

Detailed analysis of an ethylbenzene production plant

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Abstract

Ethylbenzene is a very important organic compound mainly used as feedstock to produce styrene. The objective of the present paper is to develop a process capable of producing 80,000 tons of ethylbenzene using benzene and ethylene as feedstocks. A flowsheet has been developed to maximize the overall yield of the process while minimizing costs. Thus a recycling loop is introduced to recover most of the benzene. In addition, a fourth reactor is used to convert one byproduct, diethylbenzene, back to the desired component. The reactions are carried out in gas phase and at high pressure using a beta-zeolite catalyst. The major unit operations have been modeled and optimized using Matlab and Aspen Plus. The thermodynamic model used is Redlich-Kwong-Soave. After a thorough heat integration, the process needs were reduced to 90.2 kW of electricity, 60 kW of natural gas as well as 2082 kW of cooling water. Furthermore, 192 kW of high-pressure steam is sold to a neighboring styrene plant. A detailed LCA analysis has been performed and Belgium was chosen for the localization of the plant. The economic analysis performed led to a net present value of the project close to 41,000,000 \$. Nevertheless, this analysis contains some strong hypotheses, most notably the constant prices of raw materials. The severe dependency of the profitability on the raw material prices is discussed. The total amount of money needed to start the production is 33,000,000\$. The discounted payback period is around five and a half years. Other processes are compared to the one developed. Moreover, other potential routes to produce ethylbenzene are introduced.

Keywords

Ethylbenzene - Benzene - Ethylene - Aspen Plus - Matlab - Modeling - Cost Analysis - Heat Integration - LCA

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1. Introduction

Ethylbenzene ($C_6H_5CH_2CH_3$, EB) is an essential organic compound mainly used as feedstock for styrene production. It is present in petroleum in a small proportion where it can be extracted by fractional distillation. Nevertheless, this way of production is hardly ever profitable. Instead, it can be synthesized by the alkylation of benzene with ethylene. These raw materials are obtained through several processes mainly catalytic reforming and steam cracking of naphtha. The market of ethylbenzene, its uses, and hazards as well as the most adopted production processes will be discussed. In addition, its environmental impacts and main physical properties are introduced.

Then, the description of the modeling is established. The main flowsheet of the process as well as the design of the most important units are presented. The goal of this modeling is not only to produce ethylbenzene but also to reach efficient and realistic manufacture.

Therefore, this design also includes heat integration, which is directly followed by a life cycle assessment. Afterward, an economic analysis, as well as a literature review, have been conducted.

2. Ethylbenzene context

2.1 Market and production

The ethylbenzene market is divided into different categories segmented by company, region (country), type, and application. This market's size is expected to increase significantly as demand for synthetic rubber and plastic polymers is rising. Therefore, styrene production is also increasing as it is used to produce these materials. [1]

Moreover, it is expected that the market for ethylbenzene would significantly increase by 2025. Indeed, it is expected to reach 28.2 billion\$ after growing at a compound annual growth of 4.3% for five years. The main producing and consuming regions are North America (driven by the US, Canada, and Mexico), Europe (driven by Germany, France, Italy, Spain, and the UK), the Middle East, and the Asia Pacific as shown in Figure 1. The Asia Pacific has been dominating the ethylbenzene market as it accounted for 47% of global capacity and 49% of consumption in 2019. In this region, it is used in the construction and packaging industries to manufacture paint, coating, inks, dyes, perfumes, and mostly synthetic rubber, especially in India, Japan, and China. [2]

The main producing companies are INEOS Styrolution (7.1% of world production), Royal Dutch/Shell (6.7%) in The Hague, Netherlands, Sinopec (6.2%) in the Houston, United States, and Total in Feluy and antwerpen (Belgium). INEOS Styrolution is located in North America and Western Europe. In Belgium, the main site is located in Antwerp (Zandvliet), Belgium. Furthermore, in 2016, US ethylbenzene was assessed at 670-815 \$/tonne. [3]

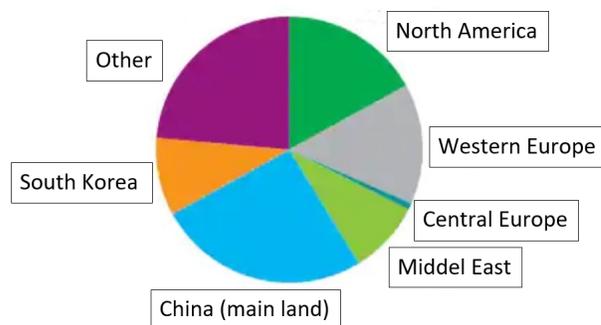


Figure 1. World consumption of ethylbenzene - 2019

2.2 Main uses

Ethylbenzene is a chemical compound mainly used as a primary building block for the production of styrene. In addition to ethylbenzene's participation in the manufacture of polymers, it is used for the manufacture of several products such as pesticides, rubber, cellulose acetate, paints, and inks. It is also used as an additive for gasoline, reducing engine knocking and increasing the octane rate. As a result, EB improves automotive engines, performance, and efficiency. It is important to mention that the use of EB for the production of styrene exceeds 95 % of its entire use. Therefore, EB production is almost completely reliant on another product, which is a drawback from a marketing perspective that might cause investors to hesitate to proceed with investments related to EB. [4]

2.3 Product Toxicity

Ethylbenzene has a high vapor pressure and low solubility in water. When it divulges in water, it moves to the air and undergoes indirect photolysis, degrading after approximately four days. EB does not persist in the environment as it is biodegradable and has moderated potential to be adsorbed in sediments. [4]

Regarding the effects of EB on human health it could be divided into short-term exposure and long-term exposure. Short-term exposure causes eyes and throat irritation. In case of higher levels of exposure, EB causes vertigo and dizziness. On the other hand, long-term exposure can lead to cancer and, irreversible inner ear and kidney damage. [5] However, since exposure is concomitant with other substances, the side effects cannot be attributed to ethylbenzene alone.

Although stable under normal conditions of use, ethylbenzene is easily flammable. The reaction of EB with strong oxidizing agents is exothermic and creates a risk of fire or explosion if handled incorrectly. Therefore, it affects aquatic species including freshwater and marine organisms. Nevertheless, it is very volatile. Thus, 99.5% will be found in the air. In soil, it is mainly decomposed by bacteria and could damage some crops. However, based on current information, it cannot be concluded that EB constitutes a danger to life or harms the environment because it does not enter the environment in a way that endangers it in the short or long term.

While ethylbenzene is not a very toxic product by itself, it does represent a significant source of pollution when converted to polystyrene. Indeed, in 2017, the recycling rate of plastics in Europe was about 30%. This leads to ocean pollution as 4.8 to 12.7 million tons of plastics end up there every year. In addition, polystyrene takes 500 years to biodegrade. [6]

2.4 Ethylbenzene process

Ethylbenzene is present in reforming gasoline alongside xylenes of which it is an isomer. However, the extraction of ethylbenzene is hardly ever profitable and it is generally preferred to synthesize it from benzene and ethylene. In industrial plants, the ratio of benzene-to-ethylene is increased to improve the selectivity for ethylbenzene and reduce the production of diethylbenzene which is a byproduct.

Depending on the catalyst, there are three ways to produce ethylbenzene. [7][8][9] First, the aluminum chloride ($AlCl_3$) process is the oldest and most widely used. It takes place in gas phase and has a yield of 40 to 45%. About 40% of worldwide ethylbenzene production still utilizes variations of this method. Second, the boron trifluoride process is no longer used. Third, the processes using zeolites are the most recent. They are generally carried out in gas phase. The process developed in this article is one of them. In a more recent development, liquid phase processes using zeolite catalysts have been introduced. These latest technologies offer low benzene-to-ethylene ratios, which can then reduce the size of the equipment and lower the production of byproducts.

A new process is currently being developed by a US-based Dow Chemical company and Italy-based Snamprogetit company for making ethylbenzene/styrene from ethane and benzene in a process that combines dehydrogenation of ethane and ethylbenzene in one unit. This new route would integrate the processes for preparing ethylene, ethylbenzene, and styrene. It is also expected to have lower costs than the conventional route to styrene. [8]

2.5 Main physical properties

Ethylbenzene appears as a clear colorless liquid with an aromatic odor at ambient temperature. It is less dense than water and insoluble in water. Hence, it floats on water. Also, its vapors are heavier than air. [10]

Furthermore, ethylbenzene is an aromatic hydrocarbon that is an inflammable and combustible liquid. This compound has several properties which are indicated in Table 1.

Table 1. Ethylbenzene characteristics

Properties	Value
Molecular weight	106.1650 g/mol
Boiling temperature T_{boil}	409.3 ± 0.4 K
Fusion temperature T_{fus}	179 ± 2 K
Critical temperature T_c	617 ± 2 K
Critical pressure P_c	36.4 ± 0.9 bar
Critical density ρ_c	2.67 mol/l
Standard vaporization enthalpy $\Delta_{vap}H$	41 ± 4 kJ/mol

3. Process description

A brief process description is explained in this section. Figure 2 is a simplified representation of the flowsheet used in this paper. Benzene (B) and ethylene (E) enter the reacting section with their respective impurities, 2% of toluene (T) and 7% of ethane (Et). B is heated and enters the first reactor while the total E flux is divided into three different streams which allow E to enter one at a time in the three reactors in series. In these reactors, the main reaction taking place is the reaction between E and B which produces ethylbenzene (EB). Two other side reactions occur: EB can react with E to form diethylbenzene (DEB) and T can react with E to form propylene (P) and EB.

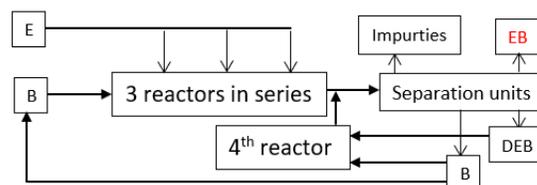
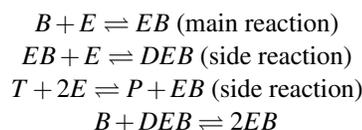


Figure 2. Simplified flowsheet

The separation units consist of one flash tank and two columns. The flash is used to separate some gases to avoid the accumulation of non-desired components within the system. The first distillation column recycles most of the unreacted B and the second one separates EB and DEB.

All the DEB and some of the recycled B are heated and fed into the fourth reactor where DEB is converted back to EB ($B + DEB \rightleftharpoons 2EB$). Finally, the inlet streams of E and B are chosen such that approximately 80,000 tons/year of EB are produced with a purity of 99.8 mol-%.

In addition, two storage units have been added. One would contain two weeks' worth of EB production. The second one would be able to contain 5 days of production and it will be placed just before the separation section to avoid ceasing the production if problems occur in the reacting section.

3.1 Thermodynamic model

This section aims to determine the most adequate thermodynamic model used to provide accurate values of thermodynamic properties for all mixtures found in the process.

Thus, liquid-vapor equilibria between benzene and ethylbenzene were plotted to select the most adapted model. This equilibrium was chosen as different ranges of experimental data corresponding to the process conditions were found in the literature [11]. Indeed, a database for constant temperatures of 180°C and 280°C was available. It was therefore possible to check the validity of the model.

Two different methods can be considered to evaluate thermodynamic properties: the residual approach or the excess approach. In the present case, different theoretical arguments promote the residual approach. First, all components are hydrocarbons. Second, some operation units operate at very high pressures and temperatures such as the reactors. Third, the composition is generally vapor except in the flash tank and the columns. Fourth, the experimental data found is rather close to the ideal solution.

For the residual approach, equations of state, EOS, were applied to pure components and mixtures. Then a fugacity coefficient was determined to study the equilibrium.

Among all the models studied with a residual approach (Peng-Robinson, Lee-Kesler, Redlich-Kwong-Soave (RKS), and Vanderwaals), the RKS method fits best the experimental data. However, at lower temperature and thus lower pressure, this model slightly differs from the experimental data as it is less adapted for this range of conditions. Consequently, a regression with these experimental data was conducted to add binary coefficients. The liquid-vapor equilibrium between benzene and ethylbenzene is illustrated in Figure 3 where the impact of the regression appears to improve the curves' behavior as they further coincide with the experimental data.

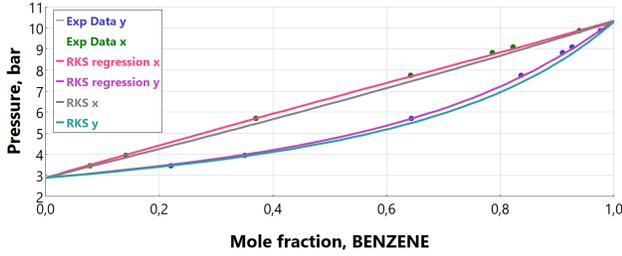


Figure 3. Equilibrium between benzene and ethylbenzene at 453.15 K

3.2 Kinetics

In this section, the reactions taking place in the studied process are introduced. The reactions follow a Langmuir-Hinshelwood adsorption-reaction model.

The main reaction taking place is the alkylation of benzene with ethylene which produces ethylbenzene.



The reaction rate of first reaction 2 can be expressed in terms of partial pressures p_i , kinetic constants k_i and equilibrium constants K_i . [12]

$$r = \frac{k_1 p_B p_E - k_{-1} p_{EB}}{(1 + K_B p_B + K_E p_E + K_{EB} p_{EB} + K_{side-react})^2} \quad (2)$$

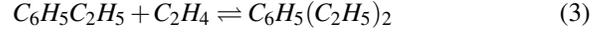
where $K_{side-react} = K_{DEB} p_{DEB} + K_T p_T + K_P p_P$

This reaction rate was simplified further:

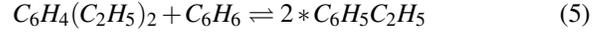
$$-r_1 = k_1 e^{\frac{-E_{a1}}{RT}} C_E C_B$$

where k_1 and k_{-1} are the rate coefficients for the forward and reverse reactions, E_{a1} the activation energy, C_E and C_B the concentrations of ethylene and benzene respectively.

Moreover, two side reactions in the first three alkylation reactors may occur. Indeed, ethylbenzene can react with ethylene to form diethylbenzene, which is a byproduct 3 and ethylene can react with toluene to form propylene and ethylbenzene 4. It is important to mention that the reaction rate of the following side reactions follow the Arrhenius law and could be simplified as well.



The fourth reaction occurring is the transalkylation of diethylbenzene which takes place in the fourth reactor:



3.3 Catalyst study

The catalyst used is β -zeolite which is a crystalline aluminosilicate whose intersecting channels are composed of 12-membered rings. A study on the catalyst's external and internal heat and mass transfers was conducted to determine if there are any diffusional limitations as it hinders the average apparent reaction rate. The approach taken to establish this catalyst study is based on the one seen in Prof. N. Job's course, Heterogeneous catalysis. [13]

First, thermal diffusion problems were evaluated in the worst-case scenario. If the catalyst is proven to be isothermal in this case then it will necessarily be the case for any other condition. Therefore, an analysis was led for a temperature of 700°C.

To do so, the external temperature gradient was studied while calculating the difference between the surface temperature of the catalyst (T_s) and the temperature of the free flow (T_e) through the external thermicity (α_e) obtained while performing a heat balance on the pellet's surface.

$$\alpha_e = \frac{k_d C_e (-\Delta H)}{h T_e} = \frac{(T_s - T_e)_{max}}{T_e} \quad (6)$$

with k_d the mass transfer coefficient [m/s], C_e the concentration of reactant in the free flow [mol/m³], h the heat transfer coefficient [W/m²K] and ΔH the enthalpy of reaction [J/mol].

Then, the internal gradient was evaluated through the Weisz criterion (first part of the equation) which determines the difference between the temperature at the center and the surface of the pellet while assuming that the concentration at the center is equal to zero. The Prater number, β_s can also be found through the second part of the formula.

$$\beta_s = \frac{(T_{c,max} - T_s)_{max}}{T_s} = \frac{(-\Delta H) C_s D_e}{\lambda_e T_s} \quad (7)$$

with D_e the effective diffusivity [m²/s], λ_e the thermal conductivity [$\frac{W}{m \cdot K}$] and C_s the concentration at the surface

$[mol/m^3]$. As the worst case is evaluated, it is assumed that $C_s = C_e$ which is equivalent to the concentration of ethylene as it is the limiting reactant.

Knowing that, $C_e = 2.11 \cdot 10^{-5} mol/m^3$ and $\Delta H = -101.64$ kJ/mol, important results obtained to evaluate if there are any thermal diffusional problems are summarized in Table 2.

Table 2. Summary for the thermal diffusion

$k_d [m/s]$	$h [\frac{W}{m^2 \cdot K}]$	$T_s - T_e$	$\beta_s [l]$	$T_{c,max} - T_s$
2.64 e-2	752	7.52 e-5	5.46 e-11	5.31 e-8

It can therefore be concluded that the catalyst is isothermal as there is no temperature gradient inside the catalyst nor at the surface.

Afterward, mass diffusion problems were evaluated at the second reactor's actual operating conditions as it is characterized by the largest temperature range. Thus, a study on the internal mass gradient was conducted while evaluating the effectiveness ratio, η_s using the Thiele modulus, ϕ_s .

$$\eta_s = \frac{\tanh(\phi_s)}{\phi_s} \quad \phi_s = \left(\frac{r_s L_p^2}{C_s D_e} \right)^{1/2}$$

where L_p is the characteristic length [m], r_s the specific reaction rate $[mol/m^3 \cdot s]$, C_s the concentration at the surface $[mol/m^3]$ and D_e the effective diffusivity $[m^2/s]$.

As η_s is very close to 1 for both temperatures ($\eta_s = 0.99$), there are no internal mass diffusional limitations. Furthermore, it also means that there are no external mass diffusional limitations. As the medium is porous, the external diffusion coefficient is greater than the internal diffusion coefficient. Thus, if there are no internal diffusion problems, there will be no external diffusion problems. It can be concluded that the catalyst operates in a chemical regime which means that there are no mass diffusion problems.

3.4 Heat exchanger design

In the assessment, it is asked to design one of process's heat exchanger to be familiar with the design method. A shell and tubes heat exchanger is designed (Figure 4).

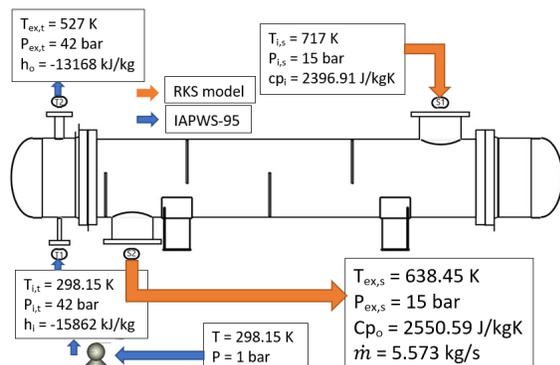


Figure 4. Heat exchanger specifications

The heat exchanger placed between the first and second reactor was chosen. This unit's goal is to cool down the stream entering the second reactor to avoid catalyst inefficiency as the reactors are adiabatic. The mixture to be cooled down passes through the shell while the water to be heated passes inside the tubes. This water is then converted into high-pressure steam. All inlet and outlet conditions were known except the mass flow rate of water which was found through simple mass balance. A cross-current model was chosen.

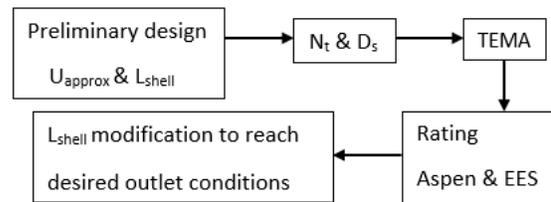


Figure 5. Methodology

Figure 5 shows the methodology applied to design a heat exchanger and refers to [14]. L_{shell} corresponds to the length of the shell, N_t to the number of tubes, and D_s to the diameter of the shell. First, the preliminary design through simple mass balance allows finding the number of tubes and the diameter of the shell.

It is necessary to determine an approximate heat transfer coefficient, U , and to select a length of the shell that gives a number of tubes close to a possible choice from the TEMA tables (available in chapter 9 of [14]). These tables correspond to actual manufacturable heat exchangers and provide a number of tubes equal to 56 and a shell diameter of 0.336 m (Figure 6).

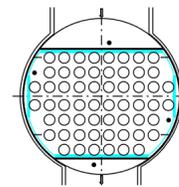


Figure 6. Cross sectional view

Then, the rating was established in both EES (manual correlations implementation) and Aspen softwares to validate the preliminary design while making sure that the outlet conditions correspond to those desired. As these softwares take into account the pressure drop and calculate a real heat transfer coefficient, the outlet conditions did not exactly coincide with the desired ones. Therefore, the length of the exchanger was adapted until the desired conditions were reached. The final results are summarized in Table 3.

Table 3. Final results of the design

L_s [m]	U $[W/m^2K]$	A $[m^2]$	D_t [m]	ΔP_s [Pa]	ΔP_t [Pa]
1.5	581	9.6	0.025	22276	19943

L_s corresponds to the length of the shell, A to the heat exchange area, D_t to the diameter of the tubes, ΔP_s to the

pressure drop in the shell, and ΔP_t to the pressure drop in the tubes. The smallest D_t was chosen in order to minimize the size of the heat exchanger and thus the cost. However, it leads to a higher pressure drop which is still acceptable.

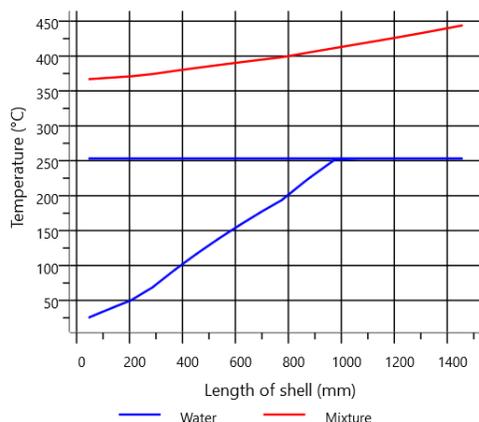


Figure 7. Streams temperature evolution along the heat exchanger

Figure 7 represents the temperature evolution along with the shell. The mixture (red) is cooled down and flows from right to left while water (blue) is heated and enters and leaves the heat exchanger on the left side as a two passes tube was chosen. The phase change of water is visible through the plateau.

3.5 Reactors

Preliminary design

The design of the four reactors is established in this section. The first three alkylation reactors in series are used to produce the main product: ethylbenzene from benzene and ethylene. Nevertheless, two side reactions have to be accounted for as ethylene can react with the product and with the impurity coming from the benzene component which is toluene. Relatively high benzene to ethylene ratio (around 8) is kept to avoid the formation of other side reactions. The reactors are placed in series to supply a new quantity of ethylene feedstock to each reactor. This also allows to minimize other side reactions (Reactions 3 and 4).

The reaction of ethylene with the main product (ethylbenzene) produces diethylbenzene. Therefore, a fourth transalkylation reactor is designed to recover EB through the reaction occurring between DEB and B. This has been established to improve the yield of the process.

The reactors were first implemented using Matlab software and then the model was validated through Aspen software.

Two different types of reactors were implemented: isotherm and adiabatic reactors. Adiabatic reactors were chosen for cost reasons. Indeed, isotherm reactors needed continuous cooling to keep the temperature constant as the reactions are exothermic. It is difficult to recover the heat through this continuous cooling and operation units thus have an important cost. Therefore, adiabatic reactors which allow an increase in the mixture temperature, are more appropriate even if it requires cooling down the mixture before it enters the following reactor. Moreover, a temperature increase in the mixture is beneficial for the size of the reactors. It leads to an increase in the reaction rates. This corresponds to the Arrhenius law which states that the faster the reaction rates are, the faster the desired conversion is achieved and the less volume is required.

For the first three adiabatic reactors in series, heat exchangers are placed between them to cool down the mixture before entering the following reactor. The temperature cannot exceed 450 °C otherwise the catalyst becomes inefficient.

By applying mass balance equations, knowing the kinetics of the reactions, neglecting the pressure drop in the reactors, and considering the evolution of the temperature in the adiabatic reactor, a model of reactors was conducted through the resolution of a system of differential equations. This system was implemented in Matlab and solved while using the function 'ODE45'. The choice of neglecting the pressure drop was proved to be correct by applying the Ergün equation to the system of differential equations and by showing that the pressure drop is smaller than 0.1% along with the reactors. This result was expected as the reactors operate at high pressure.

For the first three reactors in series, different conditions were set and specified. These conditions were then updated in the optimization. First, a ratio between ethylene and benzene feedstock was chosen to be equal to 8. Second, as the ethylene in each reactor has to be converted to 98%, an adapted volume for each reactor had to be found to reach this con-

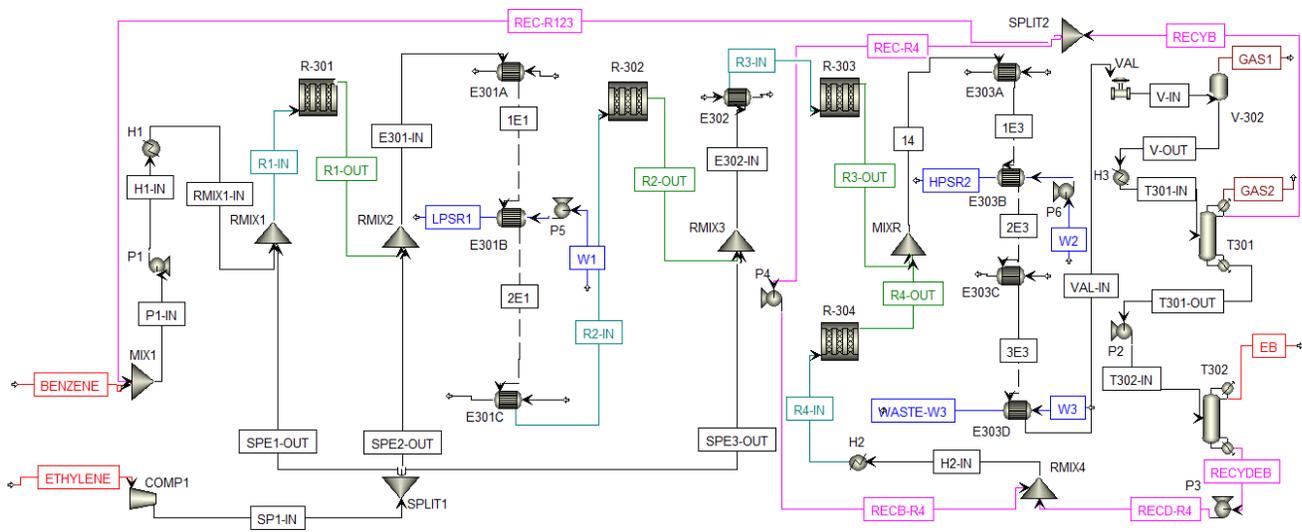


Figure 8. Process flowsheet

version. Third, the initial feedstock of ethylene and benzene was chosen considering that about 80 000 thousand tons per year of ethylbenzene has to be produced while taking into account the production of the fourth reactor. Fourth, the initial ethylene feedstock was split with a ratio of 30% in the first and third reactors and 35% in the second one. Finally, the inlet conditions of the first three reactors were fixed at 380°C and 20 bar. It is important to mention that all these conditions will be optimized and are used to understand the behavior of reactors.

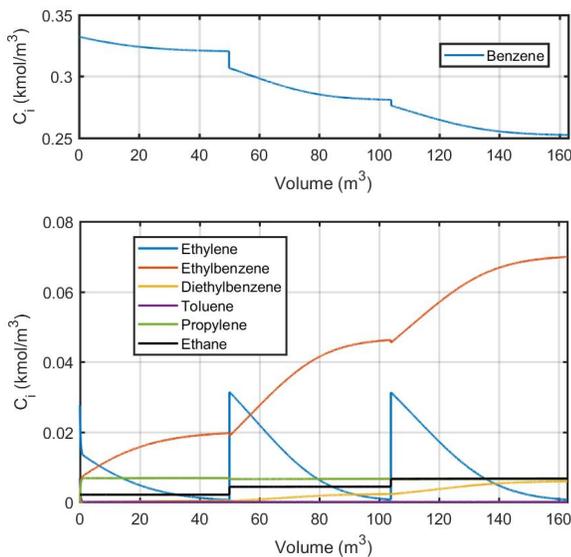


Figure 9. Concentration evolution as a function of reactor's volume in the first three reactors

The evolution of the components' concentrations as a function of the reactor's volume for the first three reactors in series is represented in Figure 9. It appears that ethylbenzene

is produced while ethylene and benzene are consumed. A quantity of ethylene that was added at each reactor's entrance, generates a jump in concentration due to the dilution and due to this additional quantity of volume. Toluene, propylene, and diethylbenzene are produced in a lower quantity by the two other side reactions. Furthermore, the small quantity of ethane present in the ethylene feedstock does not react.

Figure 10 (B) shows the evolution of the temperature in the reactors. It allows proving by analyzing Figure 9 that the higher the temperature, the faster the concentration of benzene will decrease.

These results were then compared to those found in Aspen to validate the model. The reactors were implemented in Aspen with the same conditions. In Figure 10 (B), it can be noticed that the temperature evolution in Aspen software corresponds to the one obtained while using Matlab. Moreover, Figure 11 shows the evolution of the ethylene molar fraction in the first reactor as a function of the reactor volume.

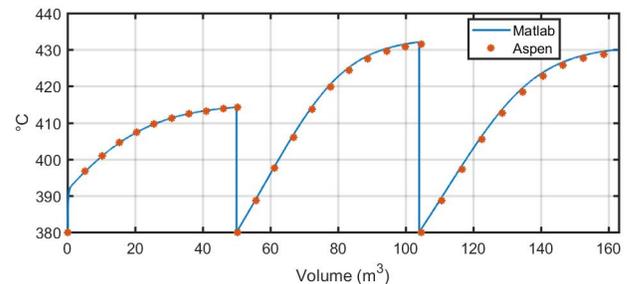


Figure 10. Matlab and Aspen of temperature evolution in the three reactors

As different values obtained coincide in both cases, the model is therefore validated. Furthermore, the reactor's volume needed to convert 98%, slightly differs (less than 1% of difference) from one case to another. The same conclusion

can also be made for the temperature profile evolution along with the reactors.

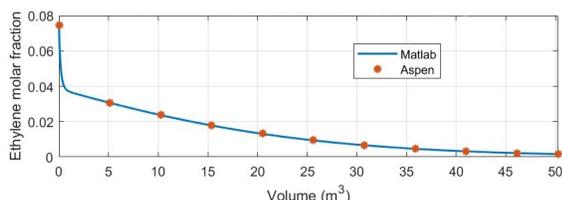


Figure 11. Comparison between Matlab and Aspen evolution of the ethylene molar fraction in the 1st reactor

In terms of the fourth adiabatic reactor, as previously mentioned, the model was first established in Matlab and then validated through Aspen implementation. The inlet of the reactor is composed of two streams: one coming from the second separation column where diethylbenzene and ethylbenzene are separated and the other coming from the recycled stream leaving the first separation column where most of the benzene is recycled. Benzene and diethylbenzene react to produce ethylbenzene and a conversion of 98 % was chosen as a first guess. The initial quantity of diethylbenzene was given by the second column and an amount of benzene was given through the recycling loop. The result of the evolution of the concentration is available in Figure 12 which displays the consumption of benzene and diethylbenzene to produce ethylbenzene.

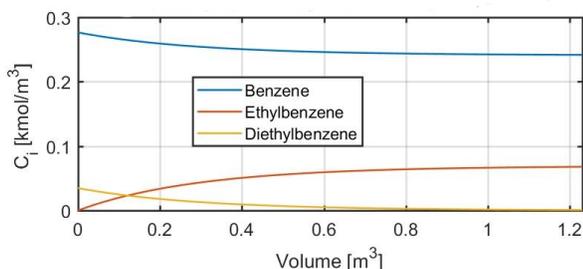


Figure 12. Concentration evolution as function of reactor's volume in the 4th reactor

These results were also confirmed by implementing this reactor in Aspen which provides exactly the same evolution.

Optimization

The optimization reactors methods were performed with the implementation of the whole process in Aspen Plus. Design specifications and sensitivity analyses were performed to find the optimal values for reactor pressure, conversion, size, and temperature.

First, a design specification was made to vary the temperature of the heat exchangers before the three adiabatic alkylation reactors to have a reactor outlet stream at a temperature between 440 and 445°C to increase the reaction rate and minimize the reactor volumes.

Then, a sensitivity analysis was performed by varying the conversion of ethylene to gauge the impact of ethylene conversion on the total cost. The two influences of conversion on cost are, first, the amount of ethylene required for the process

and second, the size of reactors. For the first one, the reason is that ethylene is a volatile component and leaves the process at the top of the flash tank making it unrecoverable. Hence, High conversion operation reduces the amount of ethylene required and therefore reduces the cost.

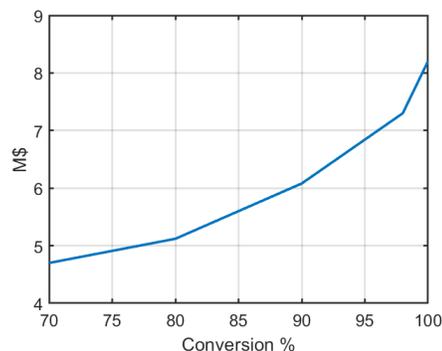


Figure 13. Capex cost of the reactors as a function of the conversion of ethylene

For the second one, the cost of the reactors increases as the conversion increases. As can be seen in the following two graphs (Figures 13 and 14), the cost of ethylene is highly dependent on conversion and should be minimized because it is a huge annual cost while the cost of the reactor is amortized over its lifetime and is correspondingly low. The conversion was set at 99.99%. The length-to-diameter ratio of the reactor was set to more than six to be in a plug flow regime.

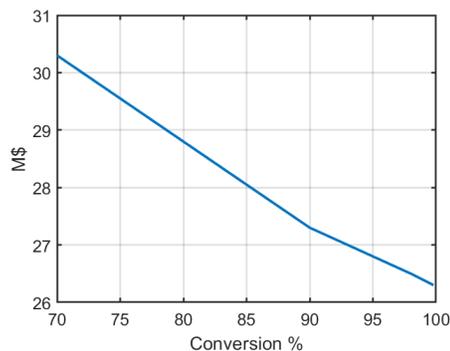


Figure 14. Annual cost of ethylene feed as a function of the conversion of ethylene

Afterward, a sensitivity analysis was performed to test the impact of reactor pressure on cost. The compression work and the reactor volumes are the two variables that are impacted by the pressure. Since compression is done in a liquid state, the cost is very low and varies in the order of hundreds of thousands of US dollars between 10 and 30 bar. As can be seen in the section on economic analysis, this cost is quite negligible. On the other hand, the cost of the reactor is the largest part of the capital cost, and increasing the pressure would lead to an overall decrease in cost. Therefore, the reactor pressure is set at a high level to reduce the size of reactors, up to 30 bar, which is the maximum pressure considered. Higher pressure was not considered for safety reasons.

In Table 4, the characteristics of the reactors are gathered.

Table 4. Summary reactors

	R-301	R-302	R-303	R-304
Length[m]	12	12	12	5
Diameter[m]	2	2	2	0.8
Volumes[m ³]	38	38	38	2.5
Pressure[Bar]	30	30	30	30
Outlet Temp[°C]	445	438	445	495

3.6 Separation

The separation part is composed of a flash tank and two distillation columns. These units are designed to separate the ethylbenzene from the other components and then recover it with a purity of 99.8%. The mixture first passes through the flash tank to remove some of the inerts. Then, it goes through column T301 (see Figure 8) where more than 99% of benzene and less than 1% of ethylbenzene pass to the top of the recycle stream while the rest goes to the bottom of the column. Furthermore, the first column consists of a partial condenser used to remove additional inerts from the process. Finally, the mixture passes through column T302 where more than 99% of ethylbenzene goes to the top of the column as a process' product containing less than 2ppm of diethylbenzene.

To design the separation units, the flash tank was first set to operate at 1.1 bar and 45°C. It must be operated at a low temperature to avoid losing too much benzene in the fuel gas, as can be seen in Figure 15. The temperature is set at 45°C and not lower because the water is fed at 25°C and the average temperature difference for the heat exchangers is 20°C. Using a refrigerant fluid instead of water lowers the temperature and minimizes benzene losses. However, it increases the total cost of the process as refrigerants are quite expensive and are therefore not used.

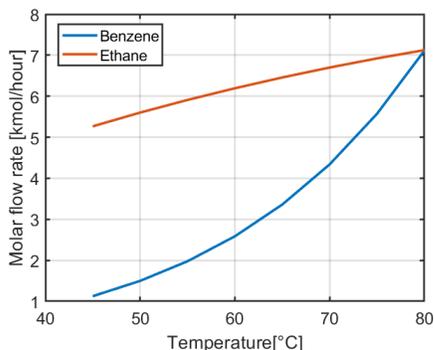


Figure 15. Evolution of the molar flow rate that goes in the flue gas at 1.1 bar as a function of the temperature of the flash

Working at low pressure increases the amount of inerts removed, which is desired, but increases benzene losses as represented in Figure 16. Due to the curves' profile, it was decided to make two removal of ethane at 1.1 bar in the process to minimize the benzene losses while maximizing the removal of inerts. The first one was made in the flash tank where about 60% of ethane is removed and the second one in column T301 where 70% of the remaining ethane leaves the process in the

GAS stream. There is a compromise between removing ethane as much as possible and losing as little benzene as possible. The choice made seems to be close to the optimum in terms of cost as only 1.5% of benzene losses occur overall to remove 90% of the ethane.

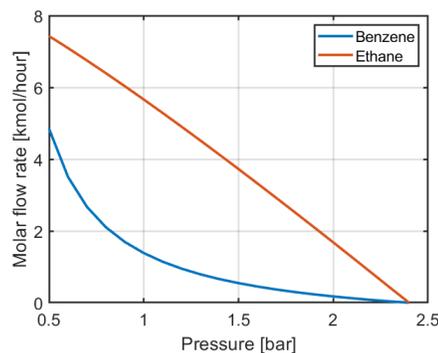


Figure 16. Evolution of the molar flow rate in the flue gas as a function of the pressure in the flash tank at a temperature of 45°C

In terms of columns, the first question was whether they were sieve tray columns or packed bed columns. Thus, the calculation methods developed in the Turton book [15] were applied and the results obtained are shown in the following Figure 17. The cost of the columns is impacted by the ratio of length-to-diameter which increases the total cost. This effect on the cost is represented when the ratio is higher than 20 and when the ratio is higher than 25, that is why two jumps are seen in the graph when the number of stages increases. Indeed, in reality, this ratio has an impact on the cost in a continuous way and not by jumps as seen in this case. The same behavior of the curves is observed for column T302. Therefore, packed columns are chosen because they are smaller than sieve tray columns meaning that the ratio length-to-diameter is less important which tends to decrease the cost. However, this conclusion is not represented in Figure 17 when the number of stages is high because it was considered that the investment cost is affected by a maximum coefficient that occurs with the length-to-diameter ratio greater than 25. With a more appropriate dependence of this ratio on cost, the orange line would always be higher than the blue one in Figure 17 because the columns of sieve trays are larger. Moreover, the cost of packaging is not so expensive compared to the cost of sieve trays when the calculation methods developed in Turton book are applied.

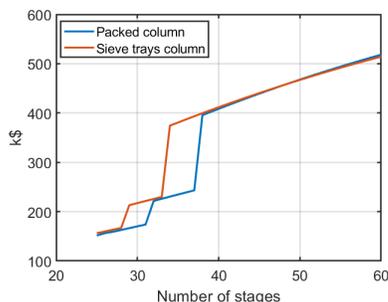


Figure 17. Capex cost of column T-301 as a function of the number of stages

Afterward, the columns were designed in Aspen using the radfrac model. The column outlets were set with the values previously mentioned and the columns were designed in terms of reboiler duty and number of stages to meet these specifications. Indeed, the radfrac columns model only requires two variables input when their inlet and outlets are known which makes it easily applicable when data are lacking. The main objectives are to design the columns to reduce their capital cost and to reduce the reboiler duty requirement. Reducing the reboiler duty is primordial as the process has a limited amount of energy to share with the columns. Concerning the heat transfer, the cold stream from the condenser in column T302 partially provides the heat required by the reboiler in column T301. The remaining heat required is provided by low-pressure steam. The energy supplied by these streams must be greater than the energy required in the reboiler (T301). On the other hand, the amount of heat required by the reboiler in T302 is supplied by high-pressure steam. The simplistic way that is used to design the columns is as follows, as the cost of the columns is less than 1% of the total cost, the goal is just to minimize the reboiler duty by increasing the number of stages until the reboiler duty reaches a certain plateau. Indeed, at this plateau, increasing the number of stages becomes quite useless since it does not reduce the required duty significantly. This happens at 30 stages for column T301 because from 30 stages to 60 stages, the reboiler duty decreases only by 5% as can be seen in Figure 18. The same idea is followed for column T302, for which the number of stages is 46.

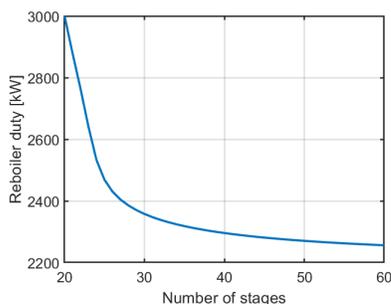


Figure 18. Reboiler duty as a function of the number of stages for the first column

Then, the pressure of the columns was defined. The element which influences the choice of the pressure is that the

temperature increases with the pressure. Column T301 is more optimal at low pressure because the temperature of its reboiler is lower at low pressure, it increases the amount of heat that can be brought to its reboiler. Moreover, a dense fluid requires more energy to evaporate which leads to an increase in the reboiler duty which is to be avoided. Concerning column T302, it is the opposite. It is more optimal at high pressure because the temperature of its condenser increases with the pressure, it increases the amount of heat that it can transfer to the reboiler in column T301. In all cases, concerning the columns it is the heat transfer that must be optimized as the capital cost of the columns is low. Maximizing the amount of excess energy produced by the process by reducing the reboiler duty of the columns. Table 5 summarizes the values of the different variables regarding the columns.

Table 5. Summary for the columns

	T301	T302
Column type	Packed	Packed
reflux ratio	0.404	0.885
reboiler duty [kW]	2200	1970
condenseur duty [kW]	2027	1632
column height[m]	21	32
diameter[m]	1.15	1.1
Pressure [bar]	1.1	3

3.7 Heat integration

The heat integration aims at minimizing energy consumption while maintaining the same product specifications. It consists of a pinch analysis that determines the amount of hot and cold utilities required and a heat exchanger network that minimizes the amount of utilities consumed and the number of heat exchangers required. Heat transfer between hot and cold streams is performed to meet the target temperatures while making sure that the golden rules are not violated [16]. These rules are: only hot utilities can be used above the pinch, only cold utilities can be used below the pinch and no heat can be transferred across the pinch. A hot stream is characterized by a target temperature lower than the supply temperature. Whereas, a cold stream has a higher target temperature and thus needs to be heated up. Therefore, one must know how to combine these different streams to maximize heat recovery.

A pinch analysis is first performed to identify the pinch temperature and is represented by a Grand Composite Curve (GCC) as illustrated in Figure 19. This pinch temperature separates the process into two regions: the heat sink region above the pinch where only hot utilities can be supplied as no cooling is required and the heat source region below the pinch where only cold utilities are supplied as no heating is required.

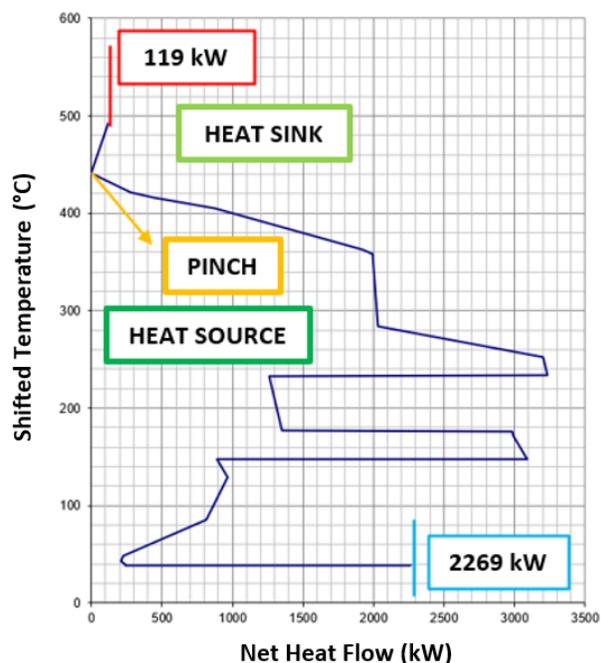


Figure 19. Grand Composite Curve

Following this analysis, it appears that the pinch temperature is obtained at 441.53°C. It also shows that there is a need to provide 119.73 kW of hot utilities and 2269 kW of cold utilities after heat integration. This process requires thus external heat and external cooling. To minimize energy requirements, a heat exchanger network has been designed to carry out heat transfer between different streams while combining them. The final process is illustrated in Figure 8.

To exchange as much heat as possible within the process, heater H1 can be replaced by heat exchangers E303C, E303A, and E301A whereas heater H3 can be replaced by the heat exchanger E301C. In terms of the heater H2, it can be partially replaced by the heat exchanger E302. However, the amount of heat provided could not bring the stream to the pinch temperature as E302 has a lower temperature, 422°C. Therefore about 20 kW of hot utilities are still required. This explains why the total amount of hot utilities required is equal to about 140 kW and not 119.73 kW.

There are also two other important heat transfers. First, the reboiler in the first column (T301) is heated by the condenser in the second column (T302) and the remaining heat required is supplied by the high-pressure steam (HPSR2) produced by the heat exchanger E303B. In terms of the reboiler in T302, it cannot be heated by the condenser in T301 as its temperature is too low. Thus, low-pressure steam (LPSR1) and high-pressure steam (HPSR2) are used to heat it.

After conducting this network, it can be concluded that the process requires about 140 kW of hot utilities and about 2080 kW of cold utilities. Indeed, around 55kW of cooling water is required for E303D as the temperature is too low to be recovered and the remaining cold utilities correspond to the amount required by the condenser in T301. Furthermore, more or less

190 kW of high-pressure steam produced at 244°C can be sold or used in the styrene process which is generally built in parallel to the ethylbenzene process. This value comes from the 2269 kW found through the pinch analysis (2269 kW = 2080 kW of cold utilities + 189 kW of HPS). A summary highlighting improvements achieved through the heat integration is available in Table 6. While analyzing this table, it can be noticed that about 85% of energy could be saved through this heat integration.

Table 6. Comparison of results obtained before and after heat integration

[kW]	Before	After
H1	4955	0
H2	760	139
H3	468	0
E303D	-55	-55
R T301	2200	0
C T301	-2025	-2025
R T302	1970	0
C T302	-1629	0

4. Life cycle assessment

Nowadays, the environmental impact of a plant is an essential parameter. This is why a tool such as the life cycle assessment (LCA) of a substance is crucial. A LCA is a technique used to evaluate the environmental aspects associated with a product during its life cycle. It is therefore a cradle-to-grave approach to a product by meticulously examining each stage of its production process. The most important application of LCA is to analyze the contribution of life cycle stages to the overall environmental load, usually to prioritize product or process improvements. To do so, a LCA consists of four steps which will be detailed throughout this section: defining the purpose and scope, life cycle inventory analysis (LCI), life cycle impact assessment (LCIA), and results interpretation. [17]

4.1 Implementation of the project

For the production of ethylbenzene, it is important to know which raw materials are needed and how they are produced. The two products concerned are ethylene and benzene. Ethylene is produced by dehydrogenation of ethane from natural gas in the USA and the Middle East, from coal in China, and naphtha in Europe. Benzene is obtained by extractive distillation of the C6 fraction (whose olefins have been selectively hydrogenated beforehand). [18]

Ethylene is the most consumed intermediate product in the world and is produced by steam cracking of fractionated naphtha in Europe. During the production of ethylbenzene, the plant simultaneously produces a fuel gas that may be useful for energy integration. In addition, natural gas will be used as an energy source for the heat supply. To cool the different

streams, the main option is water used as a heat transfer fluid. However, in certain situations, cooler ethylene or benzene streams are heated in heat exchangers instead of water, which will reduce energy and water consumption.

The first discussion focuses on these feedstocks and their environmental impacts through a powerful program used for LCA: **Simapro**. To obtain results with Simapro, several data had to be provided: the definition of the raw materials and their transport, the electrical consumption of the pumps and compressors, and the energy demand of the heat exchangers. The plant itself does not produce CO_2 emissions as no reaction produces CO_2 as would a combustion process. Nevertheless, there are indirect emissions from the transportation of raw materials, their production, and the generation of electricity, as well as from the various units.

The model applied by the program is the CML-IA. This is an environmental assessment methodology that contains characterization factors for life cycle impact assessment. For all numerical values, the program will use the Ecoinvent database. This method includes different impact categories. [19]

4.2 Impact of demands on the plant

Figure 20 shows the environmental impact of producing 1 kg of ethylbenzene.

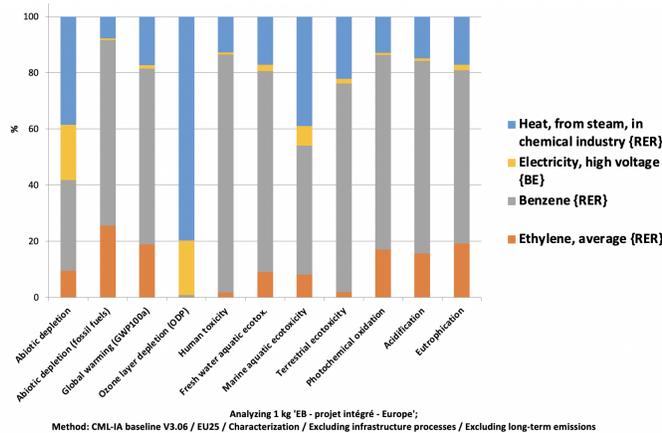


Figure 20. Impact of demands on the plant

The first two columns concern abiotic depletion. The first column represents mineral extraction and the second represents fossil fuel extraction. These factors are determined for each extraction based on global reserves and their unit is kilograms of antimony equivalents per kilogram of extraction for fossil fuels and megajoules for minerals.

As far as the consequences on living organisms are concerned, benzene has a greater impact than ethylene because, for example, the demand for benzene by the plant is almost three times higher than its demand for ethylene. In terms of energy, it is the demand for heat that has a greater impact than the electricity demand. In terms of the impact on human toxicity, freshwater aquatic ecotoxicity, and terrestrial ecotoxicity, benzene is responsible for about 70 to 80%.

As for global warming, it is the emission of greenhouse gases

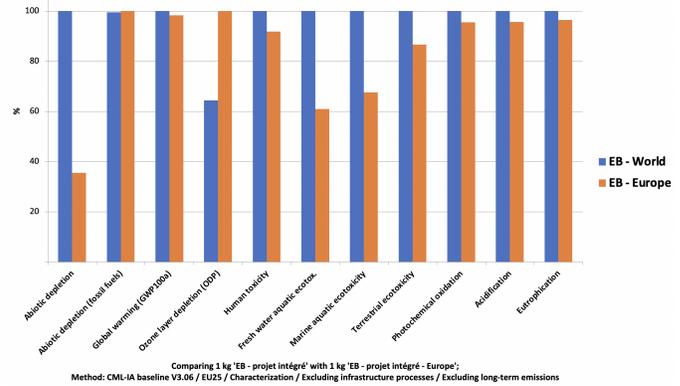


Figure 21. Comparison of the integrated project model from a European and World perspective

in the area that is taken into account. To determine this, the impact of the plant's emissions is considered. The factors are expressed in terms of global warming potential over a 100-year horizon (GWP100), expressed in kilograms of carbon dioxide per kilogram of emission. In addition, ozone depletion is expressed in kilograms of trichlorofluoromethane equivalent (CFC-11) per kilogram of emission.

For the last impact categories concerning the different toxicities, the units are expressed in equivalents of 1,4-dichlorobenzene per kilogram of emission and the impacts are more or less identical to human toxicity, freshwater aquatic ecotoxicity, marine aquatic ecotoxicity, and terrestrial ecotoxicity.

For photo-oxidant formation, its unit is ethylene equivalent per kilogram of emission. For acidification, it is sulfur dioxide equivalents per kilogram of emission. Finally, for eutrophication, it is phosphate equivalents per kilogram of emission.

4.3 Choice of location

Once the discussion of the environmental impacts of the plant is completed, the choice of plant location is feasible. The first criterion for choice is how the necessary feedstock is produced. As previously explained, there are two ways to do this, but the steam cracking technique has been preferred over the use of coal. As a result, the decision to avoid countries, such as China, using this manufacturing process is logical. The second criterion is that the ethylbenzene market in Europe has been growing for the last five years. [20] In addition, the following histogram 21 affirms that the plant would have a lower environmental impact on average in Europe.

At first glance, the key information in this graph is that the comparison of a robust indicator such as global warming confirms the viability of the plant project given the small gap.

The final choice was made in Belgium, more precisely in Antwerp. This is a good choice because Ineos could provide the raw material. [21]

This is a right choice because the demand for energy and raw material could be directly met by the Antwerp chemical site. Belgium is one of the world's largest exporters of ethylbenzene, exporting almost 90% to its neighboring countries. If

demand should arise, this country could exploit the remaining quantity.

5. Economic analysis

This section investigates the economical feasibility of the process described in this article. The capital expenditures (hereafter CAPEX) also called fixed capital investment and operational expenditures (hereafter OPEX) were computed. In addition, a cash flow analysis was performed. The methodology developed in the Turton book [15] was used as well as lectures given by Prof. G. Léonard from the University of Liège [22].

5.1 CAPEX

The estimation of the CAPEX can be decomposed into three main steps. First, the price of each piece of equipment is calculated at ambient pressure and using carbon steel as material. Equation 8 is used where K_1, K_2 and K_3 are empirical constants available in the reference book [15]. A is a sizing factor characteristic of the equipment, for instance, the surface area of a heat exchanger or the volume of a reactor.

$$\log_{10}(C^0) = K_1 + K_2 \log_{10}(A) + K_3 \log_{10}(A)^2 \quad (8)$$

The next step accounts for the real operating conditions of the equipment using two factors. The first one F_p takes into account the pressure increase. This pressure factor is especially relevant for the reactors where the pressure is 30 bar. In addition, a material factor F_m allows using different materials than carbon steel. The last parameter to consider is inflation. It is estimated using the CEPCI, Chemical Engineering Plant Cost Index. The final equation used to compute the price of a module is equation 9 where B_1 and B_2 are constants available in the reference book. The CEPCI was equal to 394.3 in 2001 and 774.5 in November 2021. The prices given in the reference book date back to 2001.

$$C_{module} = C^0 \cdot (B_1 + B_2 \cdot F_m \cdot F_p) \cdot \frac{CEPCI \text{ NOW}}{CEPCI \text{ 2001}} \quad (9)$$

The final step is to account for additional costs such as installation and transport of the pieces of equipment. The last cost computed is called "Grass root" and abbreviated C_{GR} . It is calculated while using equation 10 where $C_{module,i}$ is computed through equation 9 and C_i^0 can be found through equation 8.

$$C_{GR} = 1.18 \cdot \sum_{i=1}^n C_{module,i} + 0.5 \cdot \sum_{i=1}^n C_i^0 \quad (10)$$

The total CAPEX is finally estimated at 21,592,560\$. The following pie chart 5.1 represents the main contributions to the CAPEX.

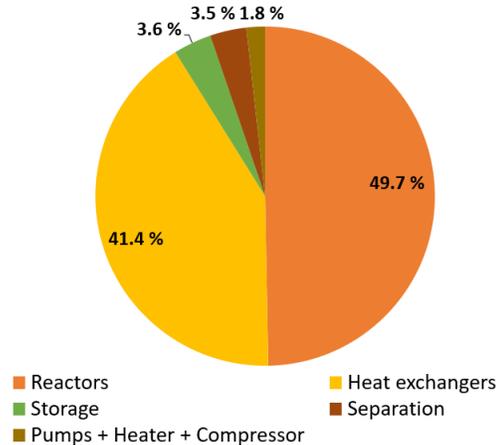


Figure 22. Percentage distribution of CAPEX

A detailed cost estimation is available in the Table 7.

Table 7. Detailed contributions to the CAPEX

Equipment	cost [k\$]	Equipment	cost [k\$]
R-301	2,757.6	P3	26.8
R-302	2,757.6	P4	29.6
R-303	2,757.6	P5	19.6
R-304	587.5	P6	40.5
T-301	197.1	E301A	567.4
T-302	308.4	E301B	578.2
V-301	113.4	E301C	583.1
COMP1	96.8	E302	609.9
STOR1	462.3	E303A	250.6
STOR2	184.6	E303B	279.8
H-301	16.2	E303C	4,340.7
P1	66	E303D	172.2
P2	20.4		

5.2 OPEX

All costs presented in this section are annualized. The total cost of manufacturing can be approximated with equation 11 where the constants are deduced from Prof. G. Léonard's lectures [22]. The different contributions are the cost of the raw materials C_{RM} , the waste treatment cost C_{WT} , the cost of utilities C_{UT} , the depreciation d_k , the cost of labor C_{OL} and general expenses labeled C_{GE} . Each term will be discussed in the section.

$$COM = \frac{(C_{RM} + C_{WT} + C_{UT} + d_k)}{0.810} + \frac{C_{OL}}{0.366} + \frac{C_{GE}}{5.548} \quad (11)$$

The cost of raw materials includes benzene and ethylene. The price of raw materials has enormously increased in the past months mainly due to geopolitical tensions. The prices upon which the cost was evaluated are 1.35\$/kg for ethylene [23] and 1.15\$/kg for benzene [24]. In addition, the price of the zeolite catalyst used was included as well. It was assumed that the catalyst has to be changed once in two years. The price

of the catalyst is 2.25\$/kg. The amount of catalyst needed in the reactors is 54.5 tons.

The waste treatment cost was arbitrarily approximated at 50,000\$ per year. The water used in the process is not contaminated as it is used in separated circuits. No real wastes are generated during the process as the fuel gas is burnt on-site to produce heat.

The labor cost was estimated based on the number of operators required to run the plant. It was assumed that one operator works 49 weeks per year and 5 shifts each week. This means that one single operator will do 245 shifts per year. For each working position, 3 shifts are needed per day leading to 1095 shifts per year. Consequently, 4.5 operators (1095/245) are needed per working position. The remaining question is the number of working positions within the plant. It is based on equation 12 where N_{WP} represents the number of working positions and N_{np} the number of non-particulate processing steps. As the plant does not contain any solid, no particulate processing step is needed, thus $P=0$. A total of 17 operators are needed.

$$N_{WP} = (6.29 + 31.7 \cdot P^2 + 0.23 \cdot N_{np})^{0.5} \quad (12)$$

The average salary in the chemical industry is one of the highest in Belgium among all the sectors. It was decided to take an average salary of 65,000 \$/year for the purpose of this exercise [25][26].

The cost of utilities can be broken down into different contributions. The plant needs 90.2 kW of electricity costing approximately 0.363 \$/kWh [27], 2082 kW of cooling water costing approximately 0.7 \$/GJ [15] (taking the inflation into consideration) and 140 kW of natural gas at 110 \$/MWh [27]. It is clear from the source that natural gas and electricity prices have skyrocketed in the last few months. All the contributions correspond to a total cost of 414,000 \$/year. Nevertheless, 192 kW of high-pressure steam is produced and sold for 170,000 \$/year. It was estimated that the price is 30\$/GJ using the Turton book with the CEPCI correction. Moreover, the fuel gas produced is burnt as well and represents roughly 80 kW of natural gas saved. This reduces a lot the cost of utilities.

The depreciation corresponds to the value of the pieces of equipment lost each year. The depreciation time is 6 years. A linear depreciation was considered to lead to the annual depreciation is equal to the fixed capital investment divided by 6.

The general expenses include all the remaining costs that have not yet been integrated. This includes, among other things, the administration, distribution, research, and patent costs. It can be approximated to a fraction of the fixed capital investment [22].

Table 8 represents the different contributions of equation 11 without taking the constant into consideration.

Table 8. Detailed contributions to the OPEX

OPEX	cost [k\$]	OPEX	cost [k\$]
C_RM	129,725	C_OL	3,196.7
C_WT	61.7	C_GE	3,891.9
C_UT	300.4		
d.k	4,442.9	COM	140,246.7

The total annual cost of manufacturing, taking into account the coefficient in equation 11 was estimated at 140,246.7 k\$. The following pie chart represents the different contributions. The main important contribution is the raw materials contribution which accounts for more than 90% of the entire cost of manufacturing.

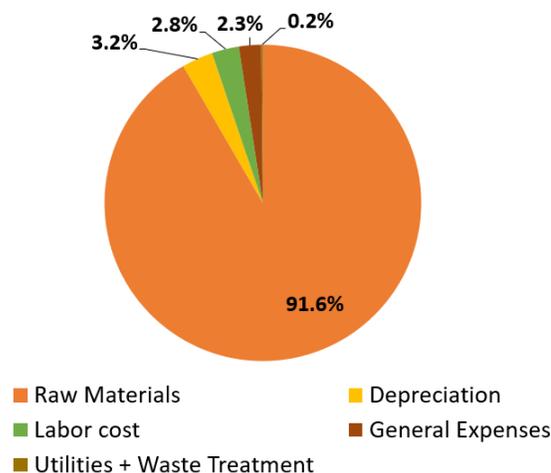


Figure 23. Percentage distribution of OPEX

5.3 Dependency on raw materials prices

The price of the raw materials is quite volatile [24][23]. The profitability of the plant depends severely on those prices as was stressed in Figure 23. To identify when the plant would be profitable or not, a graph was drawn 24. It shows the evolution of the ethylbenzene price concerning the benzene price. Moreover, four different lines were drawn representing each a different ethylene price. The plant designed in this article makes a profit as soon as the selling price of ethylbenzene is above the line for a given price of ethylene, benzene, and ethylbenzene. No relevant prices were found online for the ethylbenzene. Nevertheless, as stated in the introduction, the majority of ethylbenzene is used to produce styrene. On the 6th May 2022 in Rotterdam [28], the price of styrene was around 2.017 \$/kg. The situation chosen to make the analysis is a selling price of ethylbenzene of 1.75 \$/kg as styrene could be obtained with a yield of 91 % using a new catalyst [29]. The chosen situation is represented by a green circle in Figure 24.

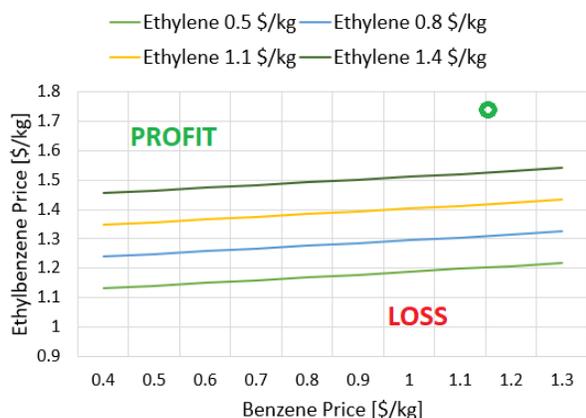


Figure 24. Break-even curves

5.4 Cash flow analysis

The cash flow analysis aims at assessing whether a project can be profitable or not for given conditions by looking at the cash flow generated from operations. The discounted cash flow diagram is shown in Figure 25. Some hypotheses were made to perform the analysis. It was assumed that building the plant would take 3 years and that the plant would produce for 20 years after start-up. For this study, the prices of the raw materials are kept constant: benzene at 1.15 \$/kg, ethylene at 1.35\$/kg, and ethylbenzene at 1.75 \$/kg. This leads to yearly revenue of 143,500,000 \$ for a production of 82,000 tons a year of ethylbenzene. The profit generated by the plant can be computed using equation 13 where R the revenue, COM_{d_k} the yearly total manufacturing cost without the depreciation, d_k the depreciation, and t the tax rate of 25% in Belgium [30].

$$\text{Profit}_{\text{net}} = (R - COM_{d_k} - d_k) \cdot (1 - t) + d_k \quad (13)$$

Equation 14 can be used to compute the discounted cash flow, DCF . The discounted interest rate i' is computed based on the inflation f and the number of years k and the interest rate i set to 10% per year. The inflation value has been set to 3% [31]. This value was taken because it seems reasonable to think that the energy prices will not continue to increase for the 25 years of the analysis. Indeed, the inflation experienced in 2022 is much higher than the decades before as shown in the reference. This increase is due, to a large extent, to the increase in energy prices.

$$DCF = \frac{CF}{(1+i')^k} \quad \text{with} \quad i' = \frac{1+i}{1+f} - 1 \quad (14)$$

Figure 25 will now be discussed. At the end of year 1, a piece of land equivalent to 65,000 m^2 is bought for roughly 1,000,000 \$ [32]. During year 2, 60% of the fixed capital investment is spent. During year 3, the remaining 40% is used as well as the working capital. It has been estimated that the working capital needed to start the production is 2/12 of the total manufacturing cost which corresponds to two months of spending. Thus, the total amount of money needed before starting the production is known and is close to 33 M\$. At

the beginning of year 4, the plant starts its production, and ethylbenzene begins to be sold. The depreciation starts at year 3 and lasts for 6 years. The time needed to recover the discounted payback period is roughly five and a half years. It corresponds to the time required, after start-up, to recover the fixed capital investment without the land. At the end of the 20th year of production, the plant stops. The land and the working capital are recovered for roughly 24.4 M\$. The salvage value has been neglected. The net present value of the project is close to 41 M\$. Ceteris paribus, the project would have a net present value of zero if the price of ethylbenzene is at 1.667 \$/kg.

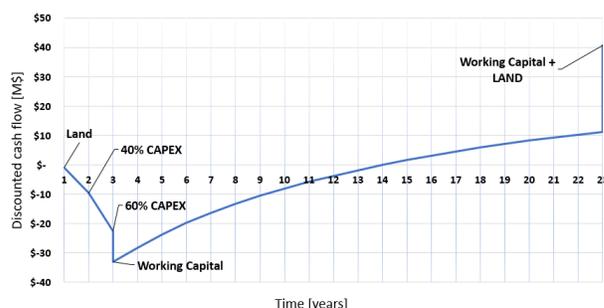


Figure 25. DCF analysis

The limit of this analysis has to be stressed. The raw materials prices do fluctuate through time and the dependency of the profitability on these prices has already been introduced.

5.5 Economic feasibility

As stated several times during the analysis, the profitability of the plant depends heavily on the feedstock as well as on ethylene prices. It can be noted the currency used throughout the analysis is the USD. This choice was made because all the relevant formulae were given in dollars. In addition, the fluctuation of the EUR/USD pair is avoided.

6. Literature review

Production of EB on an industrial scale is only done based on alkylation and transalkylation processes. More often, ethylene reacts with benzene as vapor in catalytic bed reactors producing ethylbenzene and diethylbenzene. Diethylbenzene can be converted into ethylbenzene in a transalkylation reactor leading to a very high overall selective process. The described process is the one used in this project even though others use different feedstocks or a different reaction phase. It is inconceivable to determine which approach is the best from an economic and environmental perspective because such a decision requires detailed sources to run a comparative analysis considering the contribution of time, geolocation, and the environment violation limits. However, in the following study, the accessible sources are exploited to compare this article's process to alternative and similar processes to identify whether it is promising and efficient.

6.1 Similar Process

It is relevant to compare the performance of the process described at the beginning of this article with similar processes to find possibilities for improvement or to validate the optimal operating conditions. The key parameters to consider when comparing two processes should be independent of time and geolocation to be adequate and relevant. As a result, Figure 26 represents a mass balance comparison that specifies the required reactants usage to produce a certain quantity of EB.

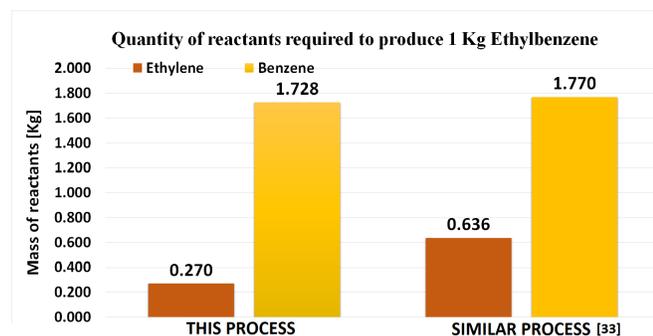


Figure 26. Reactant usage comparison with a similar vapor based process [33]

The comparison shows that for a similar purity of 99.9% EB, this process is more efficient. It uses 57.5% less ethylene and 2.3% less benzene to produce 1 kg of EB. The difference between the process of this project and the compared similar one is evinced by the flowsheet itself. The other process uses only one alkylation reactor and one transalkylation reactor with relatively broad assumptions such as that the only byproduct of the alkylation reaction is diethylbenzene. Also, it relies on a 100% pure feed of benzene and ethylene. The catalyst used for both processes is zeolite. However, the most important difference in the reaction phase is that a similar process reacts to a vapor phase ethylene with liquid phase benzene. Whereas, this process was based on a vapor phase reaction unit. [33]

6.2 Liquid phase Alkylation of ethylene and benzene

There are various liquid alkylation processes to produce ethylbenzene, one of the best processes is the alkylation using zeolite catalyst. In this section, a comparison was made to exploit the advantages and disadvantages of two liquid processes compared to the process of this project which is vapor-based.

Firstly, before getting in-depth it was relevant to run the same comparison made for a similar process and quantitatively investigate the efficiency of these processes in terms of reactant usage. The processes considered in the study are:

- J.MacDonald, R.Roda, M.Beresford (2005)[34] labeled "Liquid 1" in Figure 28
- Q.han S.Sharma, G.Pandu, (2017) labeled "Liquid 2" [35]

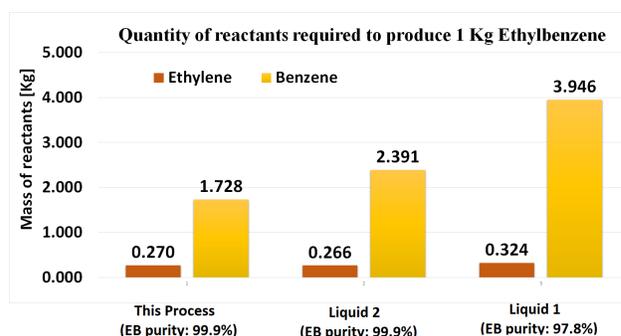


Figure 27. Reactant usage comparison between liquid based alternative processes and this process

The study shows that this process makes better usage of the reactants leading to the highest EB purity. The (L1) process uses more ethylene and benzene than the vapor and the (L2) processes. It also has the lowest EB purity. To have an idea about the differences between all of these processes, Table 9 provides a list of relevant differences.

Table 9. Important differences between Liquid 1 (L1), Liquid 2 (L2) and the this process (V)

	V	L1	L2
Reaction phase	V	L	L
Ethylene Purity %	93	1	99.9
Benzene Purity %	98	99	100
Reactors Number	4	9	7
EB purity %	99.93	97.8	99.97
Columns Number	2	2	2
Byproducts considered	DEB, Prop	DEB	DEB
Catalyst	Zeolite	Zeolite	Zeolite

Figure 28 compares the (L1) process energy requirements with the one of this process (V). The importance of the comparison was to determine which process requires more energy and most likely has a higher environmental impact. This process requires less energy to produce ethylbenzene. This conclusion proves that this process is promising compared to the available sources online, especially as it leads to higher purity, more efficient usage of its reactant, and a less energy requirement. It is relevant to mention that as shown in Table 9, this process uses almost the least pure feedstock and gives a high purity. Therefore it is expected to be even more dominant in terms of cost and benefits as the cost of such plants is strongly related to the feedstock and energy utility.

It would be more convenient to study and compare this process to better and more reliable sources that include all the aspects of such plants and provide the data required to make a more quantitative analysis of the performance.

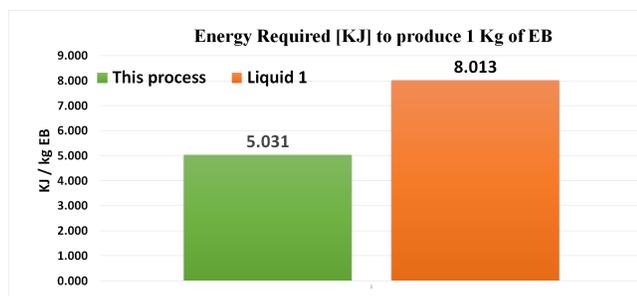


Figure 28. Comparison of energy requirements between (L1) and this process

6.3 Alkylation of benzene with ethanol

Ethylene is not the only high-value chemical used to produce ethylbenzene. The interest in finding alternatives to ethylene comes from the fact that some options can provide less environmental impact and better sustainability. In this section, ethanol was investigated as an adequate alternative that could be obtained by the fermentation of sugar deriving from biomasses. [36]

For the sake of proving that ethanol could be an industrial alternative instead to ethylene, it was necessary to check its conversion towards ethylbenzene. If and only if the conversion is similar or better, then it could be considered as a real substitute. Figure 30 and 29 present a comparison of ethanol and ethylene conversion towards ethylbenzene with added benzene. [37]

Ethanol shows better conversion towards ethylbenzene with relatively fewer side products, making it a better alternative. The study shows that at a high temperature of 400 degree Celsius ethanol leads to 17 wt% EB whereas, ethylene at the same temperature leads to 15 wt%. regardless of the conversion towards EB, ethanol show remarkable less weight percent byproducts formation for over all the temperatures and especially for propylbenzene. However, the question remains why is it not already used on an industrial scale as it is better from a performance, economic, and environmental perspective? The answer is due to the released water contributed from its usage that not only has negative effects on the catalyst performance but also its lifespan. The drawback just mentioned could not be compromised in any terms. It can result in a cost increase that could not be compensated by its conversion benefits. Interests toward substituting ethylene may continue even though optimizing the ethylene source can also be sufficient to enhance the process of ethylbenzene production.

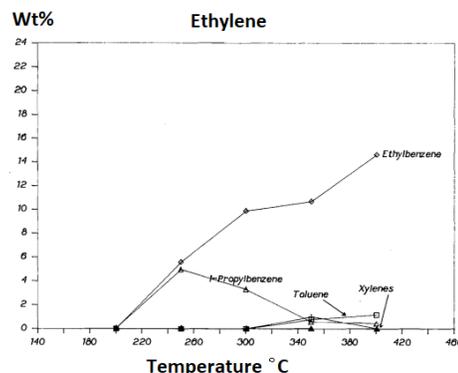


Figure 29. Ethylene conversion towards ethylbenzene [36]

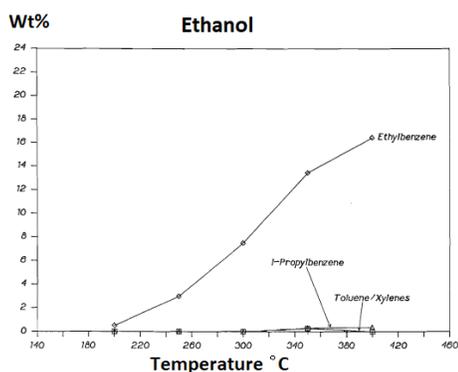


Figure 30. Ethanol conversion towards ethylbenzene [36]

6.4 Feedstock alternative

To compare feedstocks, it is interesting to do this under two axes of comparison: yield and environmental impact. This analysis focuses on coal, biomass, oil, and natural gas. The first quantitative comparison is on the percentage yield for the same ethylene production. All values are listed in the following Table 10. [38]

Feedstock	Yield [%]
Biomass	< 10
Natural gas	20
Cracking naphtha	30

Table 10. Yield of the different feedstock

These data are understandable, but before choosing the optimal raw material for the process, it is important to look at the environmental impact of these materials. For this purpose, a comparative bar chart 6.4 was made. It is a comparison between the different energy sources for the production of 1000 MJ of energy.

Figure 31 provides a good comparison from an environmental point of view.[39] All impact categories are presented with their respective units. It is important to find a good balance between the yield and the impact of a resource even if sometimes the yield will be considered as the main criterion for the choice of the feedstock.

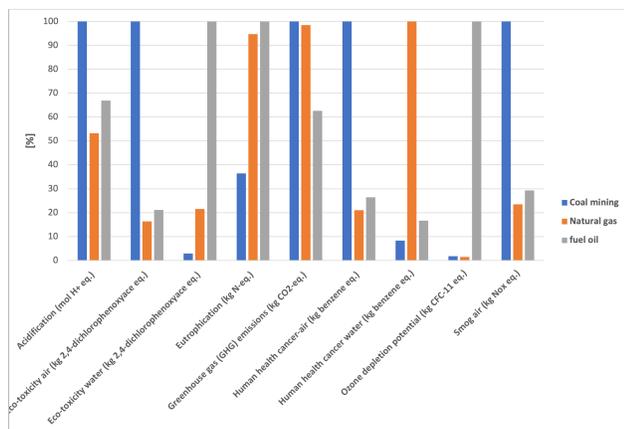


Figure 31. Comparison from an environmental point of view

6.5 Feedstock Sources

When it comes to supplying feedstock different technologies compete based on two approaches. The first one is the economical approach and the second one is the environmental approach. A feedstock source must provide the best possible price and the least environmental impact to be reliable. During the last few years, the technology of crude oil steam cracking was strongly optimized and almost impossible to challenge. On the other hand, the increasing awareness towards healthier environmental sources such as natural gas, biomass, and waste streams could be considered for the production of high-value chemicals (HVC) like ethylene. The reason behind that is the famous depleting risk of fossils as well as the global objective to react as soon as possible with different suggested scenarios to maintain the CO_2 concentration on the planet within a certain range before it becomes impossible to keep it at relatively acceptable rates. It will become impossible due to the fact that CO_2 remains in the atmosphere for 300 to 1000 years. thus, once emitted it remains [40]. The importance of this topic forces new policies and regulations every couple of years, pushing industries to compromise the price for environmental wellness. All of which makes the comparison of HVC production techniques and sources based on the rate of CO_2 emission relevant.

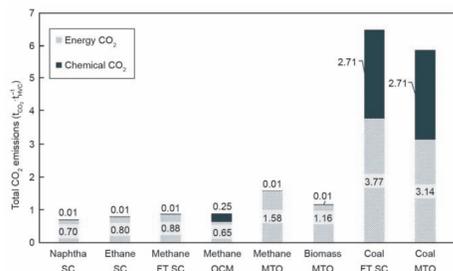


Figure 32. HVC Production methods comparison based on CO₂ emission

The study represented in Figure 32 compares different sources such as methane, crude oil, biomass, and naphtha for

different technologies such as steam cracking (SC), Fischer-Tropsch Steam cracking (FT SC), Oxidative coupling of methane (OCM) and Methanol to olefins (MTO) based on CO_2 emission. Even though some of these methods are on a lab scale, for example, in the case of OCM, the study proves that naphtha steam cracking is the best industrial option from an environmental perspective having the least chemical and energy contributed CO_2 emission.[41]

7. Conclusion

Ethylbenzene is a crucial compound for the manufacture of many commodities, it is mainly used to produce styrene. Its demand is greatly and rapidly increasing therefore it is necessary to determine the most efficient way to design its production process. Throughout this article, different aspects were evaluated to do so.

First and foremost, it was decided to use the Redlich-Kwong-Soave model to determine pure components and mixtures properties as it provided the most appropriate values and corresponded the most to the studied process.

Then, adiabatic reactors were implemented while making sure that their operating conditions and their dimensional measurements were optimal. The aim was to minimize the volume for cost reasons while increasing the reaction rate. The same approach was conducted for the separation units. Furthermore, the design of the heat exchangers used was also performed.

Afterward, the overall process was enhanced through a heat integration which allowed to maximize energy recovery while performing a pinch analysis followed by a heat exchanger network. This integration shows that around 85% of energy could be saved.

Through a life cycle assessment, it was concluded that the designed process does not have a significant impact on the environment especially if the plant is built in Europe. Thus, it was decided to base the plant in Belgium as raw materials could be easily provided by other companies such as Ineos.

The economic feasibility analysis of the ethylbenzene process was established while using formulas found in Turton book and using values found online and/or obtained after discussion with engineers in the industry. The study led to a production that is not profitable. Indeed, more than 20 million dollars are lost each year which approximately corresponds to 19 million euros.

Finally, a literature review was realized to compare different existing technologies to the one studied. Indeed, it is highly important to do so to validate the optimal operating conditions or to find further improvements. Moreover, alternative feedstocks were also discussed.

For further improvement, it could have been more interesting to only work in the liquid phase as current ethylbenzene production plants generally function in the liquid phase as it is more beneficial.

8. Acknowledgment

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Appendix

Stream Name	Units	BENZENE	EB	ETHYLENE	GAS1	GAS2	HPSR2	LPSR1	R1-IN	R1-OUT	R2-IN
From			T302		V-302	T301	E303B	E301B			
To		MIX1		COMP1					R-301	RMIX2	R-302
Phase		Liquid	Liquid	Vapor	Vapor	Vapor	Vapor		Vapor	Vapor	Vapor
Temperature	C	25.00	181.60	25.00	43.62	43.66	244.23	180.32	382.67	448.15	360.00
Pressure	bar	1.10	3.00	20.00	1.10	1.10	35.00	10.00	30.00	30.00	30.00
Enthalpy Flow	kW	1305.93	553.51	1210.33	-87.03	-19.59	-10487.42	-1785.47	8466.14	8466.14	8044.16
Mole Flows	kmol/hr	96.74	94.58	103.81	7.67	3.69	160.00	27.00	257.45	230.42	266.76
TOLUENE	kmol/hr	1.93	0.00	0.00	0.00	0.00	0.00	0.00	1.93	0.00	0.00
ETHANE	kmol/hr	0.00	0.00	7.27	5.27	2.00	0.00	0.00	3.22	3.22	5.77
ETHYLENE	kmol/hr	0.00	0.00	96.54	0.00	0.00	0.00	0.00	28.96	0.00	33.79
WATER	kmol/hr	0.00	0.00	0.00	0.00	0.00	160.00	27.00	0.00	0.00	0.00
BENZENE	kmol/hr	94.81	0.07	0.00	1.12	0.94	0.00	0.00	221.80	197.68	197.68
ETHYL-01	kmol/hr	0.00	94.51	0.00	0.09	0.00	0.00	0.00	0.10	25.19	25.19
1:4-D-01	kmol/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.48	0.48
PROPY-01	kmol/hr	0.00	0.00	0.00	1.19	0.75	0.00	0.00	1.43	3.37	3.37
O-DIE-01	kmol/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.48	0.48

Stream Name	Units	R2-OUT	R3-IN	R3-OUT	R4-IN	R4-OUT	REC-R4	REC-R123	RECB-R4	RECD-R4	RECYB
From		R-302	E302	R-303	H2	R-304	SPLIT2	SPLIT2	P4	P3	T301
To		RMIX3	R-303	MIXR	R-304	MIXR	P4	MIX1	RMIX4	RMIX4	SPLIT2
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	437.14	375.00	446.33	487.00	495.36	43.66	43.66	49.13	235.90	43.66
Pressure	bar	30.00	30.00	30.00	30.00	30.00	1.10	1.10	30.00	30.00	1.10
Enthalpy Flow	kW	8044.16	7893.52	7893.52	942.77	942.77	199.89	1799.05	203.46	-19.92	1998.94
Mole Flows	kmol/hr	232.98	269.31	235.51	26.73	26.73	14.40	129.56	14.40	12.34	143.96
TOLUENE	kmol/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHANE	kmol/hr	5.77	8.31	8.31	0.12	0.12	0.12	1.04	0.12	0.00	1.16
ETHYLENE	kmol/hr	0.01	33.80	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WATER	kmol/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
BENZENE	kmol/hr	167.73	167.73	140.54	14.11	2.71	14.11	126.99	14.11	0.00	141.10
ETHYL-01	kmol/hr	51.30	51.30	71.89	0.43	23.24	0.01	0.10	0.01	0.42	0.11
1:4-D-01	kmol/hr	2.40	2.40	5.70	5.70	0.00	0.00	0.00	0.00	5.70	0.00
PROPY-01	kmol/hr	3.37	3.37	3.37	0.16	0.16	0.16	1.43	0.16	0.00	1.59
O-DIE-01	kmol/hr	2.40	2.40	5.70	6.22	0.52	0.00	0.00	0.00	6.22	0.00

Stream Name	Units	RECYDEB	T301-IN	T301-OUT	T302-IN	V-IN	V-OUT	VAL-IN	W1	W2	W3	WASTE-W3
From		T302	H3	T301	P2	VAL	V-302	E303D				E303D
To		P3	T301	P2	T302	V-302	H3	VAL	P5	P6	E303D	
Phase		Liquid		Liquid	Liquid		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	230.84	80.00	142.66	142.85	43.62	43.62	45.00	25.00	25.00	25.00	40.46
Pressure	bar	3.00	1.10	1.10	3.00	1.10	1.10	30.00	1.10	1.10	1.10	1.10
Enthalpy Flow	cal/sec	-26.07	1991.00	185.67	187.36	1435.57	1522.60	1435.57	-2167.85	-12846.50	-12043.60	-11987.55
Mole Flows	kmol/hr	12.34	254.57	106.92	106.92	262.24	254.57	262.24	27.00	160.00	150.00	150.00
TOLUENE	kmol/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHANE	kmol/hr	0.00	3.16	0.00	0.00	8.43	3.16	8.43	0.00	0.00	0.00	0.00
ETHYLENE	kmol/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WATER	kmol/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	27.00	160.00	150.00	150.00
BENZENE	kmol/hr	0.00	142.12	0.07	0.07	143.24	142.12	143.24	0.00	0.00	0.00	0.00
ETHYL-01	kmol/hr	0.42	95.04	94.93	94.93	95.13	95.04	95.13	0.00	0.00	0.00	0.00
1:4-D-01	kmol/hr	5.70	5.70	5.70	5.70	5.70	5.70	5.70	0.00	0.00	0.00	0.00
PROPY-01	kmol/hr	0.00	2.34	0.00	0.00	3.53	2.34	3.53	0.00	0.00	0.00	0.00
O-DIE-01	kmol/hr	6.22	6.22	6.22	6.22	6.22	6.22	6.22	0.00	0.00	0.00	0.00

Figure 33. Stream Table