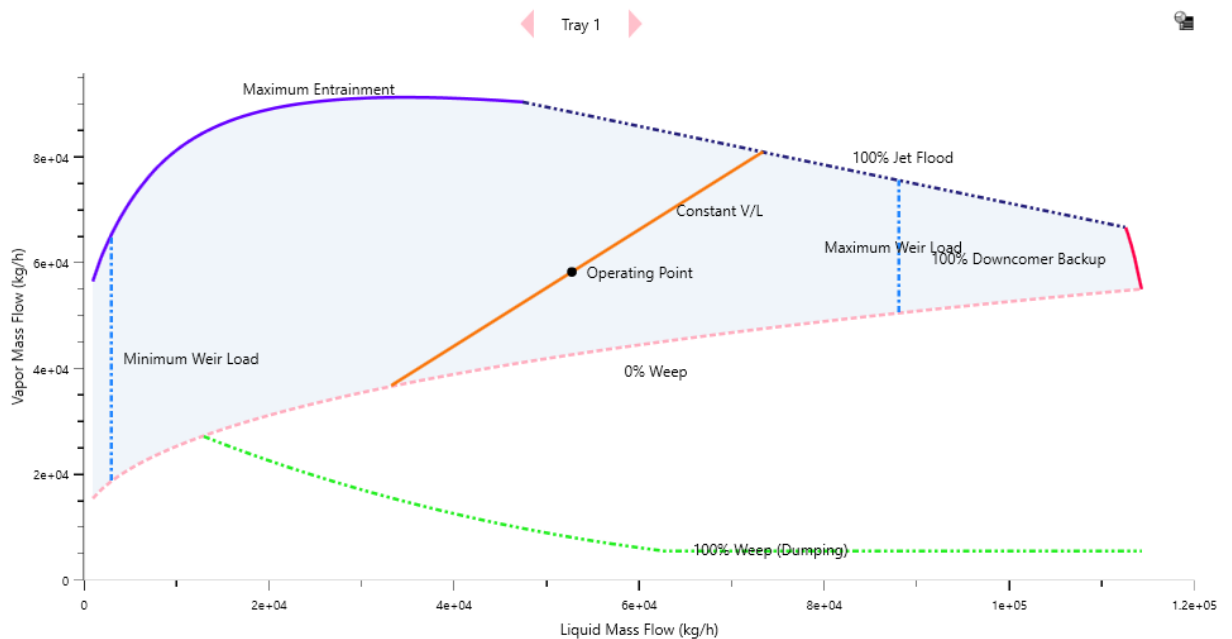


Figure 5. 1. The hydraulic plot of the first stage of column K-860 from Aspen HYSYS.

The column specification diagram as temperature, pressure, composition, etc. can easily be generated in HYSYS with the calculation of phase equilibrium relationship.



Figure 5. 2. Temperature profiles with trays number of column K-860 from Aspen HYSYS.

Figure 5. 2 represents the temperature profile versus the tray position. The profile shows a significant temperature rise close to the bottom of the column. This outcome, according to the model, is validated by thermal analysis of the column operation as the fluid on the tray is at its bubble temperature and knowing that the low boiling point components remain at the higher trays, the temperature profile naturally takes that kind of shape.



Figure 5. 3. Pressure profiles with trays number of column K-860 from Aspen HYSYS.

The above figures exhibit, as said, the variations in various parameters against the tray position of the distillation column from top to bottom. Figure 5. 3 shows that the pressure increases from top to bottom.



Figure 5. 4. Mass composition versus tray position profile of the column K-860 from Aspen HYSYS.

The feed and reflux stream of the splitter is composed largely of propane and propene, therefore can be considered a binary mixture. The steady-state mass compositions, shown in Figure 5. 4, of propene are about 99.19% at the top and 18.1% at the bottom. Therefore the propane mass composition at the first stage results -% and at the last stage -%.

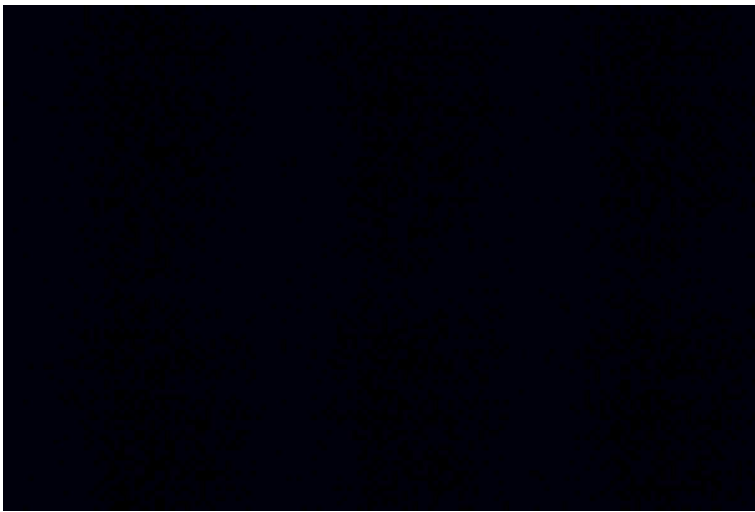


Figure 5. 5. Tube and shell stream temperatures of the heat exchanger W-862 from Aspen EDR.

The heat exchanger temperature profile show in Figure 5. 5 includes both fluids: the distillate and the water. As the plot shows the cold stream is the water and thus the hot is the distillate.

Table 4. 3, where the heat exchanger values are collected, can be contrasted with the plot to ensure that it is well simulated. Such as the inlet and outlet temperature, -, etc.

### 5.1.2. Dynamic results

In Table 5. 2 the data streams of the process flow diagram and the steady-state simulation are compared, consequently in the tables below the temperature, pressure, and compositions of the real plant and dynamic simulation are compared. Note that the feed values before the dynamic simulation are modified using the values from the plant.

Table 5. 2. Streams variables of dynamic simulation, current plant and the accuracy.

	Feed			Splitter Bottoms		
	Plant	Sim	Acc%	Plant	Sim	Acc%
<b>T (°C)</b>	-					
<b>P (bar)</b>	-					
<b>Wt% Propane</b>	-					
<b>Wt% Propene</b>	-					
<b>Wt% Nitrogen</b>	-					
<b>Wt% Ethane</b>	-					
<b>Wt% 2-propanol</b>	-					
<b>Wt% Hydrogen</b>	-					
<b>Wt% Ethylene</b>	-					
<b>Mass flow (kg/h)</b>	-					

Table 5. 3. Streams variables of dynamic simulation, current plant and the accuracy.

		<b>T (°C)</b>	<b>P (bar)</b>
<b>Overhead After Compressor</b>	Plant		
	Simulation		
	Accuracy %		
<b>Between Exchangers</b>	Plant		
	Simulation		
	Accuracy %		
<b>Cold Water</b>	Plant		
	Simulation		
	Accuracy %		
<b>Heated Water</b>	Plant		
	Simulation		
	Accuracy %		
<b>Before Pump</b>	Plant		
	Simulation		
	Accuracy %		
<b>After Pump</b>	Plant		
	Simulation		
	Accuracy %		

As expected almost all the stream values compared are very close between them, the accuracy mean obtained is 88.1%. Since in the steady-state comparison, the stream results differences have the same explanations; In the plant, there are more components, so at the same pressure the temperature at the same vapor fraction may change.

The propane and propene compositions after distillation vary. In the simulation the separation between components is better, despite the simulation efficiency of the column has been calculated. Nevertheless, the slight difference in the mass fraction would decrease if it is recalculated neglecting the non-simulated components, and in order to study controllers, different scenarios, etc. the results obtained will help.

**5.2. Controllers**

For most control schemes, is used proportional-integral-derivative, or PID, controllers. It employs proportional, integral, and derivative control. The controller can be tuned by adjusting the controller gain,  $K_c$ , the integral time,  $\tau_i$ , and the derivative time,  $\tau_d$ . Table 5.4 shows the suggestions for initial PID tuning parameters by AspenTech. (Aspentech, 2020) and the tuning parameters of the current plant (LyondellBasell)

Table 5. 4. Aspen recommended and plant tuning parameters for the simulated controllers.

Controller	Aspen recommended		Current plant		
	$K_c$	Ti(min)	$K_c$	Ti(min)	Td(min)
-					

In this section are compared step responses for both tuning parameters. The step is an increase of 10% of the plant setpoint value. Table 5. 5 collects both setpoints of each controller.

Table 5. 5. Plant setpoints for the controllers and setpoints for the step analysis. (LyondellBasell)

Controller	Setpoint	Step setpoint
-		

The following graphs show the step responses for both tuning parameters for each controller.

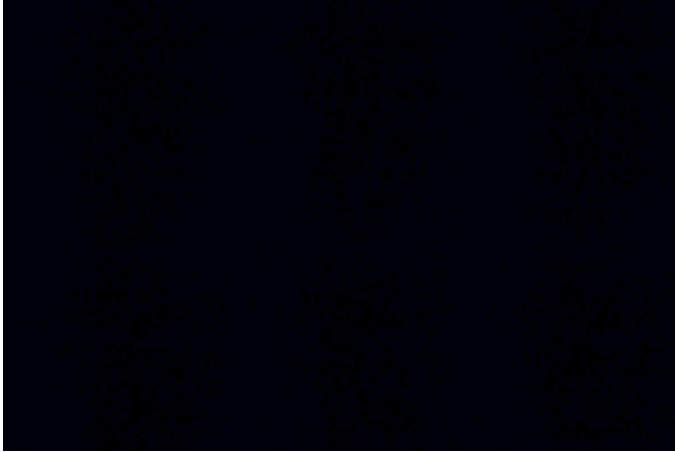


Figure 5. 6. Comparison of step responses for - controller of Aspen recommended and plant tuning parameters values.

For the - controller can be seen that the recommended parameters allow a rapid adjustment to the new setpoint while the plant parameters result in a constant oscillation.



Figure 5. 7. Comparison of step responses for - of Aspen recommended and plant tuning parameters values.

Recommended parameters for reflux controller result in a slight oscillation in the step response. The plant PI values seem to be better designed for - setpoint, at lower setpoint values the dead band oscillates continuously.



Figure 5. 8. Comparison of step responses for - controller of Aspen recommended and plant tuning parameters values.

For - controller, both step responses behave as the - controller, the plant parameters in the simulation differ from the plant results.



Figure 5. 9. Comparison of step responses for - controller of Aspen recommended and plant tuning parameters values.

For the - both tuning parameters values have a slow conversion and in the case of the recommended parameters an oscillation. Plant values seem to be better adjusted, in case of having the same results in the plant an increase of the gain parameter could improve time conversion.



Figure 5. 10. Comparison of step responses for - controller of Aspen recommended and plant tuning parameters values.



Figure 5. 11. Comparison of step responses for - controller of Aspen recommended and plant tuning parameters values.

As explained in 4.3. section the - works in cascade with the -, so the setpoint of the flowrate changes while -value changes. In this case, the step of the plant values result in a better response but the - controller produces an overshoot that, obviously, affects significantly to - setpoint.

The - controllers with the plant tuning parameters in the simulation response are entirely different from the real plant response. In this case, the simulation must be revised and improved in order to behave as the real plant.

While the other controllers, - and -, have a better step response. Nevertheless, these controllers' responses must be compared to the real plant and in the case of having small or large overshoot, slow conversion, oscillation, etc. the gain, the integral, and derivative time need to be adjusted to achieve the best response.

**5.3. Sensitivity analysis to determine optimal reflux ratio**

The main objective of this section is to study the best reflux rate for each feed flowrate because the reflux rate is an input variable that can be easily changed in the plant. The best reflux rate is focused on energy efficiency and distillate purity.

First, different scenarios are studied at the most often feed concentration. And secondly, a sensitivity analysis with two different feed concentrations is also done.

**5.3.1. Reflux flowrate analysis**

The reflux rate is the manipulating variable at different feed flowrates in a sensitivity analysis performed in order to estimate its influence on some important process parameters such as the reboiler duty and the product purity. Different scenarios are simulated to investigate the best reflux rate for each feed flowrate at the same feed concentrations. The table below collects the different scenarios simulated, these flowrates ranges are the minimum and maximum values used in the plant:

Table 5. 6. Different scenarios simulated.

Feed flow (kg/h)
Reflux (kg/h)

These simulations are performed in dynamic mode and the data is collected after a long time of simulation to guarantee that all the stream parameters and equipment are stabilized.

Next plots show the effect of the different feed flowrate and reflux situations on the reboiler heat flow, propene mass fraction at the column bottoms, and distillate.



Figure 5. 12. Reboiler heat flow at different reflux and feed flowrates.



Figure 5. 13. Propene purity in the distillate flow at different reflux and feed flowrates.



Figure 5. 14. Propene concentration in the bottom flow at different reflux and feed flowrates.

The heat flow required in the reboiler, Figure 5. 12, follows a tendency. As expected, as the reflux increases the energy demanded grows. The same happens if the amount of feed flow rate rises.

The best propene purity is obtained when the lowest feed flow and the highest reflux flowrate is simulated. Note that the improvement while these perturbations are just an increase in 1% of propene mass. The deviations concerning the purity are more remarkable for less reflux flowrate.

On the other hand, the difference in propene concentrations at the splitter bottom is more remarkable at higher reflux flowrates. More propene is lost if less feed flow enters into the column. Because if there is less amount of propane in the column the bottom flowrate will have a reduced amount of that compound, increasing the propene fraction.

Additionally to these outcomes it has been calculated the cost of the propene losses and the reboiler energy consumption. The data cost is obtained from the plant operations of December 2021. (LyondellBasell)

Table 5. 7. Electricity and propene cost.

<b>Electricity cost</b>	- €/Mwh
<b>Propene cost</b>	€ / ton





Figure 5. 15. Reboiler heat flow at different reflux, feed flowrates and feed composition.

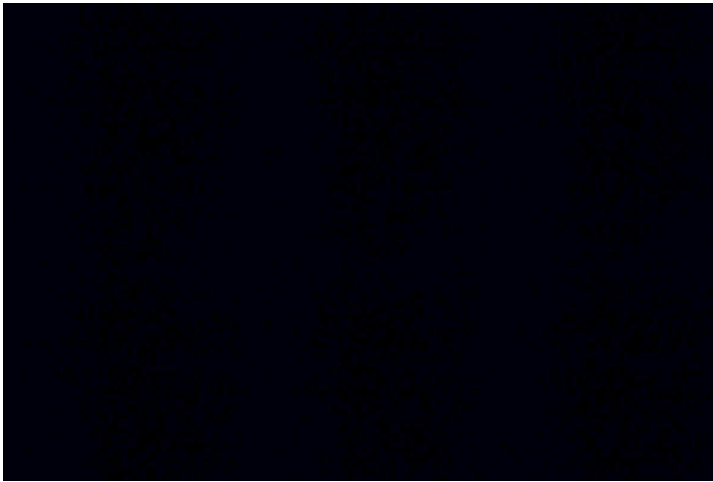


Figure 5. 16. Propene purity in the distillate flow at different reflux, feed flowrates and feed composition.

Thanks to Figure 5. 15 can be concluded that at different propene feed concentrations keeping fix other variables such as reflux and feed flowrate, the amount of energy required in the reboiler to do the distillation does not change. In other words, the reboiler heat flow is not dependent on feed composition.

Conversely, as expected the propene purity depends on the feed composition. It is not just the mass fraction that differs using different concentrations, the difference is that by varying the reflux at lower propene concentrations the purity can be improved by -%Wt.

On the other hand, as explained before by changing the reflux the propene purity can increase just -%Wt.

At larger feed flowrate is better using more reflux flowrate, even though the energy required is higher because the propene purity can be increased considerably.

This propene-propane separation handles to remove the propane before introducing the flowrate in the reactor to improve the reaction. So, it is noteworthy that this analysis must be complemented with the reactors plant simulation to reach more accurate conclusions.

**5.4. Process perturbations**

One of the purposes of the dynamic simulation is to study the stability of the process and the changes caused by perturbations to the distillation process by means of a sensitivity analysis.

To carry out this sensitivity analysis the bottom flow, the top pressure, and the feed flow have been perturbed to see the effect on propene purity (top stream) and energy consumption.

The different values are collected in the table below. Note that the italic amount is the plant data.

Table 5. 9. Perturbations in the dynamic simulation.

<b>Bottom Flow (kg/h) - 890</b>	<b>Feed Flow (kg/h) -893</b>	<b>Top Pressure (bar)</b>
---------------------------------	------------------------------	---------------------------

-

In this study it has been evaluated several streams and equipment magnitudes, however, the main magnitudes are the reboiler heat flow, the distillate purity, and the splitter top pressure. The reboiler heat flow and the distillate purity are essential variables for the process optimization while the pressure is used to ensure the safety of the operation process.

For the bottom flow variation these are the following findings:



Figure 5. 17. Effect of bottom flow on the heat flow reboiler.



Figure 5. 18. Effect of bottom flow on the propene purity.



Figure 5. 19. Effect of bottom flow on the top column pressure.

Increasing the bottom flow a -% over the plant value can be seen in Figure 5. 17 that the energy consumption is affected, the savings are -% estimated. The propene obtained in the distillate improves when the amount of bottom flow raises but the propene losses increases, however, improvements are -.

Regarding the process safety, as Figure 5. 19 shows modifying the bottom flow the column pressure -. There are no safety consequences.

Other trends are detected varying the feed flow of the process flow:



Figure 5. 20. Effect of feed flow on the heat flow reboiler.



Figure 5. 21. Effect of feed flow on the propene purity.



Figure 5. 22. Effect of feed flow on the top column pressure.

The figures above illustrate the behavior of the column in case of variation of feed rate and maintaining the rest of operating values. As supposed, as the feed flow increases the heat flow

of the reboiler increases because there is more amount of flow that requires more energy to do the separation. The purity of the distillate, Figure 5. 21, raises when there is less amount of feed.

The safety process has to be taken into account while the feed flow changes, Figure 5. 22. At lower feed flowrates the column pressure is stabilized rapidly, however, at high flowrates the pressure grows. In this simulation, the feed flow has been increased just by  $-%$ , and after a time (not plotted in this figure) the controller has managed to maintain the pressure at  $-$  bar, setpoint value.

An important analysis is the column pressure since it is a critical parameter in risk analysis. Top column pressure perturbations have been simulated:



Figure 5. 23. Effect of top pressure on the heat flow reboiler.



Figure 5. 24. Effect of top pressure on the propene purity.



Figure 5. 25. Effect of top pressure perturbances on the process.

By increasing the top pressure the reboiler heat flow and the purity have been altered. The energy consumption peak can be relevant while enlarging the pressure. Despite the initial variations in the purity, the results are similar, so the purity is not related while changes in top pressure.

For - and - bar the results of the three studied variables, including the column pressure---. Note that the setpoint has been modified but at lower pressures, the controller -.

### **5.5.Proposals**

After an evaluation of multiple process alternatives, this is a summary of the changes that can improve the plant.

Removing the -.

Usually, these types of distillation columns-.

In the previous section is concluded that -.

For each feed composition and feed flow, there is a reflux rate that can save energy and reach a better flow composition. If the plant situation differs from the scenarios presented the dynamic simulation can be used to explore other situations of interest.

Regarding the top pressure analysis, -.

Therefore, the model can be used to explore perturbations other than those studied in this thesis, especially if the feed variables have been changed.

### **5.6.HAZOP study**

This section compares the HAZOP consequences analyzed in - with the simulation consequences, in order to see if they have identified the results properly.

Table 5. 11 compares the report consequences with the simulation ones. It is not a complete HAZOP study due to the table just showing the guide word, the deviation, the causes, and the consequences. Furthermore, there are deviations and causes missing because they could not be simulated like a start-up, electric failure, etc.

The report consequences highlighted in green indicate that the report and the simulation consequences have been carried out to the same conclusion.

The node is the propene separator K860-. The values of the simulation and the report are collected in Table 5. 10.

Table 5. 10. Parameters values in the HAZOP report and simulation.

<b>Report values</b>	<b>Simulation values</b>
-	-

Table 5. 11. Comparison of the HAZOP report with the simulation consequences.

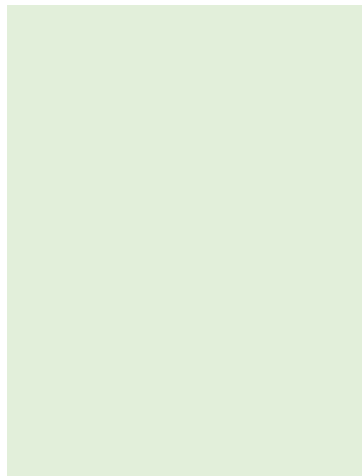
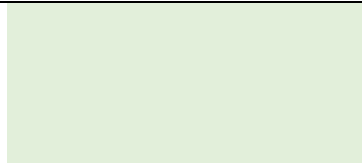
<b>PARAMETER: LEVEL</b>						
<b>GUIDE WORD</b>	<b>DEVIATION</b>	<b>CAUSES</b>	<b>CONSEQUENCES REPORT PHA</b>	<b>SIMULATION</b>	<b>SIMULATION CONSEQUENCES</b>	<b>DIFFERENCES</b>
-						

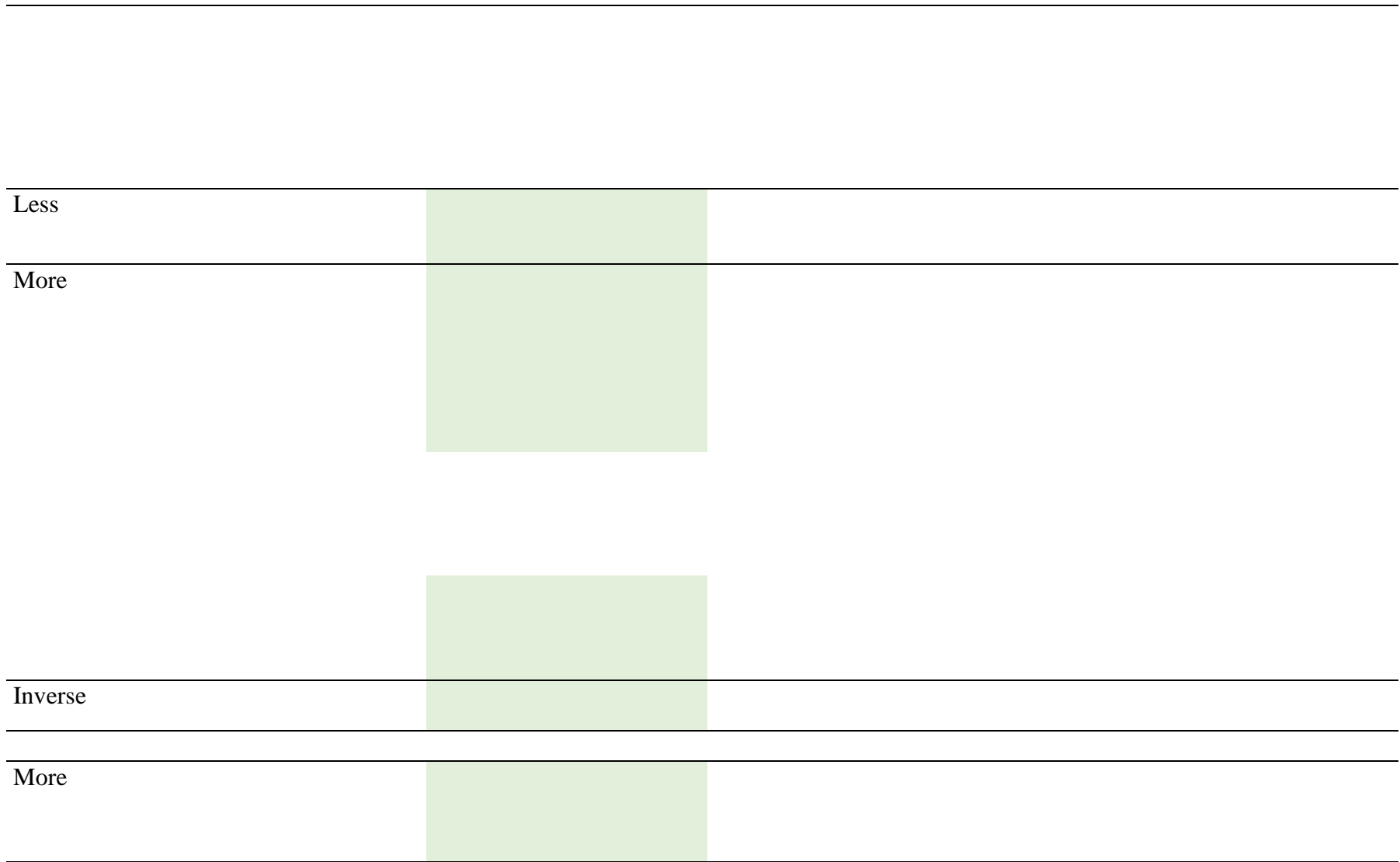
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Less

---

No





More	
Less	
More	

Less	
No	

This study has shown an alternative pathway in the study consequences. Establishing the evolution of the process variables upstream of the column and downstream of the pump has not been considered in this study. However, it has been demonstrated that the dynamic HAZOP has the same results as the traditional one done in -.

Most of the report consequences match with the simulated ones. The consequences that result different are because the simulation doesn't inform about mechanical damages, the pump outlet simulation has specifications at it is the last unit operation of the simulation, etc. The HAZOP team has proved that they have enough experience and creativity to predict the outcomes.

As the traditional HAZOP study requires additional time and effort in the deliberation of the consequences in future studies can be used this dynamic simulation.

It has been demonstrated that a simulation can help and save time in the HAZOP studies it is recommended to simulate all the plants to obtain all the nodes and complete this activity as part of the preparatory phase of a HAZOP study.

## **6. CONCLUSIONS**

A Propene-propane splitter with vapor recompression in a petrochemical plant has been simulated in steady-state and dynamic mode using Aspen HYSYS V12 tool. Both simulations have been proved to predict similar values as the current plant, the average accuracy for the steady-state and dynamic simulation are 89.2% and 88.1%, respectively. Analysis of the column data has shown results that can help in plant optimization.

Step responses of the recommended and plant tuning parameters of the controllers have shown different results. -.

On the other hand, -.

The second case study consists in investigating -.

The main conclusion is that the reboiler heat flow -.

For greater -.

If the plant situation differs from the scenarios presented the dynamic simulation can be used to explore other situations of interest.

Some other studies can be performed to see if -.

Regarding the comparative study of the consequences of the last process hazard analysis (using HAZOP methodology) with the simulation results has been explored, proving that most of the identified consequences are confirmed by the simulated ones.

### **Further proposal**

This propene-propane distillation column separates both C3 components as a recycling process. So, it is noteworthy to mention that this analysis could be further complemented with the reactors plant simulation to reach more accurate conclusions.

However, both simulations can be used to explore other situations and perturbations than those studied in this thesis, especially if -.

A way to reduce energy consumption in distillation is optimization through the implementation of advanced controllers. The major chemical industries are now competing to 54/57 optimize raw material and utility consumption in order to reduce waste, reduce emissions, and minimize pollution. An excellent tool to achieve it is implementing multivariable model predictive control (MPC).

Some researchers have proved the rentability of the MPC implementation in a propane-propene splitter. Can be used either Matlab-Simulink (Tuan et al., 2016) or eXperiment design (MPC-X) (Larsson et al., 2015) in cooperation with HYSYS.

It could be interesting to simulate the - plant in order to evaluate and optimize the current plant.

Today there is a continuous increase in the energy cost, which makes it of great importance to focus on a deeper economic study since a variation in the energy cost could completely change the project conclusions.

Another relevant study for the VRC column optimization is to perform the curves profiles of the -.

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## **APPENDIX**

### **APPENDIX A: Aspen HYSYS steady-stead**

In this section are collected several actions followed during the simulation steady-state design. All the variables and design specifications are taken from (LyondellBasell) files.

First, it is selected the components involved, has been created two components list as can be seen:

Figure A. 1. First component list.

Figure A. 2. Second component list.

The fluid package is chosen after the study of the interaction parameters between components required in this simulation:

Figure A. 3. Establishing the fluid package.

Once the components and the fluid package have been set the simulation environments must be chosen and in the model palette, a column must be selected. Once in the column subflowsheet, the condenser must be removed as appears in Figure 4. 2. The column specifications and the stream names are defined as:

Figure A. 4. Column connections, pressure, and the number of stages.

The feed streams variables have to be defined as compositions, temperatures, flowrates, and pressure. Before running the column the internals section must be completed:

Figure A. 5. Column internals.

Once the column does not ask for any other variable it is time to click 'Run' bottom, the program starts to iterate to converge and can take several minutes due to the complexity. When it stops running the result can be 'Converged' in green color or 'Unconverged' in red. If the column does not converge some variable or specification may be wrong.

One important result is the hydraulic plot of each stage, the operating point has to be inside ranges as weir load, jet flood, weep, etc.

Figure A. 6. Hydraulic plots for each column stage.

Once the column and reboiler are working properly, the main flowsheet has to be completed. This is the design decision for the compressor V-860.

Figure A. 7. Compressor V-860 design.

The 'OK' appears when all the equipment parameters and connections are completed properly.

The heat exchanger W-862 has been performed using *Aspen Exchanger Design & Rating (EDR)*. The heat exchanger is a Shell & Tube exchanger. The next pictures show the process and geometry entered:

Figure A. 8. The geometry of W-862 in the EDR.

Figure A. 9. Process of W-862 in the EDR.

In the Heat Exchanger of HYSYS has to be chosen: Rigorous Shell&Tube on the Design section and upload the EDR file created.

For the cooler W-860B the parameters stated are:

Figure A. 10. Heat exchanger W-860B design.

The Tee B-860 is an easy equipment for the simulations, HYSYS just requires the connections:

Figure A. 11. Tee B-860 design.

As the characteristic curves are missing this is the design followed:

Figure A. 12. Pump P-860A design.

All the equipment is working properly to simulate the reflux stream the recycle tool connects one column feed to one Tee outlet stream. This tool iterates all the flowsheet equipment in order to obtain a solution, this can take several minutes as well.

Figure A. 13. Connection of the reflux stream.

To conclude the steady-state simulation the W-860 heat streams must be connected, so a spreadsheet is used. The cooler heat flow will always be 10% greater than the reboiler heat flow.

Figure A. 14. Spreadsheet connections.

Figure A. 15. Spreadsheet formulas.

### **APPENDIX A: Aspen HYSYS dynamic**

For the dynamic simulation, it is important to define the base elevation relative to the ground as shown in Table 4. 4. Each valve and equipment must be defined in the Rating section. For the column apart from the base elevation before the dynamic simulation it is required the k values:

Figure A. 16. Dynamic specification of the column.

Next dynamic specifications are explained in section 4.3. The next pictures show the dynamic specification of each equipment:

Figure A. 17. Dynamic specification of the compressor V-860.

Figure A. 18. Dynamic specification of the heat exchanger W-860.

Figure A. 19. Dynamic specification of the heat exchanger W-860B.

Figure A. 20. Dynamic specification of the pump P-860A.

In the model palette there are different types of valves, these are “control valves”. The sizing and characteristics for each valve:

Figure A. 21. Dynamic specification of the valve -.

Figure A. 22. Dynamic specification of the valve -.

Figure A. 23. Dynamic specification of the valve -.

Figure A. 24. Dynamic specification of the valve -.

Figure A. 25. Dynamic specification of the valve.

For all the controllers in the model palette has been selected “PID Controller”. Table 4. 6 are collected some of the variables below.

Figure A. 26. Connections of the controller -.

Figure A. 27. Parameters of the controller -.

Figure A. 28. Connections of the controller -.

Figure A. 29. Parameters of the controller -.

Figure A. 30. Connections of the controller -.

Figure A. 31. Parameters of the controller -.

Figure A. 32. Connections of the controller -.

Figure A. 33. Parameters of the controller -.

Figure A. 34. Connections of the controller -.

Figure A. 35. Parameters of the controller -.

Figure A. 36. Connections of the controller -.

Figure A. 37. Parameters of the controller -.

Once all the controller's parameters are entered, in the Dynamics section, click on the Integrator (labeled in red) and Figure A. 39 sheet will be opened. Figure A. 39

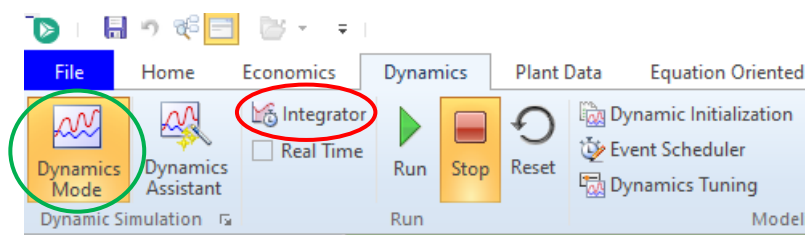


Figure A. 38. Dynamic simulation section.

To start the simulation these are the step and the acceleration selected in automatic mode.

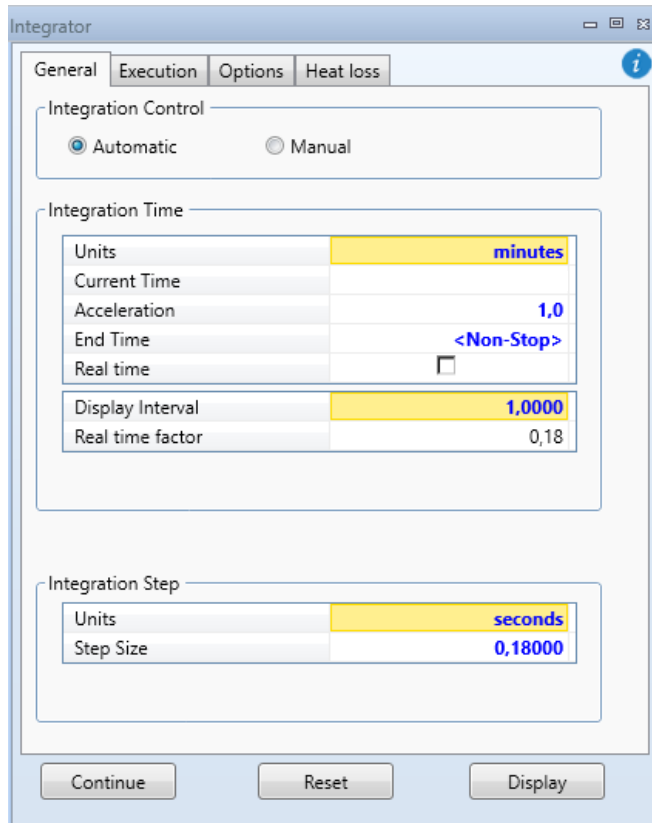


Figure A. 39. Integrator of the Dynamic simulation.

In Figure A. 38 click on the dynamic mode (labeled in green) and maybe some suggestions may appear. After solving all the suggestions the dynamic simulation will start. In each controller in the monitor section, a plot like Figure A. 40 appears.

Figure A. 40. Monitor section of the controller.

To analyze if the simulation is running properly these plots can be interesting. The next pictures show how the data is collected for the studies. The first picture is for taking steady-state data or after a fixed time of the dynamic simulation because shows the actual variable.

Figure A. 41. Data table of the current time.

If the analysis depends on the time the Datalogger is needed. Selecting “display” a plot will be created in the “historical” the value for each time can be converted in an Excel file.

Figure A. 42. Datalogger table collects values as a time function.

## APPENDIX B: Self-evaluation Questionnaire

a) Evaluate the acquired **competences** according to the **tasks** you have carried out.

<b>Degree Competences</b>		<b>Task in which you have observed the competence</b>	<b>Self evaluation [Rank 1 to 10]</b>	<b>Aspects to be improved</b>
<b>SPECIFIC COMPETENCES</b>				
A1.1	Effectively apply knowledge of basic, scientific and technological materials pertaining to engineering.	Equipment parameters calculations and design.	9	
A1.2	Design, execute and analyze experiments related to engineering			
A1.3	Be able to analyze and synthesize the continuous progress of products, processes, systems and services, whilst applying criteria of safety, economic viability, quality and environmental management. (G6)			
A1.4	Know how to establish and develop mathematical models by using the appropriate software in order to provide the scientific and technological basis for the design of new products, processes, systems and services and for the optimization of existing ones. (G5)	Development of the steady state model in Aspen Plus and the dynamic model in Aspen Plus Dynamics	8	
A2.1	Be able to apply the scientific method and the principles of engineering and economics to formulate and solve complex problems that arise in processes, equipment, installations and services, in which the material undergoes changes to its composition, state or energy content, these changes being characteristic of industrial chemistry and other related sectors such as pharmacology, biotechnology, materials sciences, energy, food and the environment. (G1)	In both simulations, the convergence of the propane-propene splitter represents a complex problem in the process simulation.	9	
A2.2	Conceive, project, calculate and design processes, equipment, industrial installations and services in the field of chemical engineering and related industrial sectors in terms of quality, safety, economics, the rational and efficient use of natural resources and the conservation of the environment. (G2)	Proposal for improvement in the current plant. The consequences simulation of the HAZOP.	9	
A2.3	Lead and technically and economically manage projects, installations, plants, companies and technological centres in the ambit of chemical engineering and related industrial sectors. (G3)			
A3.1	Apply knowledge of mathematics, physics, chemistry, biology and other natural sciences by means of study, experience, practice and critical reasoning in order to establish economically viable solutions for technical problems (I1).	Development of the simulation with the required previous calculations	9	
A3.2	Design and optimize products, processes, systems and services for the chemical industry on the basis of various areas of chemical engineering, including processes, transport, separation operations, and chemical, nuclear, electrochemical and biochemical reactions engineering (I2).	All the analysis performed in the simulation to optimize the process	9	
A3.3	Conceptualize engineering models and apply innovative problems solving methods and appropriate IT applications to the design, simulation, optimization and control of processes and systems (I3).	Simulation of the propane-propene splitter using Aspen HYSYS v12.	9	
A3.4	Be able to solve unfamiliar and ill-defined problems by taking into account all possible solutions and selecting the most innovative. (I4)	Study of different alternatives to optimize the installation	9	
A3.5	Lead and supervise all types of installation, process, system and service in the different industrial areas related to chemical engineering (I5).			
A3.6	Design, construct and implement methods, processes and installations for the integrated management of waste, solids, liquids and gases, whilst			

	also taking into account the impacts and risks of these products (I6).			
A4.1	Lead and organize companies and production and service systems by applying knowledge and abilities regarding industrial organization, commercial strategy, planning and logistics, mercantile and labour legislation, and financial and costs accounting (P1).			
A4.2	Lead and manage the organization of work and human resources by applying criteria regarding industrial safety, quality management, occupation risk prevention, sustainability and environmental management (P2).			
A4.3	Manage research, development and technological innovation whilst ensuring the transfer of technology and taking into account property and patent rights (P3).			
A4.4	Adapt to structural changes in society caused by economic, energy or natural factors so as to be able to solve any resulting problems and to contribute technological solutions with a high commitment to sustainability (P4).			
A4.5	Lead and monitor the control of installations, processes, products, certification, auditing, verification, testing and reports (P5).			
A5.1	Carry out, present and defend (once all the curriculum credits have been obtained) an original individually produced piece of work before a university panel. The work will consist of a professional integrated Chemical Engineering project that synthesizes (TFM1)			
<b>TRANSVERSAL COMPETENCES</b>				
B1.1	Communicate and discuss proposals and conclusions in a clear and unambiguous manner in specialized and non-specialized multilingual forums (G9).	Performance of weekly meetings about the state of the project	9	
B1.2	Adapt to changes and be able to apply new and advanced technologies and other important developments with initiative and entrepreneurial spirit. (G10)			
B2.1	Lead and define multidisciplinary teams that are able to make technical changes and address management needs in national and international contexts. (G8)			
B3.1	Work in a team with responsibilities shared among multidisciplinary, multilingual and multicultural teams			
B4.1	Be able to learn autonomously in order to maintain and improve the competences pertaining to chemical engineering that enable continuous professional development. (G11)	Learn how the Aspen HYSYS and Aspen EDR simulators work	10	
B5.1	Carry out and lead the appropriate research, design and development of engineering solutions in new or little understood areas, whilst applying criteria of creativity, originality, innovation and technology transfer. (G4)	Proposal of new modifications.	8	
B5.2	Bring together knowledge, make judgements and take decisions on the basis of incomplete or limited knowledge whilst taking into account the social and ethical responsibilities of professional practice. (G7)	Take decisions and establish several assumptions for the steady-state simulation.	9	
<b>NUCLEAR COMPETENCES</b>				
C1.1	Have an intermediate mastery of a foreign language, preferably English	English	8	
C1.2	Be advanced users of the information and communication technologies	Internet datasearching, on-line conferences about technical topics and on-line meetings with technical experts.	10	
C1.3	Be able to manage information and knowledge	Data and information search.	10	
C1.4	Be able to express themselves correctly both orally and in writing in one of the two official languages of the URV	Both communication with tutors and technical experts from other sites of the company.	9	

C2.1	Be committed to ethics and social responsibility as citizens and professionals			
C2.2	Be able to define and develop their academic and professional project	Weekly meetings	8	

**b) Evaluate** the final master project and suggest improvements.

<b>Key steps</b>	<b>Evaluation [Mark 1 to 10]</b>	<b>Improvement proposed</b>
Selection/assignment of the project (dissemination, communication, assignment requirements...)	9	
Stay (welcome, length, relationship, follow-up made by the company...)	10	
Follow-up made by URV tutor	10	
Other aspects to be considered (which ones...)		