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Production of Benzene by Hydrodealkylation of Toluene

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Subject:	FEL-1 Techno-Economic Assessment of a Process for Benzene Production by the Hydrodealkylation of Toluene
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Executive Summary

A conceptual process design and techno economic analysis was performed for the conversion of toluene and hydrogen to produce 100 kta of benzene in Alkyl Products Limited Company. The primary feedstock is toluene and hydrogen gas feed priced at $300/MT and $1,400/MT mixture respectively. The main product benzene is priced at $1,000/MT.

The base case evaluation using a PFR reactor and a separation system consisting of 1 flash drum, 1 PSA, and 2 distillation columns. The key design variable was optimized by maximizing the net present value (NPV), at which condition the process can provide $ 38.2MM/yr in gross chemical sales revenue. The finalized process design sequesters 7.1 MJ energy and 0.7 kg CO_2 per kg of benzene produced.

Fixed costs were dominated by capital recovery. TCI = $44.2MM, based on a 2 year construction time, an enterprise rate of 10%, after 13 years of operation the project NPV = $ 108.6MM, NPV% =16, IRR = 33%.

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1. Introduction & Overview

The hydrodealkylation (or HDA) process was designed to produce benzene by James Merrill Douglas in the 1980s [1]. The reactions are shown below: (more information may be found in Appendix A)

$$T + H_2 \rightarrow B + CH_4 \text{ (R1)} \qquad \Delta H_1 = 42\ kJ$$

$$2B \rightleftharpoons D + H_2 \text{ (R2)} \qquad \Delta H_2 = 67\ kJ$$

However, the process is not up-to-date, as there has been significant developments in chemical engineering design, and many technologies were not considered at the time, such as pressure-swing adsorption technology (PSA) and chemical process simulators software such as Aspen HYSYS. Alkyl Products Limited is planning to expand its existing benzene production by 100kta of benzene in Freeport, TX. The goal of this design report is to make the FEL-1 assessment and a conceptual design of this 100kta benzene production based on chemical process plants, economic, safety and environmental concerns. The design is based on:

(1) On the basis of Economic viability. The selection for an optimized process design will be through an net present value (NPV) calculation based on a viable economic financing plan to make sure the whole design will give the maximum profits it can achieve by the end of the plant's life.

Table 1. Chemical prices of the HDA process

Chemical Species	Price
Toluene (C_7H_8)	300 \$/MT
95% Hydrogen (H_2) + 5% Methane (CH_4)	1400 \$/MT
Fuel	4.25 \$/GJ
Benzene (C_6H_6)	1000 \$/MT
Diphenyl ($C_{12}H_{10}$)	Fuel Value
Gas Purge	Fuel Value
CO_2 Charge	40 \$/MT

(2) On the basis of safety. The use of pressurized vessels will be examined in terms of a HAZOP analysis. The risk of the plant will then be examined from a process control point of view. Chemical toxicity will also be considered.

(3) On an environmental aspect by accounting for the carbon footprint of the process.

2. Conceptual Design Process Basis

2.1 Determination of Design Variables

The two process design alternatives being considered in this report are :(1) HDA process with diphenyl exiting the plant and a pressure swing adsorber (PSA) on the gas recycle stream, and (2) HDA process with diphenyl exiting the plant and no PSA on the gas recycle stream. For both of these two alternatives, there are two feed streams to the reactor: mixed gas feed (hydrogen + methane) and toluene gas; 3 product streams: a benzene product stream, a biphenyl by-product stream, and a purge gas steam containing methane and hydrogen; two recycle streams: a liquid recycle stream containing toluene and a gas recycle stream as an opposite way to the purge stream.

Benefits of having a recycle loop include: (1) hydrogen gas must not be wasted as it is the highest costing raw material used in the HDA process; (2) the recycle loop was considered for its thermodynamic properties as a heat carrier to regulate the PFR, preventing it from overheating or having a runaway reaction. Compared with the no PSA design, PSA helps with removing methane and purifying the gas recycle stream. We will evaluate the applicability of this PSA with other design and economic considerations in this report.

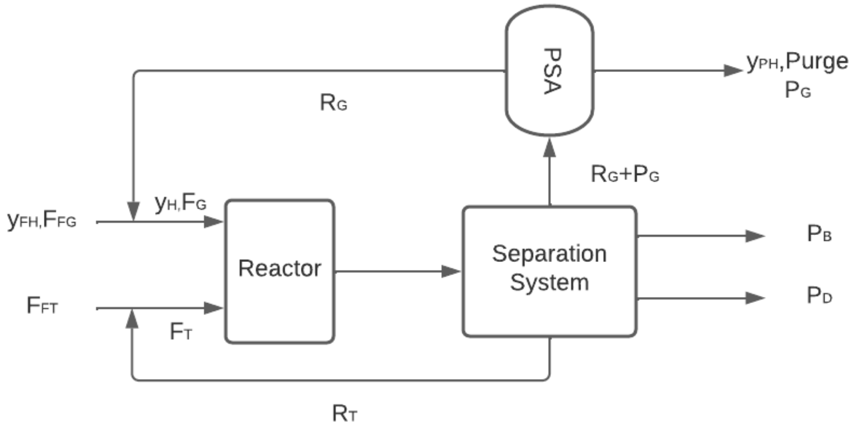


Fig 1. Flow diagram of a level-3 MATLAB HDA process with a purge stream, a PSA system, and a recycle toluene stream. F_{FT} is the toluene feed; F_H is the hydrogen gas feed, and F_{CH4} is the methane gas feed (95% H_2 and 5% CH_4 in the feed); R_G is the gas recycle stream back to the reactor; P_G is the gas purge ($P_H + P_{CH4}$), and P_B is the benzene outlet.

According to reaction kinematics (App. A), the HDA process must be performed under high temperature (550-650 °C) and high pressure (30-34 bar). This reaction was designed to take place under laboratory conditions (see App. A for a statement of process chemistry) with a hydrogen to toluene ratio (MR) of 5 to 1. A high conversion and a gas phase reaction are needed for this process, so a plug flow reactor (PFR) is used in this process. The mole balances for the two conceptual designs were used to specify the initial conditions for the reactor calculations. PFR design equations for all chemical species were solved numerically at 3 different temperatures and pressures to get several relationships among reactor outflows, reactor volume, selectivity and conversion. The operating temperature and pressure of the PFR is finally determined at 627 °C and 34 bar because it provides the largest conversion and lowest reactor volume change at these conditions (more detailed information in App. C).

The reaction conversion was determined by the Net Present Value (NPV) calculations. NPV is a method used to determine the current value of all future cash flows generated by a project, including the initial capital investment. Conversions of 0.63, 0.72, 0.82, and 0.86 were picked and plugged in both conceptual design alternatives to estimate the NPV. The results showed that when the design is finished up to level 3, the PSA system design and a conversion of 0.82 provided the best NPV of -$0.98 million (see more detailed conversion calculated values in App. E).

The preliminary operating condition for the ractor estimated above was based on the conceptual designs up to level 3, without specifications of separation and energy systems. For the level 4 to level 6 design considerations, the separation system was then specified into two distillation columns, one flash drum and one PSA system. In addition, there are 4 heat exchangers connected before the PFR reactor. The second reaction (R2) kinetics parameters were furthered revised with accurate calculations, and the new conversion is at $x = 0.75$.

Total ISBL = $12 MM

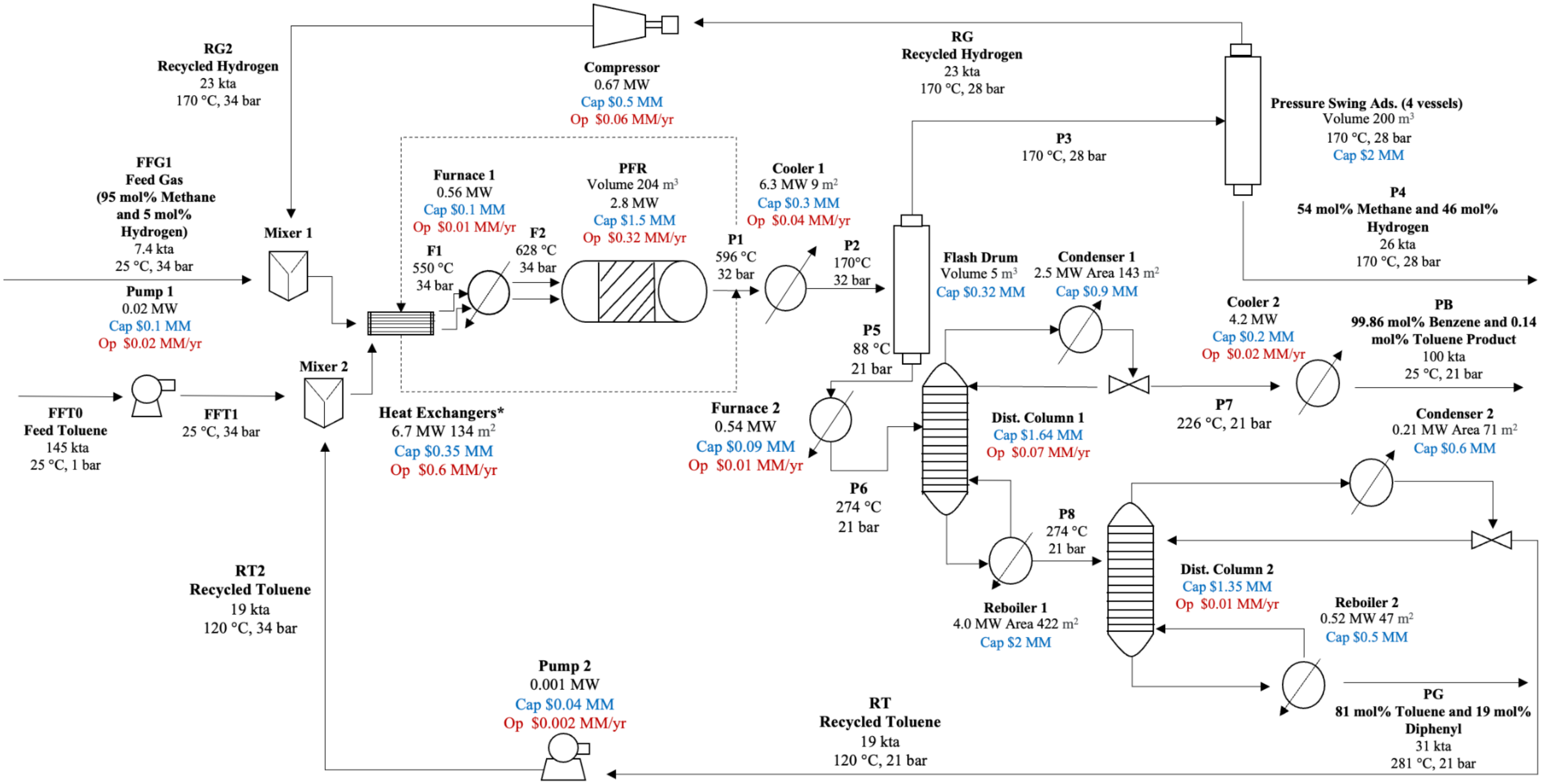


Fig 2. Process flow diagram for HDA. Equipments include: 1 PFR reactor, 2 furnaces, 2 coolers, 1 flash drum, 2 distillations columns, 1 compressor, 1 PSA system, 2 pumps, and 1 heat exchanger set (4 heat exchangers included). Total ISBL is ~$12MM and total OSBL is ~$1.3M.

Table 2. PFD stream flow parameters

Stream	Flow Rate (kg/hr)	Flow Rate $\times 10^5$(MT/yr)	Energy Flow (MW)	T (°C)	P (bar)
FFT0	16590	1.5	0.64	25	1
FFG1	842	0.07	0.3	25	1
FFT1	16590	1.5	0.67	25	34
F1	22210	2	17	550	34
F2	22210	2	17	628	34
P1	22210	2	14	596	32
P2	22210	2	3.6	170	32
P3	5582	0.5	1.6	170	28
P4	2976	0.3	3.1	170	28
P5	16630	1.5	3.1	88	21
P6	16630	1.5	5.4	274	21
P7	11416	1	3.1	226	21
P8	5768	0.5	1.3	274	21
PB	11416	1	0.65	25	21
PG	3566	0.3	0.92	281	21
RT	2198	0.2	0.2	120	21
RG	2606	0.2	1.5	170	28
RT2	2198	0.2	0.2	120	34
RG2	2606	0.2	1.5	170	34

2.2 Separation System Design

The first considered separation design is a flash separation drum that separates the mixed gas (hydrogen and methane) from the other organic compounds. To achieve a high amount of separation with lowest cooling costs, the flash drum was controlled around 30-50 °C to limit the cooling method to only cooling water. The pressure level was not lowered because the pressure build up of the reaction was easy for other separation processes to operate. Given these separation variables, the optimal separation was found at 32°C and 25 bar from ASPEN+. The flash drum in the separation system has a low impact on the economics with a total installed cost of 316327 $. This flash drum does not have any utility costs from ASPEN.

For the PSA system, zeolite 5A was used as an adsorption catalyst. In designing the PSA, four packed beds are used by 80% so there will be sufficient loading and off loading to achieve 90% recovery. In total, the PSA is designed to have a 5 minute load time and 95% load fraction. Due to the design requirements of the flash drum, the PSA system will operate at an inlet pressure of 25 bar. For optimal use of the catalyst, the PSA system will have an outlet pressure of 2 bar. Considering all of these factors, the final PSA will consist of four cylindrical beds with a 2.5 m diameter and 10.7 m length. The total mass of zeolite 5A was estimated at around 140 MT (more detailed calculations can be found in App. L).

The third separation design that took into consideration were the distillation columns. Two distillation columns are used in a direct split order: The first column separates benzene products from toluene and biphenyl because benzene has the lowest boiling point among the three chemicals, and the second column separates toluene from diphenyl because toluene has a higher boiling point (App. A).The distillation MATLAB design procedures assumed “constant molar flow” (CMO), that is, the latent heat of vaporization is independent of the mixture composition. Also, the assumption of a saturated liquid feed was made. [2] A lower vapor rate results in better performance of the distillation columns because If the distillation is conducted too rapidly, liquid-vapor equilibria will not be established in the fractionating column, and poor separation of the compounds will result. From MATLAB calculations, the distillation vapor rates of the direct split order resulted in a lower value than indirect split orders (~35% less). As a result, a direct split order was performed. The real stage numbers, reflux ratio, and boilup ratio obtained from MATLAB calculations were then adjusted in Hysys Simulation to reach high purities of benzene products and recycled toluene. For both design alternatives, the two distillation column operate at 21 bar, while the average temperature through the first column is about 240 °C, which is lower than 280°C of the second one (Hysys specified values shown in App. F). The first column contains 40 stages, with the composition of benzen at top up to 0.998. The second column contains 54 stages, with the composition of toluene at the top up to 0.991. By selecting the tray spacing of 0.55 m, the first column has a height of 22 m, while the second column has a height of 30 m. The distillate rate to feed stage flowrate ratio (V/F) of the first distillation column was calculated as 2.2, while the V/F of the second column was 0.6. These simulation results from Hysys is constructed based on preliminary calculations finished in Matlab though the final Hysys results are much different from Matlab results as perfect distillation separation is assumed in Matlab calculations (Matlab calculation details shown in App. L).

2.3 Energy Integration

For the heating system, three factors had been considered: Total cost, efficacy, and overall carbon footprint. To optimize the heating system, this report follows the heat integration to achieve a low capital cost, high efficiency, and a low carbon footprint:

As mentioned in the determination of design variables section, all feeds in the reactor must be heated to 627 °C for spontaneous reaction. After exiting the reactor, products at 595 °C must be reduced to around 30 °C to achieve a high amount of separation in the flash drum. There is about 600 °C temperature drop and 12 MW of energy being created and removed in this short process. The separation processes require a total of 25 MW of power. To get an estimate on the optimal heat exchanger size, this report used a Graphical Pinch analysis for the integrated heating system (more detail in check figure in App. G) [2]. A total surface area of 502 m^2 was calculated with a total trim power of 12 MW and a net power consumption of 897 kW. This power consumption is needed for the cooling of the benzene product stream (P_B). A total capital cost of over $23 MM was needed for this heating system, which was cost prohibitive. When a 4-heat exchanger system was added to the system, the overall process had decreased 13 MW in heating and cooling. The total capital cost was reduced by $12 MM from the previous original plan. However, Table 3 shows that the significant need of steam and cooling water still costs $ 0.4 MM yearly.

Table 3. Energy system parameters. Calculated using figure App. G.1 and values from table App. G.3.

Equipment Unit	Area (m^2)	Power (MW)	Total Cooling Water Cost ($/yr)
Reactor Heat Exchangers	135	6.7	N/A
Furnace-1	N/A	0.56	N/A
Furnace-2	N/A	0.54	N/A
Cooler-1	92	6.3	$35,176
Reboiler-1	422	4	N/A
Reboiler-2	47	0.52	N/A
Condenser-1	143	2.5	$286,960
Condenser-2	71	0.21	$53,420
Total	910	21.33	$0.4 MM

All in all, there are some advantages of having this heating system over others. First, the reduction of heat needed by this system lowers the need to use power from the power grid. The final energy use per mass product was calculated as 7.09 MJ/kg. Also, this integration reduced the need for heating water significantly by removing large amounts of cooling water (450,000 MT) used in reaction outlet coolers.

It is important to note that this heating system also uses an outside furnace to produce the reboiler steams. This furnace will heat cooling water at 54 bar to produce steam at 264 °C. This will use 5 MW of the total 40 MW heat produced by the burning of the process purge gas (P_G).

3. Process Economics

3.1 Overall Financial Plan and Costs

The financing plan of this design project consists of bonds that will be sold with a 10-year bond life. These bonds follow a 10 year depreciation schedule. An assumption demonstrates that there will be a 2-year construction period with the total capital investment (TCI) charging in full at the end of year 0. The plant life is 13 years, and there will be a salvage value of 5% of TCI at the end of plant life. In addition, the assumption states that the cost of land is negligible and the working capital (WC) is 5% of fixed capital investment (FCI).

Furthermore, there is a carbon dioxide charge at $40/MT for any amount of carbon produced in this plant. This charge includes the purge fuel burned at the outlet of the plant and any other carbon footprint electrical power use. According to the US Energy Administration in 2020, the US Power grid had a carbon footprint of 0.4 kg/kwh [3]. Therefore, for every GJ of power used from outside sources, this financial plan includes a $ 4.3 charge. By using this charge, Alkyl Products Limited can invest in the carbon capture program.

In addition, ASPEN-HYSYS provided the financial estimate for the design equipment costs with the associated installation costs in the US Gulf Region. The Appendix E. of Douglas's *Conceptual design of Chemical Processes* [1] was also used to calculate part of equipment costs. The assumed Marshall and Swift Index is 1650 in 2022.

The equipment parameters and costs in the process are shown in Table 4 and Fig. 3. The PSA system requires the largest capital cost because hydrogen gas is corrosive to carbon steels, and alternative stainless steels material are much more expensive than carbon steels. Also, the size of PSA system is big as mixed gas (hydrogen and methane) has huge production rate.

Table 4. PFD Equipment parameters

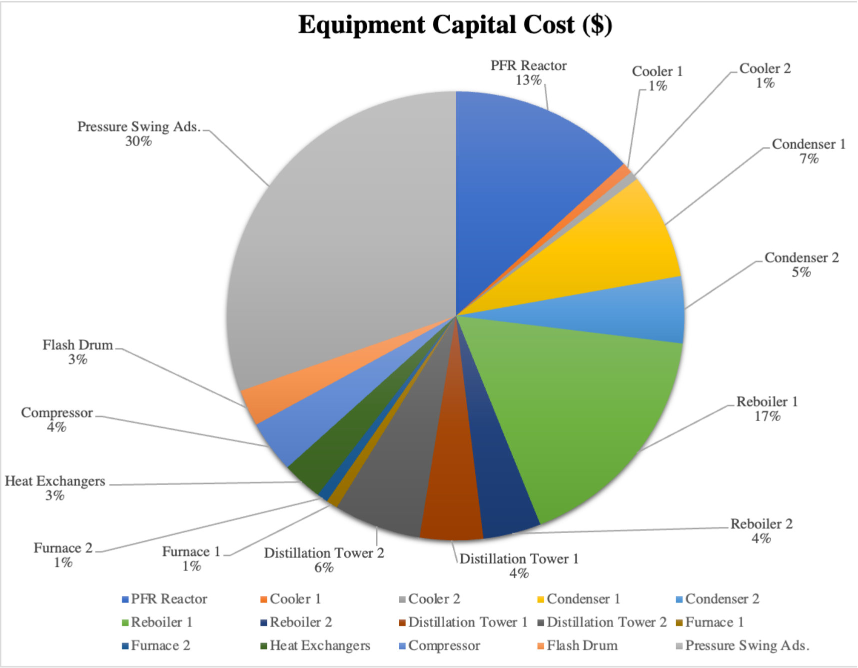
Equipment	Materials	Size	Installed Cost ($)
PFR Reactor	Stainless Steel	204 m^3	$1,582,743
Cooler 1	Stainless Steel	92 m^3	$94,389
Cooler 2	Stainless Steel	71 m^3	$76,469
Condenser 1	Carbon Steel	143 m^2	$914,452
Condenser 2	Carbon Steel	71 m^2	$580,050
Reboiler 1	Carbon Steel	422 m^2	$2,048,079
Reboiler 2	Carbon Steel	47 m^2	$494,164
Distillation Tower 1	Carbon Steel	39 m^3	$538,400

Distillation Tower 2	Carbon Steel	52 m^3	$744,900
Furnace 1	Stainless Steel	0.56 MW	$98,075
Furnace 2	Carbon Steel	0.54 MW	$94,389
Heat Exchangers	Stainless Steel	6.7 MW (4 vessels)	$346,672
Compressor	Stainless Steel	0.67 MW	$450,000
Flash Drum	Stainless Steel	15 m^3	$316,327
Pressure Swing Ads.	Stainless Steel	200 m^3(4 vessels)	$3,665,239
Total ISBL			$12 MM

Table 5. PFD Equipment Operating parameters

Operating Costs	Amount	Cost ($/yr)
Electricity	6202 MW/yr	$478,146
Cooling Water	24 MT/yr	$757,693
Other (~1% ISBL)		$120,443
Total		$1,356,283

(a)



(b)

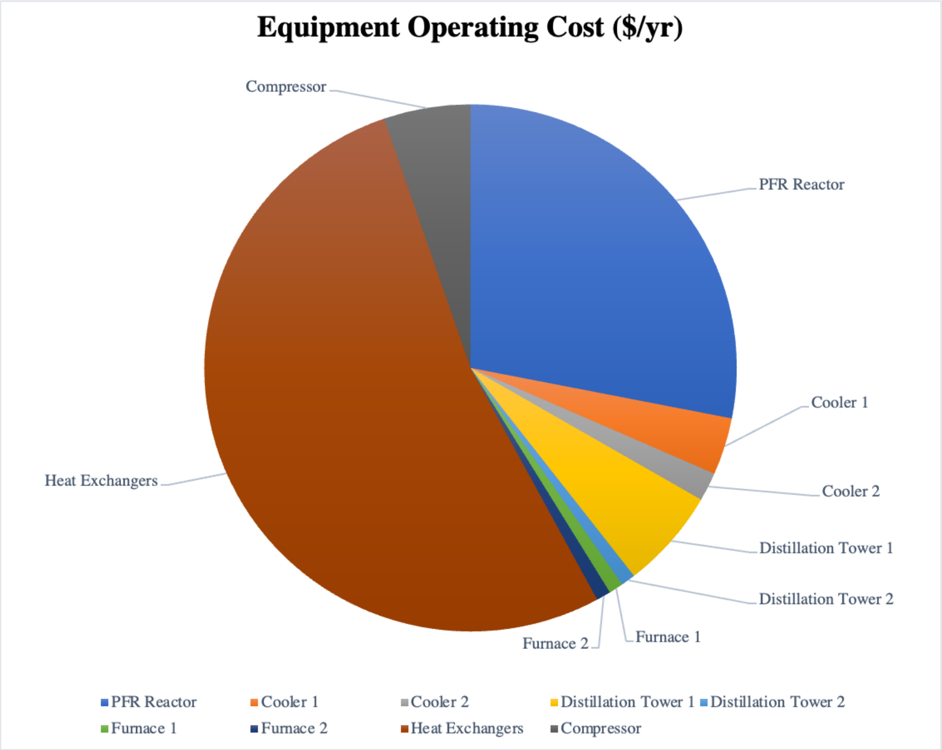


Fig. 3. Operation unit (a) installed capital cost and (b) annual operating cost diagram

3.2 Net Present Value Analysis

The profitability of the conceptual design is calculated through NPV(net present value) analysis where the calculation incorporates the total investment cost (TCI), annual revenue, depreciation, tax rate, interest rate and so on to do the calculations (see Appendix I) . Total Investment calculation is based on ISBL and OSBL and the model of factor estimates. Annual revenue is from economic potential (EP) calculation based on the amount of products produced and reactants assumed at the conceptual designed operating condition and with a concern of carbon tax. Depreciation takes a 10-year linear depreciation schedule. Administration service fee charges 10% of annual revenue. The total taxation rate is 27% and the exterperise rate is 10% annual (full calculation equations are in App. K).

By varing the key design variable (x), it is straightforward to observe the change in NPV of the PSA process alternative and without the PSA process alternative. The goal of comparing NPV between two process alternatives and at different conversion (x) is to determine the maximum profitability this design can achieve.

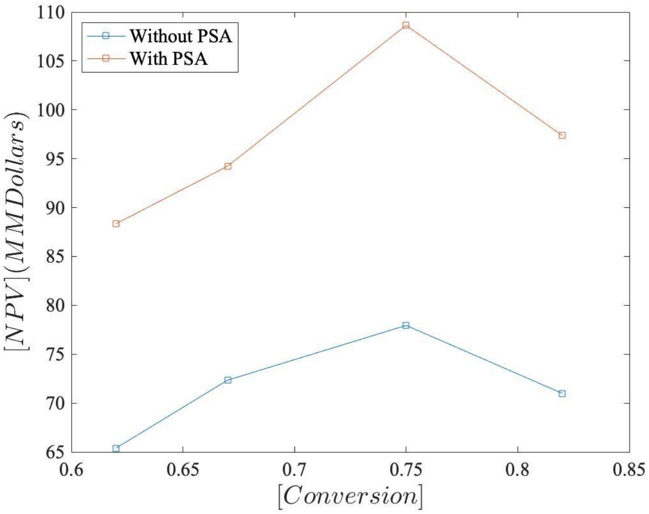


Fig 4. NPV of with a PSA and without a PSA process alternatives at different conversion. Conversion is picked at 0.62, 0.67, 0.75, 0.82. NPV has unit in MM $.

The comparisons of NPV between the HDA process with a PSA system and without a PSA system clearly shows that the with a PSA alternative gives much higher NPV overall. While the NPV of without a PSA alternative is around $78 MM, the NPV of with a PSA alternative is around $100 MM. Thus, the with a PSA alternative is absolutely a better choice than the without a PSA one. The maximum NPV occurs at x = 0.75 of the with PSA alternative, where the NPV is $108.6 MM. The corresponding NPV% is 16.37 and IRR is 32.52%.

3.3 Sensitivity Analysis

Considering the price fluctuation of raw materials, carbon tax, PSA adsorbent and so on, a sensitivity analysis is carried on to observe the effects of these fluctuation on the design's profitability..

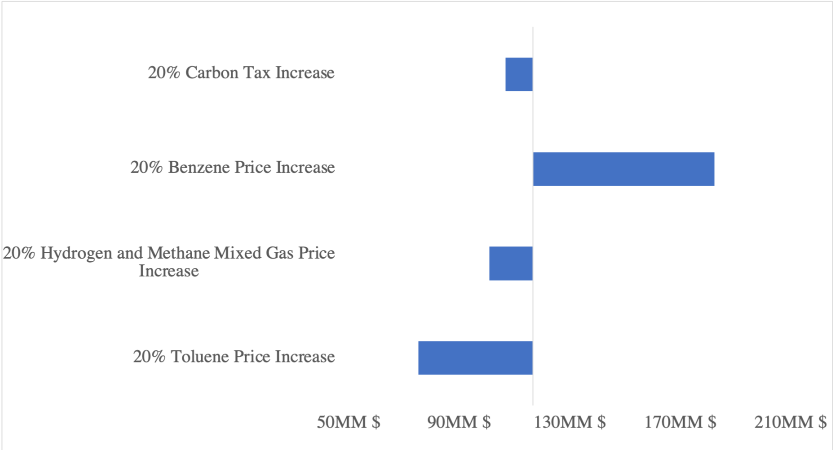


Fig 5. Sensitivity Analysis Tornado Plot (with 4 different variations)

There is also a sensitivity analysis done for the PSA unit. The main influencing factor of the cost of the single PSA unit is the price of the sorbent, zeolite 5A. However, the influence of sorbent price on the NPV of the whole design is minimal. An 20% increase on zeolite 5A only results in 0.05% decrease in total NPV value.

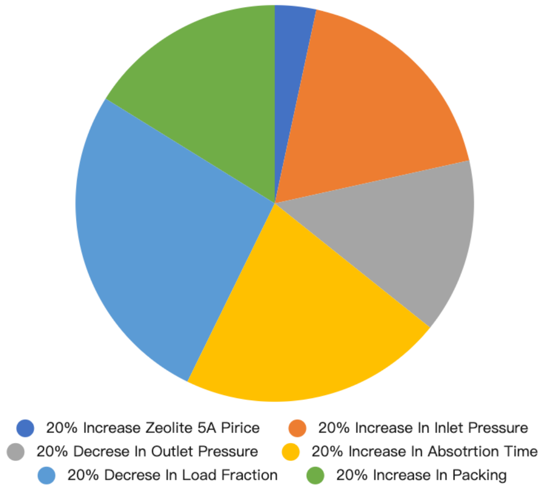


Fig 6. Sensitivity analysis on the single PSA unit. The area of each component represents the relative amount of total cost increase when there is a 20% variation on the listed variables.

Based on the several variation cases compared in the tornado diagram and PSA pie chart, it can be concluded that benzene price fluctuation brings the largest NPV variation. This probably because benzene is the main product of the reaction in a large amount and has a relatively high price in the market.

For abnormal variations such as national or global recession in 2008 and 2020, the price and interest rate of raw materials greatly increase, so the economic profitability would drop to a much lower value. As the selling price of benzene contributes most to the NPV, under the assumption of all the other chemicals prices keeping the same, the lowest acceptable benzene selling price of this report's design is \$704/MT. Once the price drops below \$704/MT, the NPV will be negative.

4. Safety and Hazard

All the chemicals used in this design have potential hazards both in the operating environment and human health. More detailed MSDS information may be found in Appendix L. From the given MSDS, the largest hazard is the flammability of the chemical species in this process: All the chemical species in this process have high flammability rates, and hydrogen contains the highest with an NFPA Fire Rating of Four. Therefore, the transportation of these chemical species and the operation of reaction present a significant high risk of fire. It is important to note that the reaction temperature of the HDA process adds another level of risk because the heat of reaction is above the auto ignition temperatures of many of the chemical species. The ignition temperatures are shown in Table 6.

Table 6. Auto Ignition temperature of chemical species in the HDA process. Data from: [4,5,6,7]

Chemical Species	Auto Ignition Temperature (℃)
Toluene (C_7H_8)	480
Hydrogen (H_2)	585
Methane (CH_4)	537
Benzene (C_6H_6)	498
Diphenyl ($C_{12}H_{10}$)	540

Also, the air contact between the reactor and the air must be limited because a possible explosion hazard might exist. To limit the air contact, this reactor needs to be buried underground or covered with a second layer of cement. Robust process control mechanisms should be used in any reactor leakage, temperature, or pressure drop control, such as adding at least two different process control loops and using a combination of physical and digital measurement devices. Such physical secondary process control mechanisms may include a viewing window and mercury barometers. A secondary containment vessel can also be used to prevent a leak or loss of pressure because the leaked product will be burned off using a flare. This reactor also needs to be built away from offices. Local emergency services should be consulted and presented with the HAZOP analysis (which may be found in Appendix K) and MSDS provided in this report before building this reactor.

Furthermore, the chemicals this reactor produces are harmful to health (especially benzene which presents an OSHA exposure limit of 5 ppm [8]). Benzene must be treated with personal protective equipment. All chemical exposure should be reported and treated with a dedicated poison control response. All local health services should be informed of the potential risks.

Moreover, one of the most common reasons that causes a reactor failure is a runaway reaction [9]. Due to the lack of cooling operations, the exponential increase of the reaction temperature in a runaway reaction makes it dangerous. To prevent a runaway reaction, the cooling jacket of this reactor must be made from non-corrosive metals, and soft water should be used. To mitigate any future risk, a secondary containment vessel may be needed. Leak and feed quality protocols are also important to act as a preventive factor.

For the separation system, the most significant hazards exist due to the pressurized nature of the separation vessels. An unplanned decomposition of such pressurized vessels may lead to rapid ignition and fire. This risk is higher in our PSA and flash drum where the high-pressure hydrogen creates an especially significant danger because hydrogen is highly corrosive. This corrosion is called hydrogen embrittlement and is most common in carbon steel, brass, and titanium [10,11,12] where the high reactivity of the hydrogen hurts the tensile strength of the metal which can lead to fractures and material failure. To avoid this, this process design uses stainless steel as the materials of equipments where hydrogen was used. This is because some types of stainless steel have shown high resistance to the hydrogen embrittlement [13]. Another possible risk factor associated with the separation systems is instrument malfunction. This happens mostly because of a valve failure or process control failure. As a result, secondary backup process control is recommended. For a more detailed analysis on safety of our separation system, a sample HAZOP analysis on Distillation Column-1 can be found in Appendix _.

Risks relating to the plant's heating and cooling systems are rarer because these are closed loop systems. However, there are still some significant risks in these operations. Corrosion is the largest threat because it is a significant factor of heat exchanger failure and malfunction. To avoid this, plugging must be conducted where the surface area reduction of heat exchangers must be balanced with the stream flow rates.

5. Conclusion

The report analysis shows that the HDA process design alternative with a PSA system on the gas recycle stream has better performance in both economic and environmental aspects compared with the no PSA design alternative. The PSA design in this report recycles 90% of the hydrogen gas from reactor outlet and purifies the recycle gas up to 99.99% hydrogen. A maximum NPV of the with a PSA design was up to \$108.6 MM at the optimal operating conditions with conversion x = 0.75. The corresponding NPV% is 16.37 and IRR is 32.52%. The maximum NPV of without a PSA design is about \$ 30 million lower than the with PSA design. The sensitivity analysis shows the fluctuation on benzene price will bring the largest overall profits variations. When assuming the market price for all the other chemicals keeping the same, the lowest acceptable price for benzene is \$704/MT, or the NPV of this design will go to negative. The two largest components of this design's TCI are the capital cost of PSA unit and the operating cost of the heat exchanger systems. Therefore, the profit of this conceptual design may be further increased by finding cheaper but corrosion-resistant material for PSA unit and improving the design of the heat exchanger system.

6. Future Work

For this HDA design process, a few design elements were not considered: First, There is not a design about a recycled reactor design model or a gas phase CSTR reactor. Furthermore, this report does not consider the recent volatility in oil markets [11] and other economic risk factors, such as market risks. As a result, we recommend a further Monte-Cristo Analysis to explore the risk associated with the finances of this report. In addition, an equity finance model should be considered as an alternative financing modal.

Certain research and development steps are also recommended for the viability of this process:
More research and experimentation must be put in the considerations surrounding the assumptions regarding constant molar overflow and ideal separation in the distillation column system. The results show that HYSYS optimization has deviated from the MATLAB ideal split distillation columns, so further testing must be conducted to confirm the viability and purity of the distillation column presented in this report. Also, some experiments should be made to consider the applicability of the NRTL reaction design package used in this report.

To implement the reactor scheme specified in this report, we recommend further experiments by using a batch reactor. The batch reactor parameters should be adjusted to have safe thermodynamics properties and prevent a possible runaway reaction.

We also recommend doing further research on the materials of construction in this report. This report did not detail the composition of the equipment materials used in this system, such as stainless steel and carbon steel. Due to large differences in steel composition, more detailed analysis must be done to determine the hydrogen compatibility of stainless steel in the use of HDA process. These research must also show that the stainless steel is able to withstand the high pressure requirements of the HDA process.

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Appendices

A. Chemical Reaction Kinetics of the Hydrodealkylation (HDA) Process

Benzene production reactions through Hydrodealkylation (or HDA) are shown below [1]:

$$T + H_2 \rightarrow B + CH_4 \quad (1)$$

$$2B \rightleftharpoons D + H_2 \quad (2)$$

T is Toluene (C_7H_8) B is Benzene (C_6H_6) and D is Diphenyl (also known as Biphenyl, $C_{12}H_{12}$). The first reaction (1) follows the reaction rate expression below:

$$r_1 = k_{0,1}\, e^{\frac{-\Delta E_1}{RT}} [C]\, [H]^{0.5} \quad (3)$$

$k_{0,1}$ is the reaction prefactor, ΔE_1 is the activation energy, T is temperature in Kelvin , [T] and [H] is the concentration of Toluene and Hydrogen. $k_{0,1}$= 1.188 x 10^{14} (units in $\frac{1}{h}\sqrt{\frac{L}{gmol}}$). The activation energy equals 52.0 kcal/mol. This reaction has a heat of reaction of 41760 J/mol.

The second reaction (2) follows the reaction rate expression below:

$$r_2 = k_{0,2}\, e^{\frac{-\Delta E_2}{RT}} P^2 (y_B^2 - \frac{y_D y_H}{K_{eq}}) \quad (4)$$

$k_{0,2}$=1.1647 x 10^{-5} gmol/$(L \times Pa^2 \times h)$, ΔE_2=30.19 kcal/mol, y_B , y_D , y_H are the gass mole fractions of benzene, diphenyl and hydrogen. Then, the equilibrium constant can be calculated as follows:

$$log_{10}[K_{eq}(T)] = -\frac{734.92}{T} - 8.1046 + 3.1294\, log_{10}(T) - 7.0804 \times 10^{-4} T + 8.523 \times 10^{-8} T^2 \quad (5)$$

$$K_{eq} = \frac{y_D y_H}{y_B^2} \quad (6)$$

Constraints:

The reactor is bound by a temperature of 550-650 ℃ and a pressure of 30-34 bar. The hydrogen-to-toluene ratio of 5:1 is used for these reactions in the lab environment. The boiling points of reactants and products in this process are listed in table 1 below.

Table A.1. The physical properties for all species in the HDA process

Species	Molar Mass (g/mol)	Heat of Combustion ΔH° (kj/mol)	Boiling Temperature (℃)
Hydrogen (H_2)	2.016	286	-253
Methane (CH_4)	16.04	890	-162
Benzene (B)	78.11	–	80

Toluene (T)	92.14	–	111
Diphenyl (D)	154.21	6248	255

B. Level 2 Design Balances [1]

B.1 With Purge Stream Without PSA:

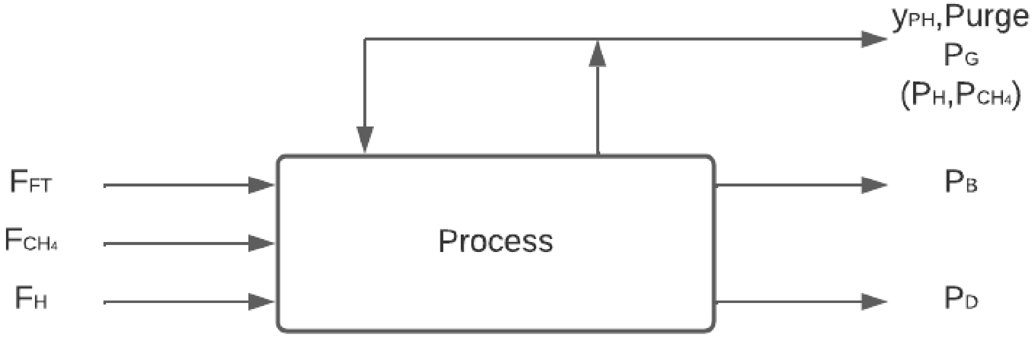


Fig B.1. Flow diagram of a level-2 HDA process with a purge stream. F_{FT} is the toluene feed; F_H is the hydrogen gas feed (95 mol% H_2 and 5 mol% CH_4); P_G is the gas purge (P_{CH4} + P_H); P_D is the diphenyl outlet, and P_B is the benzene outlet. [1,2]:

Benzene Balance:
in - out + generated - consumed = 0

$$0 - P_B + F_{FT} - 2P_D = 0$$

$$F_{FT} = P_B + 2P_D$$

Hydrogen Balance:
in - out + generated - consumed = 0

$$F_H - P_H + P_D - F_{FT} = 0$$

Methane Balance:
in - out + generated - consumed = 0

$$F_{CH_4} - P_{CH_4} + F_{FT} = 0$$

Variables = 7 (F_{FT}, F_H, F_{CH_4}, P_B, P_D, P_H, P_{CH_4})

Equations = 3
Degrees of freedom = 7-3 = 4

Using selectivity to solve:

$$S = \frac{P_B}{F_{FT}}$$

$$F_{FT} = \frac{P_B}{S}$$

Benzene Balance:

$$F_{FT} = P_B + 2P_D$$

$$\frac{P_B}{S} = P_B + 2P_D$$

$$P_D = P_B \left(\frac{1-S}{2S}\right)$$

Hydrogen Balance:

$$F_H - P_H + P_D - F_{FT} = 0$$

$$F_H - P_H - P_B \left(\frac{1+S}{2S}\right) = 0$$

Methane Balance:

$$F_{CH_4} - P_{CH_4} + F_{FT} = 0$$

$$F_{CH_4} - P_{CH_4} + \frac{P_B}{S} = 0$$

Purge Flow Balance:

$$P_H = P_G\, y_{PH}$$

$$P_{CH_4} = P_G\,(1 - y_{PH})$$

B.2 With Purge Stream and an PSA:

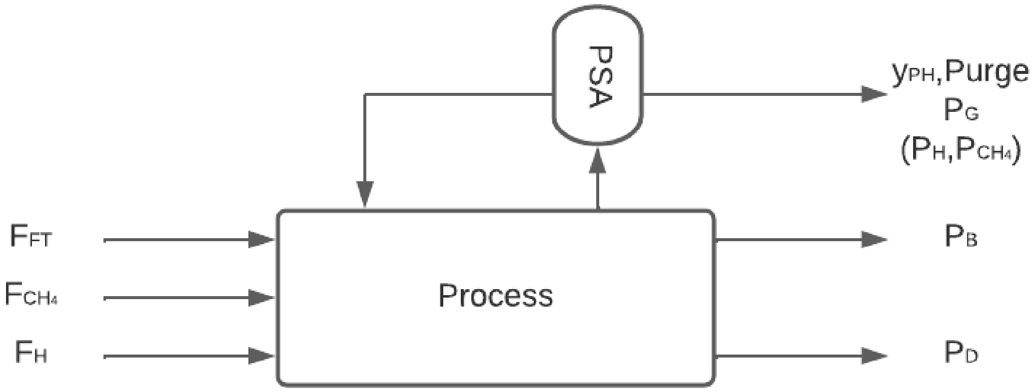


Fig B.2. Flow diagram of a level-2 HDA process with a purge stream and a PSA system. F_{FT} is the toluene feed; F_H is the hydrogen gas feed (95 mol% H_2 and 5 mol% CH_4); P_G is the gas purge (P_{CH4} + P_H); P_D is the diphenyl outlet, and P_B is the benzene outlet. [1,2]:

Benzene Balance:
in - out + generated - consumed = 0

$$0 - P_B + F_{FT} - 2P_D = 0$$

$$F_{FT} = P_B + 2P_D$$

Hydrogen Balance:
in - out + generated - consumed = 0

$$F_H - P_H + P_D - F_{FT} = 0$$

Methane Balance:
in - out + generated - consumed = 0

$$F_{CH_4} - P_{CH_4} + F_{FT} = 0$$

Variables = 7 (F_{FT}, F_H, F_{CH_4}, P_B, P_D, P_H, P_{CH_4})
Equations = 3
Degrees of freedom = 7-3 = 4

Using selectivity to solve:

$$S = \frac{P_B}{F_{FT}}$$

$$F_{FT} = \frac{P_B}{S}$$

Benzene Balance:

$$F_{FT} = P_B + 2P_D$$

$$\frac{P_B}{S} = P_B + 2P_D$$

$$P_D = P_B\left(\frac{1-S}{2S}\right)$$

Hydrogen Balance:

$$F_H - P_H + P_D - F_{FT} = 0$$

$$F_H - P_H - P_B\left(\frac{1+S}{2S}\right) = 0$$

Methane Balance:

$$F_{CH_4} - P_{CH_4} + F_{FT} = 0$$

$$F_{CH_4} - P_{CH_4} + \frac{P_B}{S} = 0$$

Purge Flow Balance:

$$F_{FH} - P_G y_{PH} + P_B\left(\frac{1-s}{2s}\right) = 0$$

$$\frac{F_{FH} + P_B\left(\frac{1-s}{2s}\right)}{y_{PH}} = P_G$$

B.3 Without purge stream (gas separation system included):

Fig B.3. Flow diagram of a level-2 HDA process without a purge stream and with a gas separation system. F_{FT} is the toluene feed; F_H is the hydrogen gas feed, and F_{CH4} is the methane gas feed (95% H_2 and 5% CH_4 in the feed); P_{CH4} is the methane outlet; P_{H2} is the hydrogen outlet; P_D is the diphenyl outlet, and P_B is the benzene outlet.

Benzene Balance

$$0 - P_B + F_{FT} - 2P_D = 0$$

Hydrogen Balance:

$$F_H + P_D - P_H - F_{FT} = 0$$

Methane Balance:

$$F_{CH_4} - P_{CH_4} + F_{FT} = 0$$

Variables = 7 (F_{FT}, F_H, F_{CH_4}, P_B, P_D, P_{CH_4}, P_H)
Equations = 3
Degrees of freedom = 7-3 = 4

Using selectivity to solve:

$$S = \frac{P_B}{F_{FT}}$$

$$F_{FT} = \frac{P_B}{S}$$

Benzene Balance:

$$F_{FT} = P_B + 2P_D$$

$$\frac{P_B}{S} = P_B + 2P_D$$

$$P_D = P_B \left(\frac{1-S}{2S}\right) = 1.28 \times 10^6 \left(\frac{1-S}{2S}\right) \left[\frac{kmol}{yr}\right]$$

Hydrogen Balance:

$$F_H - P_H + P_D - F_{FT} = 0$$

$$F_H - P_H - P_B \left(\frac{1+S}{2S}\right) = 0$$

Methane Balance:

$$F_{CH_4} - P_{CH_4} + F_{FT} = 0$$

$$\frac{0.05}{0.95} F_H - P_{CH_4} + \frac{P_B}{S} = 0$$

$$P_{CH_4} = 3.37 \times 10^4 + \frac{1.31 \times 10^6}{S} \left[\frac{kmol}{yr}\right]$$

B.4 Without purge stream (gas separation system and diphenyl recycle stream included):

Fig B.4. Flow diagram of a level-2 HDA process without a purge stream, with a gas separation system and a diphenyl recycle. F_{FT} is the toluene feed; F_G is the hydrogen gas feed (95% H_2 and 5% CH_4); P_{CH4} is the methane outlet, and P_B is the benzene outlet.

Benzene Balance: (bottom left)

$0 - P_B + F_{FT} = 0$

Hydrogen Balance:

$F_H - F_{FT} = 0$

Methane Balance:

$F_{CH_4} - P_{CH_4} + F_{FT} = 0$

Variables = 5 (F_{FT}, F_H, F_{CH_4}, P_B, P_{CH_4})

Equations = 3

Degrees of freedom = 5-3 = 2

Using selectivity to solve:

$S = \frac{P_B}{F_{FT}}$

$F_{FT} = \frac{P_B}{S}$

Benzene Balance:

$F_{FT} = P_B + 2P_D$

$\frac{P_B}{S} = P_B + 2P_D$

$P_D = P_B\left(\frac{1-S}{2S}\right) = 1.28 \times 10^6 \left(\frac{1-S}{2S}\right) \left[\frac{kmol}{yr}\right]$

Hydrogen Balance:

$F_H - F_{FT} = 0$

$$F_H - \frac{P_B}{S} = 0$$

$$F_H = \frac{1.28\times10^6}{S}\ [\frac{kmol}{yr}]$$

Methane Balance:

$$F_{CH_4} - P_{CH_4} + F_{FT} = 0$$

$$F_{CH_4} - P_{CH_4} + \frac{P_B}{S} = 0$$

Selectivity = $S = \frac{P_B}{F_{FT}} = 1$

We calculated the flow rates in this design based on the benzene mass and the mole balances we derived (See Appendix B.1 for balances); the calculated flow rates are shown in table B.1.

Table B.1. Flow rate values calculated from the mole balances in the selected level-2 design

Flow Rate	Mass Flow Rate × 10^6 (kg/s)	Molar Flow Rate × 10^4 (kmol/s)
P_B	3.17	146
F_{FT}	3.78	4.1
F_G	0.36	20.5
F_{H_2}	0.2	19.5
F_{CH_4}	0.16	1
P_{CH_4}	0.82	5.1

From the figure B.5, we found the maximum economic potential at $y_{PH} = 0.71$ *and* $y_{FH} = 0.7$.Then we calculated the values of P_G *and* P_H,where $P_G = 1.7 \times 10^5\ kmol/s$ *and* $P_H = 1.2 \times 10^5 kmol/s.$

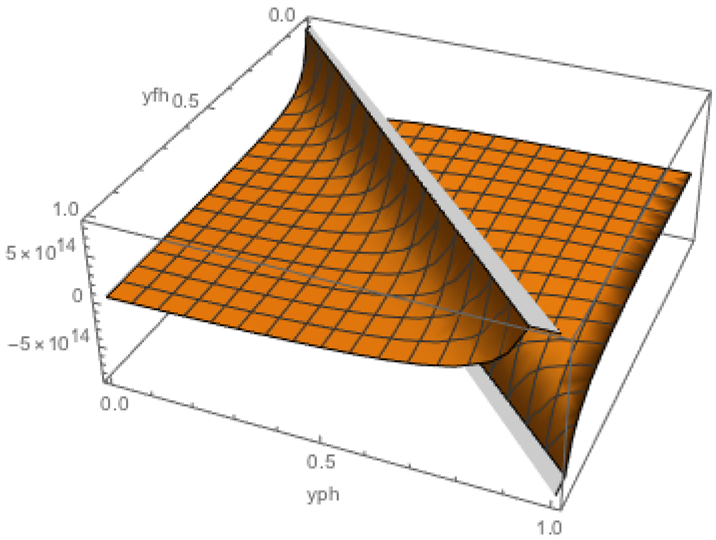


Fig B.5. Plot of the economic potential with respect to yph, yfh in the level-2 design system. yfh is the y axis, yph is the x axis, and economic potential is the z axis.

The several reasons that we selected this level-2 design are shown below:

1. To maximize the profits from the process, we will try to have a high selectivity. We will try to achieve high selectivity due to the economic potential being greater on an level two design basis:

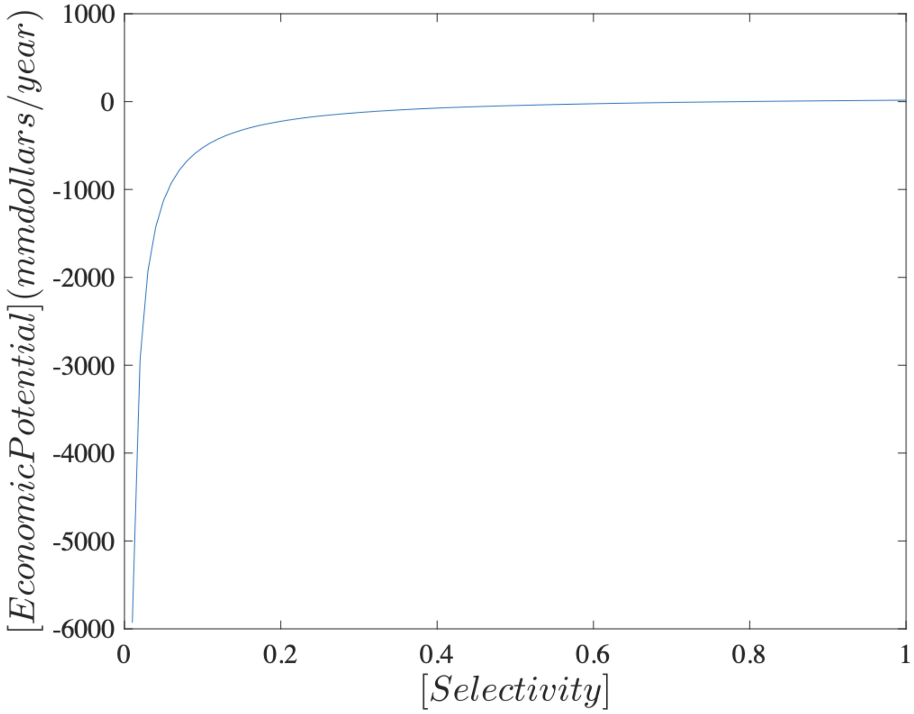


Fig B.6. The relationship between the economic potential and the process selectivity for the level two flowsheets. yph value equals to 0.95 and yfh value equals to 0.5.

C. Plant Design Basis

C.1 Level-2 Design

The considered Level-2 processes include 1 process plant. The HDA process in this case includes 2 feed streams: a mixed stream of 95 mol% hydrogen gas and 5 mol% methane gas, and a toluene gas stream. There are three separate product streams: a benzene product stream, a biphenyl by-product exit stream, and a purge gas stream containing methane and hydrogen. Moreover, some amount of the hydrogen gas will be recycled back to the process plant as an opposite way to the purge stream. We calculated the flow rates in this level-2 design based on the benzene mass and the mole balances we derived (See Appendix B.2 for balances).

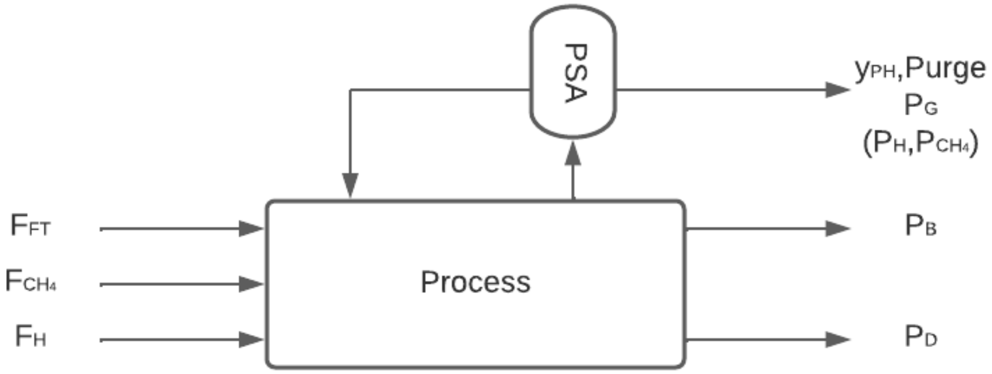


Fig. C.1. Flow diagram of a level-2 HDA process with a purge stream and a PSA system. F_{FT} is the toluene feed; F_H is the hydrogen gas feed (95 mol% H_2 and 5 mol% CH_4); P_G is the gas purge (P_{CH4} + P_H); P_D is the diphenyl outlet, and P_B is the benzene outlet. [1,2]

There were a few different considerations in the making of the final level 2 design. One of the decisions made in making the level 2 flow sheet was if a gas purge stream was going to exist. In making this decision we considered the following:

This reaction was designed to take place under laboratory conditions (see Appendix A for a statement of process chemistry) with a hydrogen to toluene ratio (MR) of 5 to 1. To limit the hydrogen costs and recycle most of the hydrogen, we considered a few options: the first is to purify the gas stream before it is used in the process. However, This is too cost prohibitive because the low temperatures in this separation process makes it not competitive in the cost considerations. Therefore, the separation of the gas stream would be done after the reaction takes place.

We found some advantages of this design process. First, the unreacted hydrogen that comes from the reactor is reentered back into the reactor. Second, it has a high adaptability, which comes from the selectivity of the process. Selectivity (s) is defined as the ratio of the toluene used in the process (F_{FT}) to benzene produced in the plant (P_B). Under the saturated nature of the use of the unreacted hydrogen, the amount will vary based on the selectivity of the reactor in the design. Based on our level 3 Douglas Design hierarchy, we chose an optimal selectivity. However, the selectivity can change based on different operating conditions.

We made the decision to add the PSA on the purge stream and not add to the inlet gas stream because based on the process thermodynamics. Due to the high thermodynamic load on the reactor, the extra methane acted as a heat carrier. Therefore, a limited amount of methane in the inlet gas stream was kept.

C.2 Level-3 Design

We used level-3 processes to evaluate the applicability of an PSA separator and the selection of the final process decisions by applying the MATLAB conceptual design and the Aspen Hysys simulations. The MATLAB conceptual design was conducted first, and the simplified level 3 process diagram is shown in Fig. C.2 (See more considered design choices and mole balances in Appendix D).

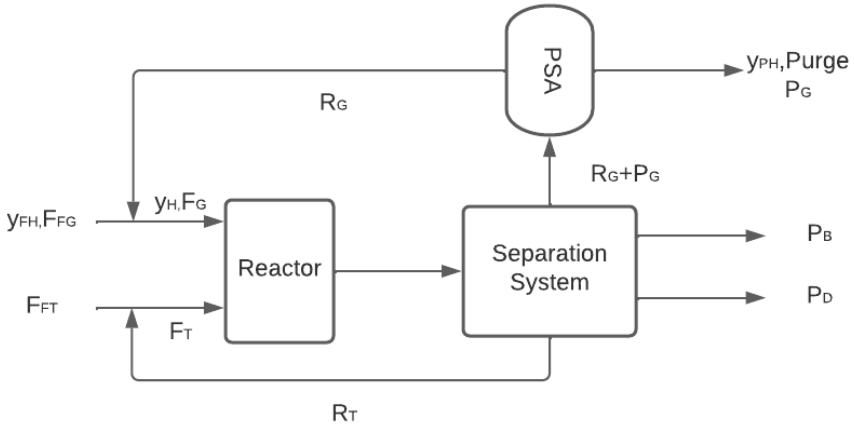


Fig C.2. Flow diagram of a level-3 MATLAB HDA process with a purge stream, a PSA system, and a recycle toluene stream. F_{FT} is the toluene feed; F_H is the hydrogen gas feed, and F_{CH4} is the methane gas feed (95% H_2 and 5% CH_4 in the feed); R_G is the gas recycle stream back to the reactor; P_G is the gas purge ($P_H + P_{CH4}$), and P_B is the benzene outlet.

Using the process diagram as a guide, we first solved the mole balances of Fig. C.2 using selectivity (amount of benzene produced leaving the reactor divided by the amount of toluene reacted in the reactor) and reactor conversion the amount of toluene reacted in the reactor divided by the amount of toluene fed into the reactor) as variables (more details in Appendix D.2). These mole balances were then used to specify the initial conditions for the reactor calculations. Then, the set of PFR design equations for all chemical species (more details in Appendix D.4) were solved at a specific temperature and pressure. To do this, MATLAB's ode45 function was used. In this numerical solving of the PFR design equations, an initial condition using the reaction mole balances was used as the basis. The solution of this numerical solving technique gave a range of species reaction concentration conditions for different volumetric sections of the reactor. Using these reactor calculations, we were able to determine the outlet flow rates in terms of our key design variables selectivity and conversion, which are correlated with the reactor size, temperature, and pressure. The comparison of these key design variables was the criteria we used in this report.

For the Level 3 design decisions, our final design has one PFR reactor. In this process we selected a PFR reactor because both reactions (R1 and R2) occurred simultaneously in gas phases. Under these circumstances, the PFR design equations (see Appendix D.4) were used to model volume as a function of selectivity or conversion. Also, we applied two recycle streams for toluene and hydrogen in this system. We decided that the reactor should be operated adiabatically with a heat carrier. The external heat carrier was used to cool the reactor when the temperature increased during the purification of recycle streams.

The optimized PFR reactor was designed under 3 criteria: selectivity, conversion, and reactor volume. We used MATLAB software to solve the PFR design equations at different reactor temperatures and pressures, and it was applied under the reaction constraints (see appendix A). From Fig. C.3, we can see that a high conversion cannot be reached if there is no significant increase in the reactor volume under the temperature lower than 600°C. We selected the reactor temperature of 627°C because it gave us the largest conversion with lowest reactor volume change. Also, we found that the reactor pressure did not affect the relationship between reactor volume and conversion a lot, but higher pressure resulted in a higher conversion with less reactor volume change. As a result, we chose the reactor pressure of 34 bar.

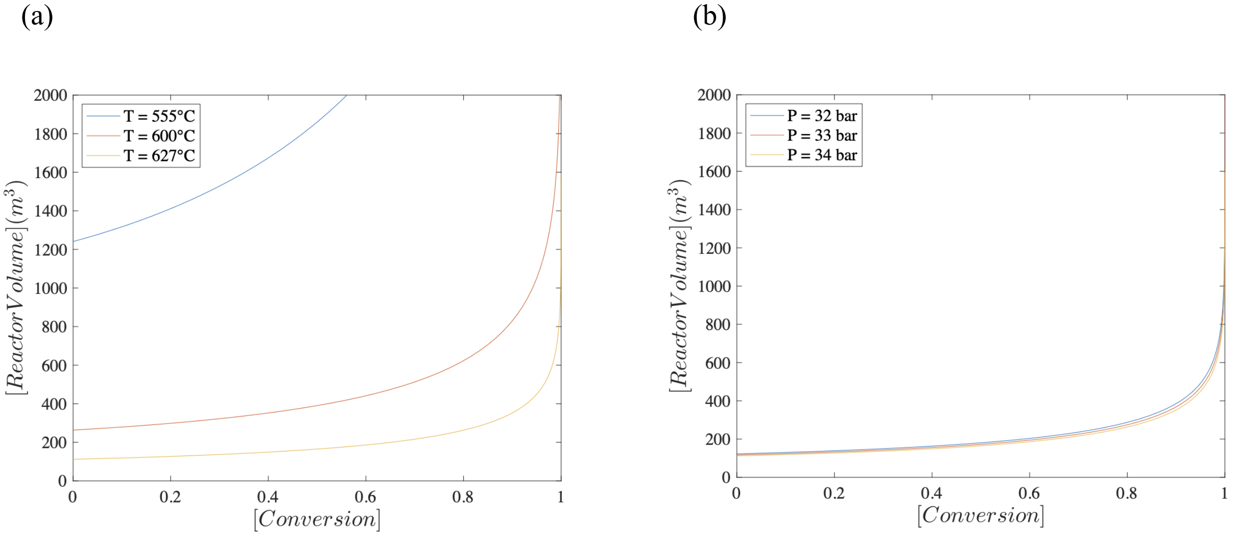


Fig C.3. The relationship between reactor volume and conversion at 3 different (a) temperatures and (b) pressures in level 3 balances. Reactor volume increases as conversion decreases.

From Fig C.3., we found that selectivity decreased from 1 to 0.81 as the conversion increased in different reactor temperatures and pressures. We can see that a larger temperature can sustain a higher selectivity for a given conversion. These results are consistent with the fact that reaction R1 has a higher activation energy than R2's forward reaction. Therefore, as the temperature increases, the ratio of the rate of R1 to the rate R2 increases exponentially. This was also a reason why we chose to operate our reactor at 627°C. However, the higher temperature leads to increased utility costs and safety risk. To examine these factors, we also examined the conversion's relationship with our economic and safety considerations.

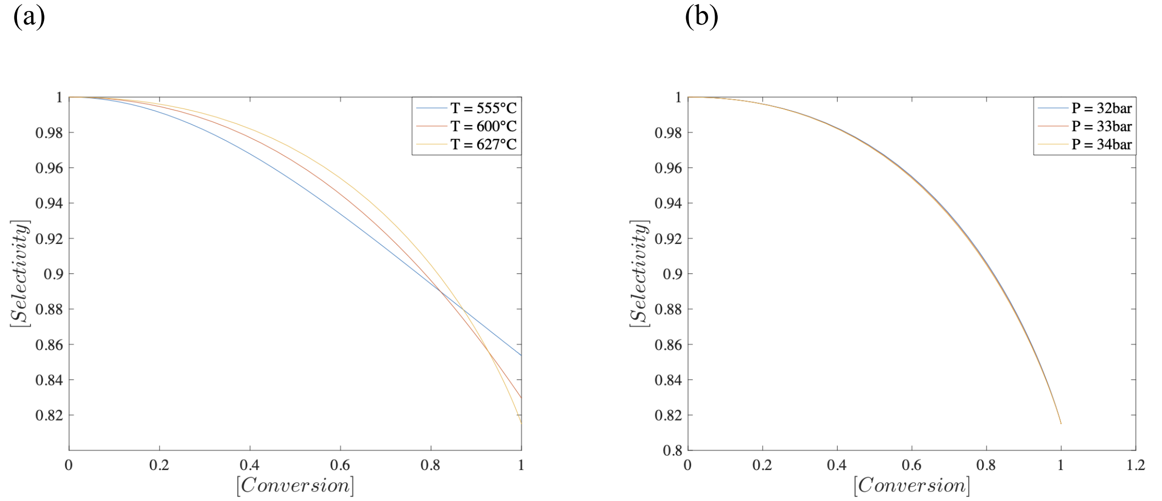


Fig C.4. The relationship between selectivity and conversion at 3 different (a) temperatures and (b) pressures in level 3 balances. Selectivity decreases as conversion increases.

After HYSYS was set up, the process type and the conversion were determined based on the Net Present Values from the economic section. We first briefly drew the trend of NPV change over conversion, finding the maximum NPV we can achieve and did the subsequent calculations and analysis based on the corresponding conversion at that NPV as we believe that will be the best profitability we can make. The Net Present Value (NPV) is a method used to determine the current value of all future cash flows generated by a project, including the initial capital investment. We picked conversions of 0.63, 0.72, 0.82, and 0.86 and plugged them in both conceptual designs to calculate the NPV. We found that the design with the PSA system and a conversion of 0.82 provided the best Net Present Value of -$0.98 million (see more detailed conversion calculated values in Appendix E). Then we ran the HYSYS simulation based on this conversion by adjusting the reactor volume and inputting the MATLAB design fresh feed values to compare the values in both conceptual designs. The results showed that the HYSYS simulation converges with the MATLAB conceptual design, with an average deviation in the flow rates of 1% and the deviation of reactor volume of 77% (see more detailed comparison values in Appendix E tables).

Table C.1. Hysys conceptual design stream flows with PSA system

Stream	Flow Rates (kg/hr)	Flow Rates $\times 10^5$(MT/yr)	Energy Flows (MW)	T (°C)	P (kPa)
FFT0	15000	1.3	0.59	25	101.3
FFG0	681	0.06	0.5	25	101.3
FFT1	15000	1.3	0.61	26	3401
FFG1	681	0.06	0.36	327	3400
FFT	15000	1.3	7.3	627	3400
FFG	681	0.06	1	627	3400
Mixout	20210	1.8	0	623.2	3400
Reactout	20210	1.8	10	595.6	3200
Cooledreactout	20210	1.8	4.5	295.6	3200
FHC	4231	0.4	-2.6	170	2800
FBT	15980	1.4	3.6	170	2800
PG	2952	0.2	-3.3	170	2800
PB	12700	1.1	5.6	360	2800
RT	3276	0.3	0.38	170	2800

RG1	1279	0.1	0.73	170	2800
RT1	3260	0.3	0.38	170	2800
RG2	1269	0.1	0.73	170	2800
RT2	3260	0.3	0.38	170.4	3400
RG3	1269	0.1	2.8	570	2800
RT3	3260	0.3	1.6	627	3400
RG4	1269	0.1	3.1	629.6	3400

Table C.2. Hysys conceptual design equipment parameter values with PSA system

Equipment	Size	Installed Cost ($)
PFR Reactor	420 m3	$1,120,000
Cooler	985 m3	$927,040
Compressor-1	0.33 MW	$2,013,200
Compressor-2	0.86 MW	$2,105,300
Pump-1	0.02 MW	$100,400
Pump-2	0.001 MW	$37,500
Furnace-1	6.7 MW	$831,970
Furnace-2	0.65 MW	$174,800
Furnace-3	2.1 MW	$337,610
Furnace-4	1.2 MW	$213,890
Total ISBL		$ 7.9 MM

Table C.1 reports all of the streams associated with the final HYSYS conceptual design with the PSA system at conversion of 0.82. Table C.2 demonstrates the results of parameters used in each equipment in the final Hysys conceptual design with the PSA system.

D. Level 3 Design Balances

D.1 Without PSA:

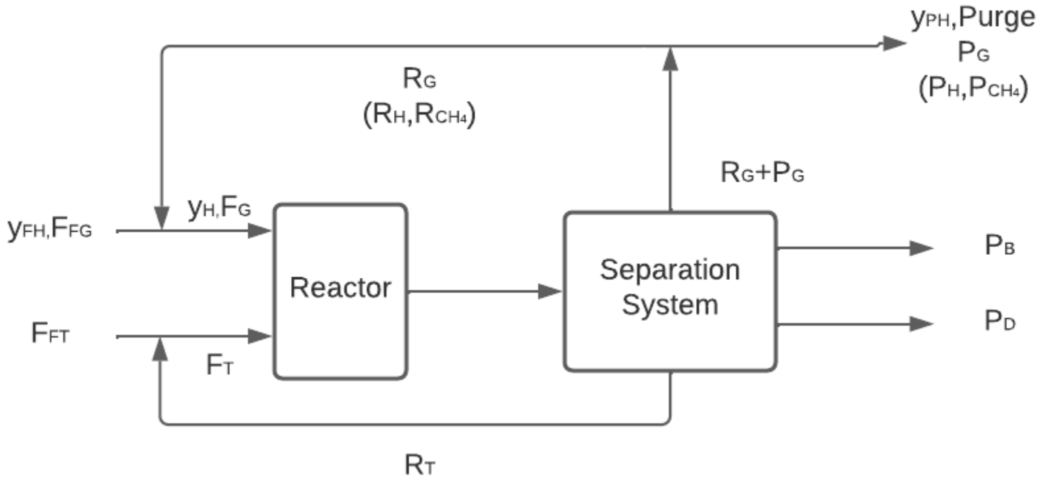


Fig D.1. Flow diagram of a level-3 HDA process with a purge stream and a toluene recycle stream. F_{FT}, F_{FG} (95% H_2 + 5% CH_4) are the fresh toluene and gas feed; R_G ,R_T are the recycle stream back to the reactor; F_G , F_T are the feeds to the reactor (fresh feed+recycle stream); P_G is the gas purge ($P_H + P_{CH4}$); y_{FH}, y_{PH} , y_H are the mol fraction of hydrogen in F_G and P_G and F_T; and P_B , P_D are the benzene and diphenyl outlet.

Reactor design considerations:

Selectivity: $S = \frac{P_B}{F_{FT}}$

There are several assumptions for this gas phase reactor design:

1. Constant mass density of process stream
2. No volume of mixing

Overall mole balances on the whole system for each component:

Benzene Balance:

$- P_B + \xi_1 - 2\xi_2 = 0 (13)$

$\xi_2 = \frac{1}{2} \times (F_{FT} - P_B) (14)$

We define purge composition of $H_2\ as\ y_{PH}$

Hydrogen Balance:

$F_{FG} \times y_{FH} - P_G \times y_{PH} - \xi_1 + \xi_2 = 0\ (15)$

Toluene Balance:

$F_{FT} - \xi_1 = 0$ (16)

Methane Balance:

$F_{FG} \times (1 - y_{FH}) - P_G \times (1 - y_{PH}) + \xi_1 = 0$ (17)

Reference components are selected to be toluene and benzene. The balances on the non-reference components are shown below:

Hydrogen Balance:

$F_{FG} \times y_{FH} - P_G \times y_{PH} - F_{FT} + \frac{1}{2} \times (F_{FT} - P_B) = 0$ (18)

Methane Balance:

$F_{FG} \times (1 - y_{FH}) - P_G \times (1 - y_{PH}) + F_{FT} = 0$ (19)

Variables = 7 (F_{FT}, F_{FG}, P_B, y_{FH}, P_D, P_G, y_{PH})

Equations = 4

Degrees of freedom = 7-4 = 3

Recycle Balances:

Toluene Recycle Balances:

The feed toluene balance is shown below:

$F_{FT} + R_T = F_T$

We defined the conversion x as the conversion of toluene over the reactor:

$x = \frac{F_T - R_T}{F_T}$

As a result, R_T can be expressed as:

$R_T = F_T \times (1 - x)$

Then the feed toluene balance can be expressed as:

$F_{FT} + F_T \times (1 - x) = F_T$

Since F_{FT} can be expressed in terms of P_B and s, R_T can be shown as:

$F_T = \frac{F_{FT}}{x} = \frac{P_B}{x \times s}$

$R_T = \frac{P_B \times (1 - x)}{x \times s}$

Hydrogen Recycle Balances:

The ratio of feed hydrogen to toluene (MR) in this process is 5:1. The balances are shown below:

$F_G \times y_H = MR \times F_T$, where $F_G = F_{FG} + R_G$ (20)

Then we get the hydrogen balance below:

$F_{FG} \times y_{FH} + R_G \times y_{PH} = MR \times F_T$ (21)

Afterwards, we calculate the flow rate of the purge stream back to the reactor (R_G) using the molar ratio of hydrogen to benzene (MR) and the feed toluene balance:

$R_G = \frac{1}{y_{PH}}\left(\frac{MR \times P_B}{x \times s} - F_{FG} \times y_{FH}\right)$ (22)

As a result, F_G can be expressed as:

$$F_G = F_{FG} + \frac{1}{y_{PH}}\left(\frac{MR \times P_B}{x \times s} - F_{FG} \times y_{FH}\right)$$

D.2 With PSA:

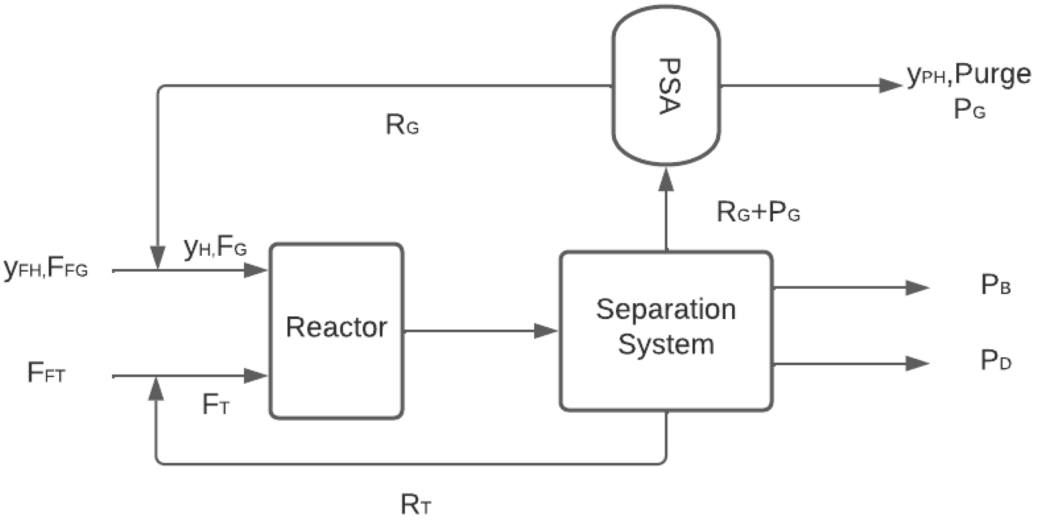


Fig D.2. Flow diagram of a level-3 HDA process with a purge stream, a PSA system, and a recycle toluene stream. F_{FT} is the toluene feed; F_H is the hydrogen gas feed, and F_{CH4} is the methane gas feed (95% H_2 and 5% CH_4 in the feed); R_G is the gas purge stream back to the reactor; P_G is the gas purge ($P_H + P_{CH4}$), and P_B is the benzene outlet.

Overall mole balances on the whole system for each component:
Benzene Balance:
$- P_B + \xi_1 - 2\xi_2 = 0$(13)
$\xi_2 = \frac{1}{2} \times (F_{FT} - P_B)$(14)

We define purge composition of H_2 as y_{PH}

Hydrogen Balance:
$F_{FG} \times y_{FH} - P_G \times y_{PH} - \xi_1 + \xi_2 = 0$ (15)

Toluene Balance:
$F_{FT} - \xi_1 = 0$ (16)

Methane Balance:
$F_{FG} \times (1 - y_{FH}) - P_G \times (1 - y_{PH}) + \xi_1 = 0$ (17)

Reference components are selected to be toluene and benzene. The balances on the non-reference components are shown below:

Hydrogen Balance:
$F_{FG} \times y_{FH} - P_G \times y_{PH} - F_{FT} + \frac{1}{2} \times (F_{FT} - P_B) = 0$ (18)

Methane Balance:
$F_{FG} \times (1 - y_{FH}) - P_G \times (1 - y_{PH}) + F_{FT} = 0$ (19)

Variables = 7 (F_{FT}, F_{FG}, P_B, y_{FH}, P_D, P_G, y_{PH})
Equations = 4
Degrees of freedom = 7-4 = 3

Recycle Balances:
Toluene Recycle Balances:
The feed toluene balance is shown below:
$F_{FT} + R_T = F_T$
We defined the conversion x as the conversion of toluene over the reactor:

$x = \frac{F_T - R_T}{F_T}$

As a result, R_T can be expressed as:

$R_T = F_T \times (1 - x)$

Then the feed toluene balance can be expressed as:

$F_{FT} + F_T \times (1 - x) = F_T$

Since F_{FT} can be expressed in terms of P_B $and\ s$,R_T can be shown as:

$F_T = \frac{F_{FT}}{x} = \frac{P_B}{x \times s}$

$R_T = \frac{P_B \times (1-x)}{x \times s}$

With the PSA system, 90% of the feed hydrogen to the PSA was recovered. As a result, the off-gas of PSA contains 10% of the entering hydrogen and all of the entering methane gas.

$F_{FH} - P_G y_{PH} + P_B\left(\frac{1-s}{2s}\right) = 0$

$\frac{F_{FH} + P_B\left(\frac{1-s}{2s}\right)}{y_{PH}} = P_G$

$R_G = 9 P_G y_{PH}$

As a result, F_G can be expressed as:

$F_G = F_{FG} + R_G$

D.3 Reactor Design Balance Equations:

Toluene Balance:

$qC_{T0} - qC_T + Vr_1 = 0$

Benzene Balance:

$- qC_B - Vr_1 + Vr_2 = 0$

Hydrogen Balance:

$qC_{H_2 0} - qC_{H_2} - Vr_1 + Vr_2 = 0$

$qP_{tot} = F_{tot} RT$

$$C_i = \frac{F_i}{q}$$

$$C_i = \frac{F_i P_{tot}}{F_{tot} RT}$$

$$y_i = \frac{F_i}{F_{tot}}$$

$$\frac{dF_T}{dV} = -r_1$$

$$\frac{dF_H}{dV} = -r_1 + r_2$$

$$\frac{dF_B}{dV} = r_1 - 2r_2$$

$$\frac{dF_{CH_4}}{dV} = r_1$$

$$\frac{dF_D}{dV} = r_2$$

$$\frac{dF_{tot}}{dV} = 0$$

D.4. Level 3 Stream Mass Flow Rate and Composition without PSA Figures

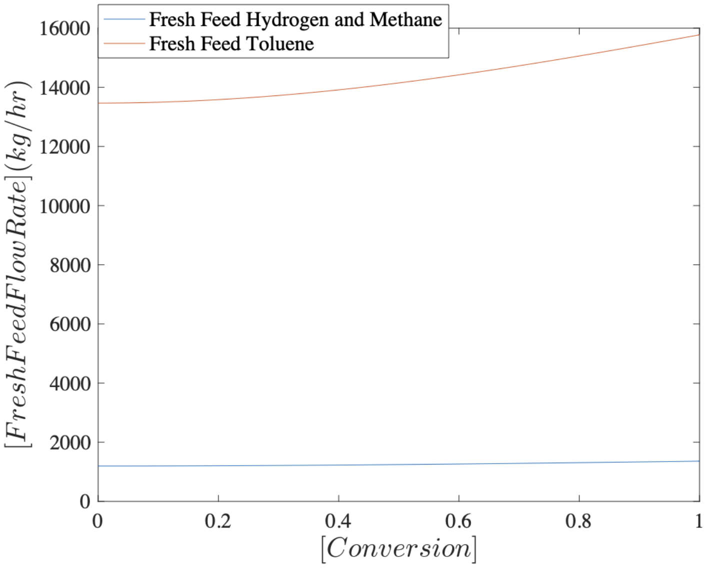


Fig D.3. The relationship between fresh feed mass flow rates and conversion in level 3 design without a PSA system.

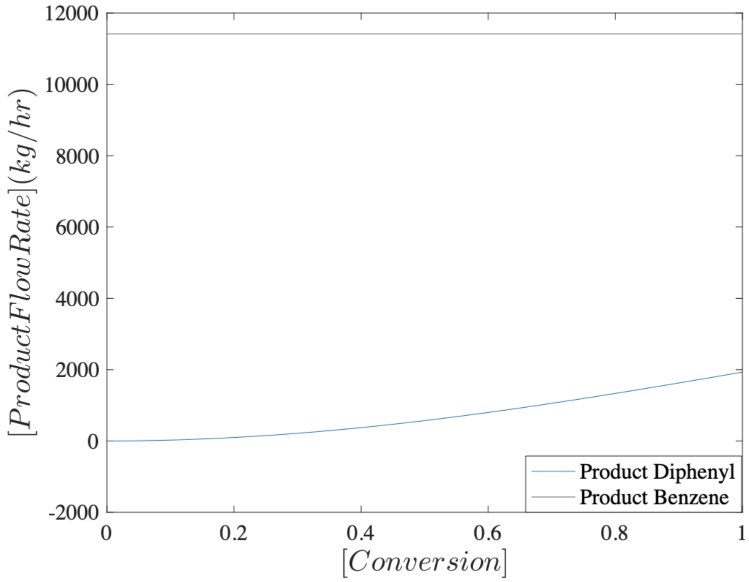


Fig D.4. The relationship between product mass flow rate and conversion in level 3 design without a PSA system.

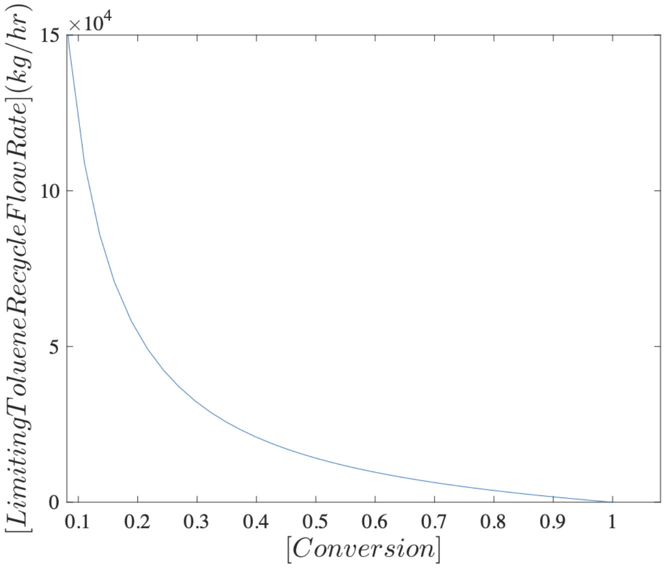


Fig D.5. The relationship between toluene recycle mass flow rate and conversion in level 3 design without a PSA system.

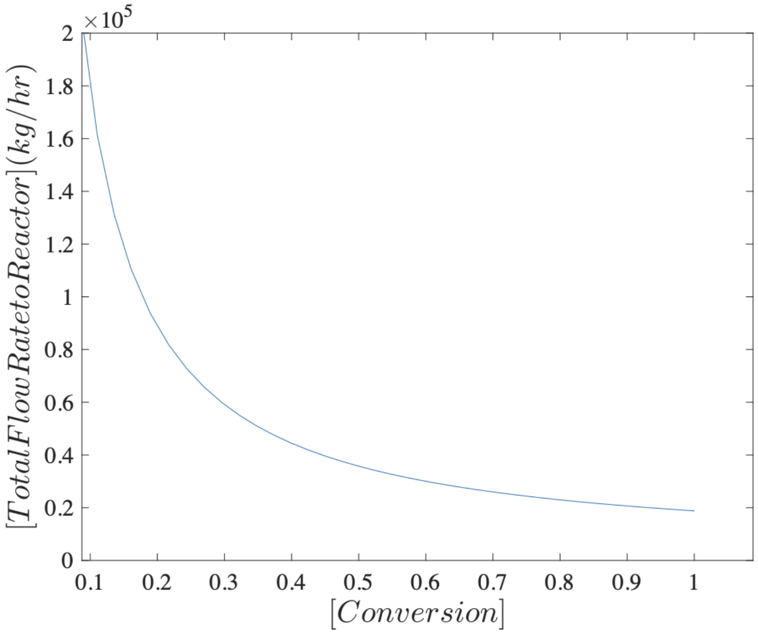


Fig D.6. The relationship between total mass flow rate into the reactor and conversion in level 3 design without a PSA system.

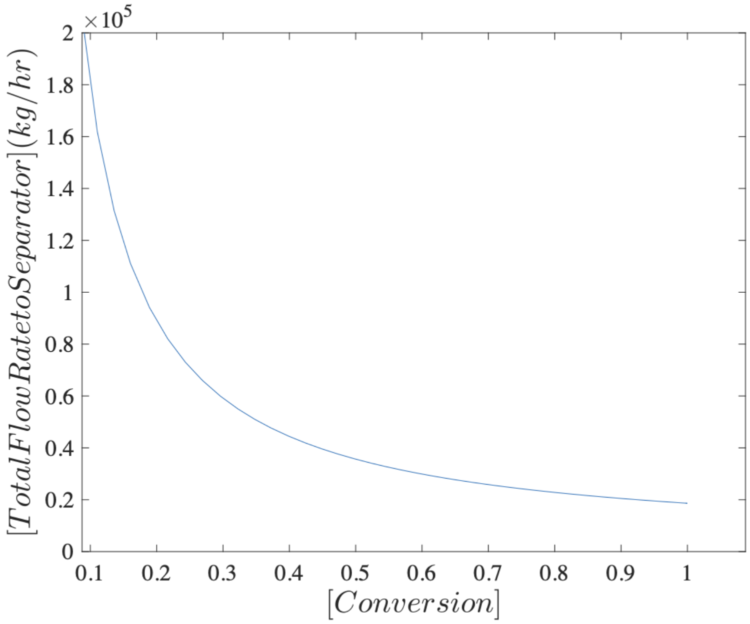


Fig D.7. The relationship between total mass flow rate into the separator and conversion in level 3 design without a PSA system.

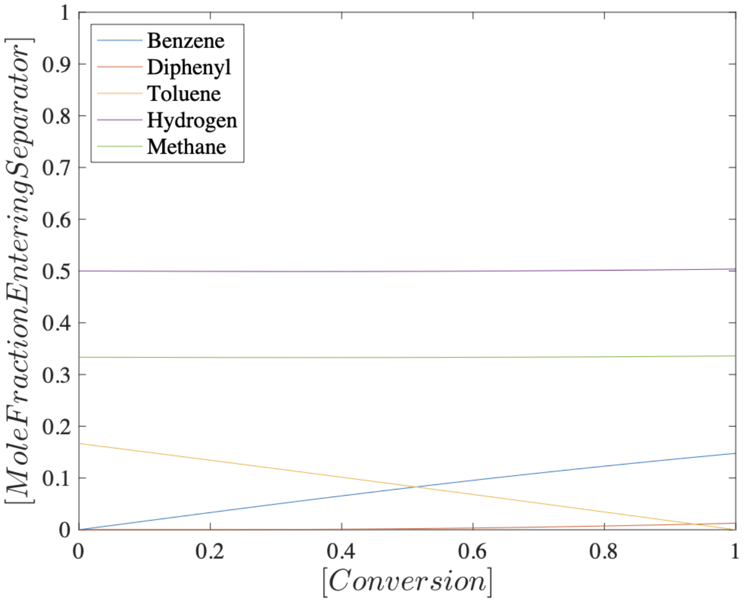


Fig D.8. The relationship between different component mole fractions into the separator and conversion in level 3 design without a PSA system.

E. Level 3 Stream Mass Flow Rate and Composition with PSA Figures

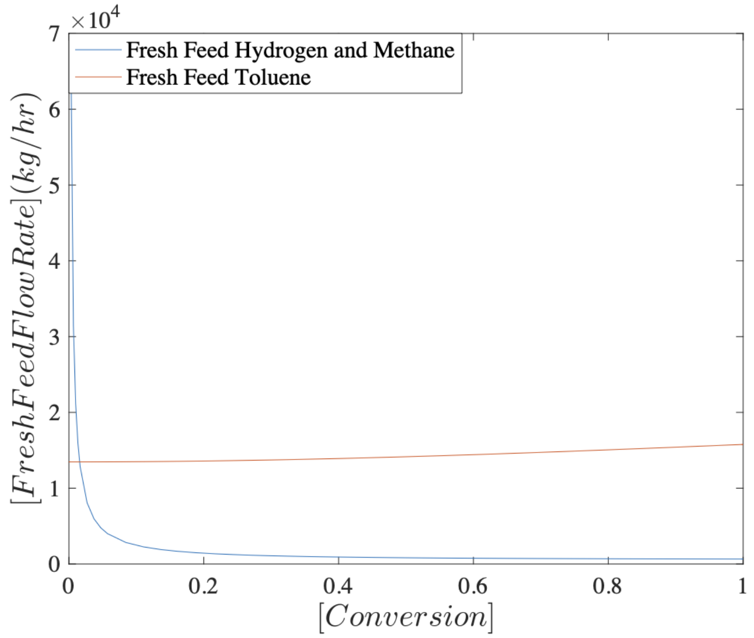


Fig E.1. The relationship between fresh feed mass flow rates and conversion in level 3 design with a PSA system.

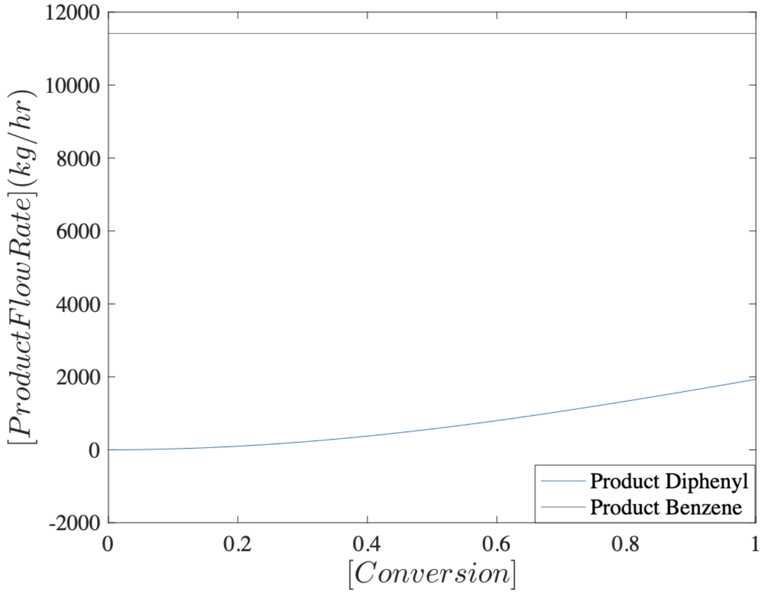


Fig E.2. The relationship between product mass flow rates and conversion in level 3 design with a PSA system.

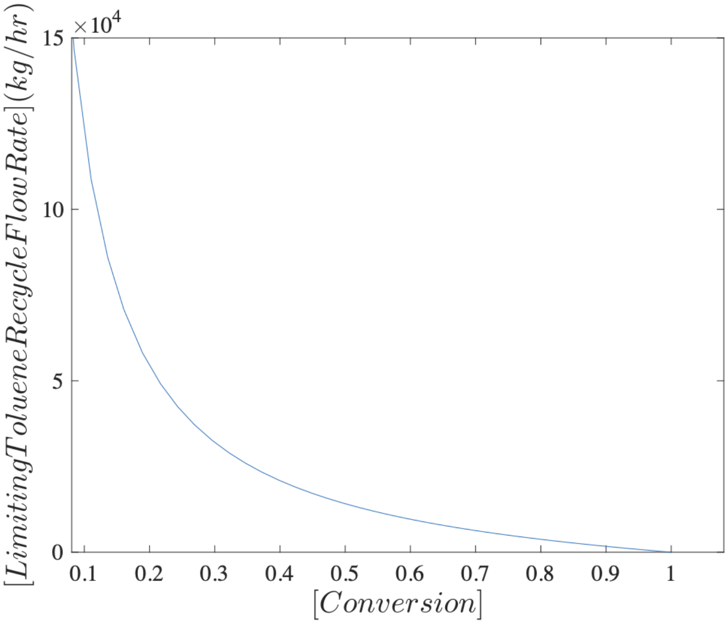


Fig E.3. The relationship between toluene recycle mass flow rate and conversion in level 3 design with a PSA system.

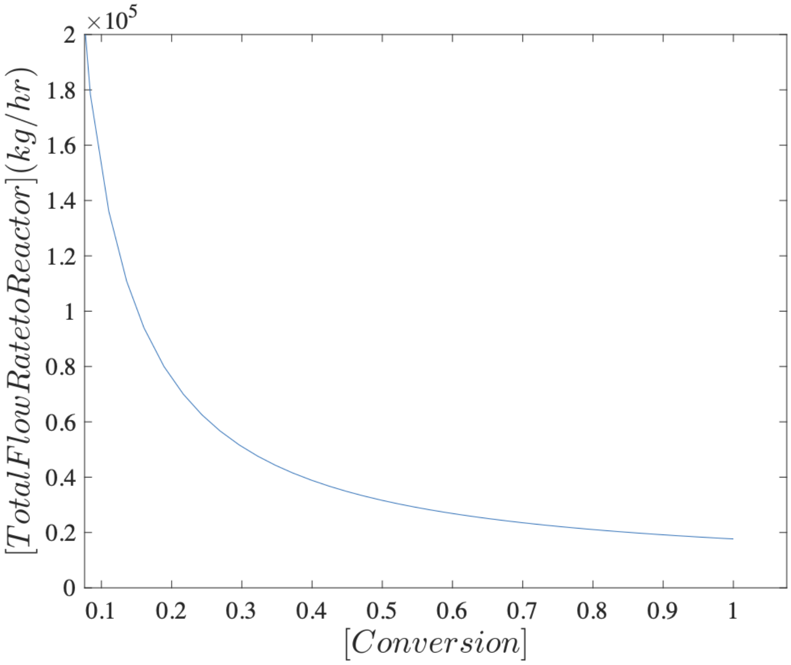


Fig E.4. The relationship between total mass flow rate into the reactor and conversion in level 3 design with a PSA system.

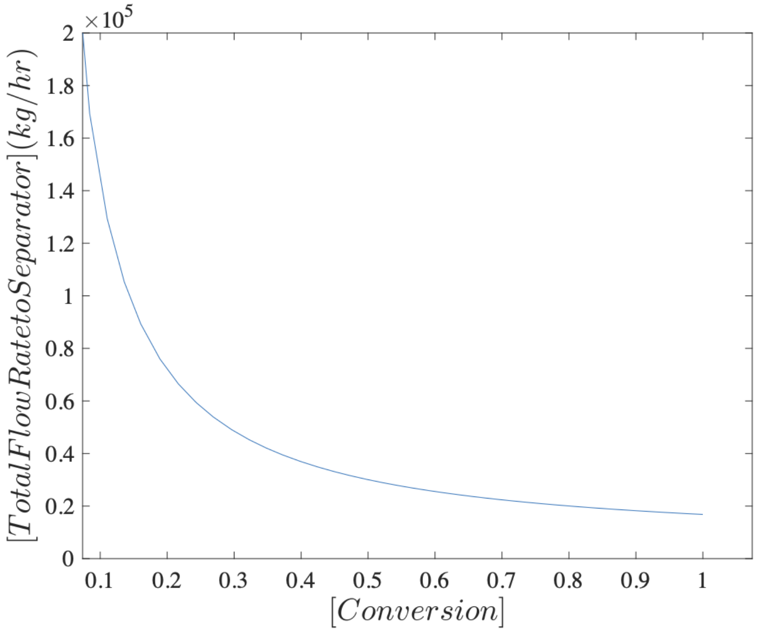


Fig E.5. The relationship between total mass flow rate into the separator and conversion in level 3 design with a PSA system.

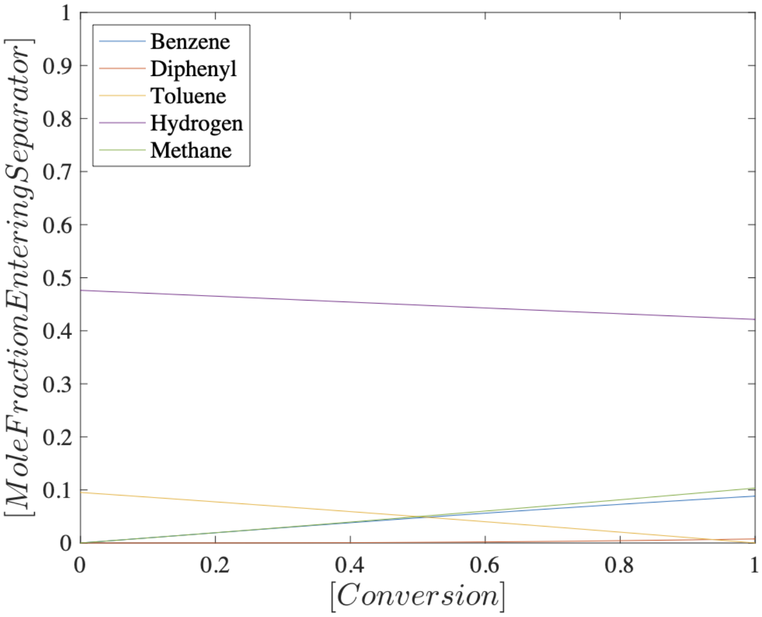


Fig E.6. The relationship between different component mole fractions into the separator and conversion in level 3 design with a PSA system.

Table E.1. Mass flow rate values from MATLAB conceptual design with PSA

	$x = 0.72$		$x = 0.82$		$x = 0.86$	
Mass Flow Rate	Mass Flow Rate $\times 10^4$ (kg/hr)	Mass Flow Rate $\times 10^4$ (MT/yr)	Mass Flow Rate $\times 10^4$ (kg/hr)	Mass Flow Rate $\times 10^4$ (MT/yr)	Mass Flow Rate $\times 10^4$ (kg/hr)	Mass Flow Rate $\times 10^4$ (MT/yr)
F_{FT}	1.45	12.70	1.50	13.14	1.52	13.32
F_{FG}	0.070	0.61	0.068	0.60	0.067	0.59
R_G	0.49	4.29	0.49	4.29	0.49	4.28
R_T	0.56	4.91	0.32	2.8	0.25	2.19
F_G	0.30	2.63	0.27	2.37	0.26	2.28
F_T	2.01	17.61	1.82	15.94	1.77	15.51
P_G	0.27	2.37	0.28	2.45	0.28	2.45
P_B	1.14	9.99	1.14	9.99	1.14	9.99
P_D	0.085	0.74	0.13	1.14	0.15	1.314

Table E.2 Comparisons between MATLAB conceptual design and HYSYS simulation in different design variables

At conversion$x = 0.82$

Variables	MATLAB		HYSYS	
	Without PSA	With PSA	Without PSA	With PSA
F_{FG} (kg/hr)	1305	677	1313	681
P_G (kg/hr)	3277	2772	3595	2952
P_B (kg/hr)	11415	11415	12720	12700
$Reactor\ Volume$ (m^3)	204	204	1020	870

At conversion$x = 0.72$

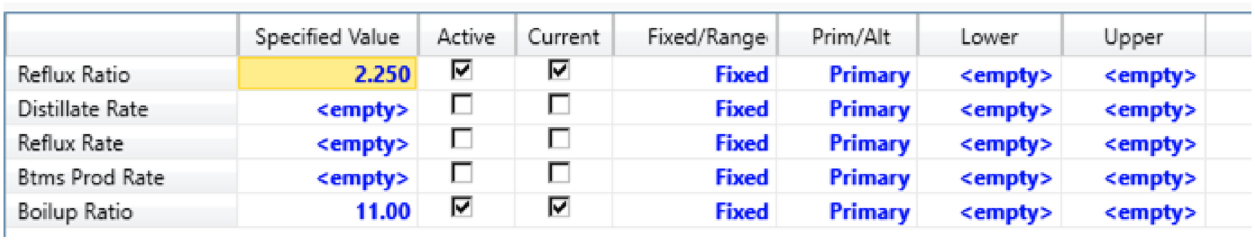
Variables	MATLAB		HYSYS	
	Without PSA	With PSA	Without PSA	With PSA
F_{FG} (kg/hr)	1268	698	1276	702
P_G (kg/hr)	3164	2702	3488	2910
P_B (kg/hr)	11415	11415	12300	12300

$Reactor\ Volume$ (m^3)	151	151	770	710

At conversion $x = 0.63$

	MATLAB		HYSYS	
Variables	Without PSA	With PSA	Without PSA	With PSA
F_{FG} (kg/hr)	1248	732	1256	737
P_G (kg/hr)	3103	2680	3428	2889
P_B (kg/hr)	11415	11415	12080	11980
$Reactor\ Volume$ (m^3)	115	115	620	620

F. Separation System Data Tables

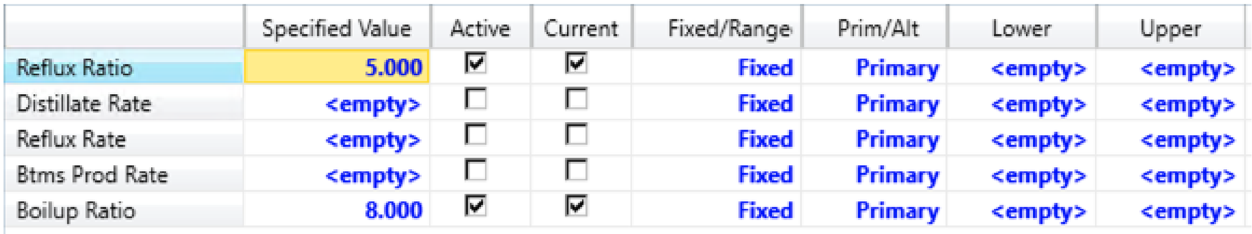


	Specified Value	Active	Current	Fixed/Range	Prim/Alt	Lower	Upper
Reflux Ratio	2.250	☑	☑	Fixed	Primary	<empty>	<empty>
Distillate Rate	<empty>	☐	☐	Fixed	Primary	<empty>	<empty>
Reflux Rate	<empty>	☐	☐	Fixed	Primary	<empty>	<empty>
Btms Prod Rate	<empty>	☐	☐	Fixed	Primary	<empty>	<empty>
Boilup Ratio	11.00	☑	☑	Fixed	Primary	<empty>	<empty>

Fig F.1. Hysys with PSA distillation column 1 specified values

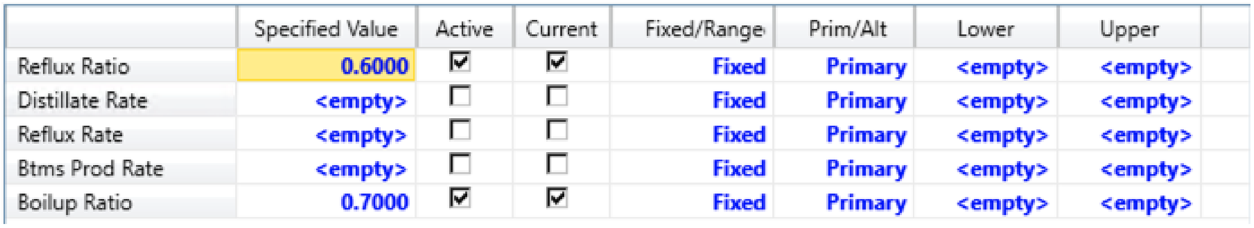
	Specified Value	Active	Current	Fixed/Range	Prim/Alt	Lower	Upper
Reflux Ratio	0.6000	☑	☑	Fixed	Primary	<empty>	<empty>
Distillate Rate	<empty>	☐	☐	Fixed	Primary	<empty>	<empty>
Reflux Rate	<empty>	☐	☐	Fixed	Primary	<empty>	<empty>
Btms Prod Rate	<empty>	☐	☐	Fixed	Primary	<empty>	<empty>
Boilup Ratio	1.000	☑	☑	Fixed	Primary	<empty>	<empty>

Fig F.2. Hysys with PSA distillation column 2 specified values



	Specified Value	Active	Current	Fixed/Range	Prim/Alt	Lower	Upper
Reflux Ratio	5.000	☑	☑	Fixed	Primary	<empty>	<empty>
Distillate Rate	<empty>	☐	☐	Fixed	Primary	<empty>	<empty>
Reflux Rate	<empty>	☐	☐	Fixed	Primary	<empty>	<empty>
Btms Prod Rate	<empty>	☐	☐	Fixed	Primary	<empty>	<empty>
Boilup Ratio	8.000	☑	☑	Fixed	Primary	<empty>	<empty>

Fig F.3. Hysys without PSA distillation column 1 specified values



	Specified Value	Active	Current	Fixed/Range	Prim/Alt	Lower	Upper
Reflux Ratio	0.6000	☑	☑	Fixed	Primary	<empty>	<empty>
Distillate Rate	<empty>	☐	☐	Fixed	Primary	<empty>	<empty>
Reflux Rate	<empty>	☐	☐	Fixed	Primary	<empty>	<empty>
Btms Prod Rate	<empty>	☐	☐	Fixed	Primary	<empty>	<empty>
Boilup Ratio	0.7000	☑	☑	Fixed	Primary	<empty>	<empty>

Fig F.4. Hysys without PSA distillation column 2 specified values

G. Heating System and Tables

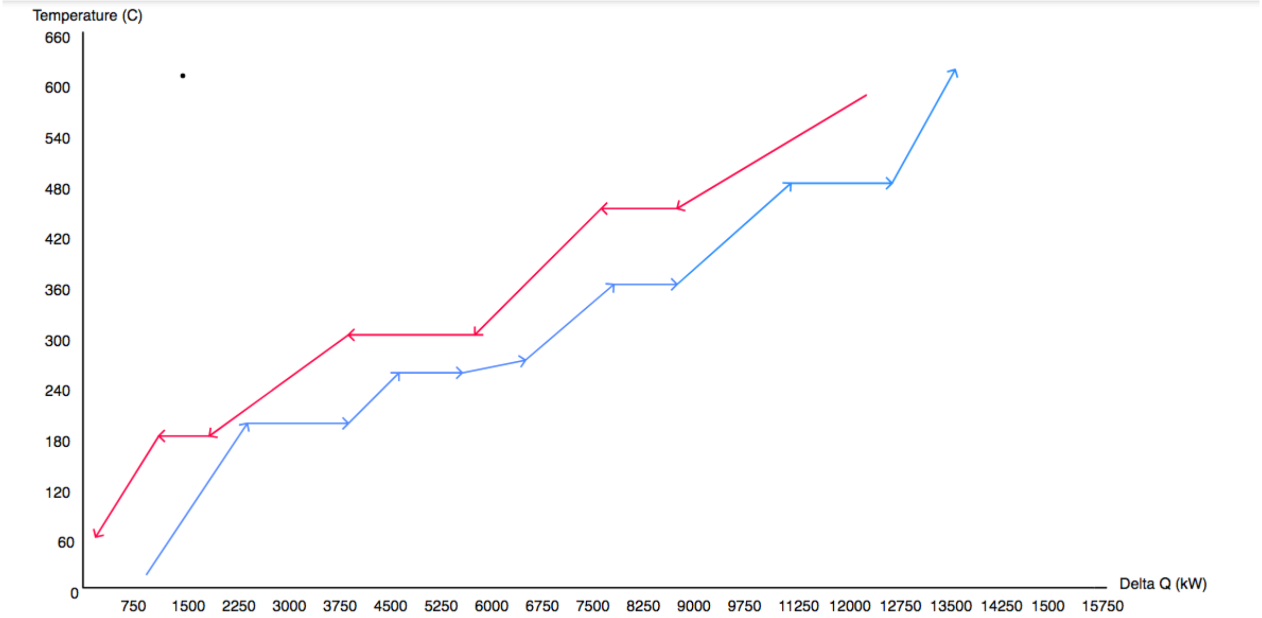


Fig G.1. Final heat integration plot. Red represents the cooling and blue represents the heating vectors. The vectors were calculated using the values of G.2. The total applicable trim area for this graph was measured as 12 MW.

Table G.2. Final heat system table with no trimming

Exchanger	**Start T (°C)**	**End T (°C)**	**CpF (kW/°C)**	**Phase Change**	**Q (kW) at Phase Change**	**Q1 (kW)**	**Q2(kW)**	**dQ (kW)**
Heater-1	26	627	4.7 - 11.2	Yes	1500	596	7387	6791
Heater-2	27	627	2.2	No	N/A	-256	1012	1269
Heater-3	121	627	0.67- 1.2	Yes	163	142	804	662
Heater-4	30	67	7.9	No	N/A	39	33	292
Heater-5	30	88	6.5	No	N/A	2166	2704.	538
Reboiler-1	266	268	5.2	Yes	904	6154	11802	4744
Reboiler-2	268	272	4.9	Yes	347	-62	817	532
Cooler-1	595.6	30	1.5 - 7.8	Yes	1919.5	11802	-1145	-12948
Cooler-2	226	26	4	No	N/A	269	1637	-1055
Condeser-1	226	226	4	Yes	1043	787	1830.98	-2855

Condeser-2	266	266	N/A	Yes	531	484	1015	-531

Table G.3. Typical properties for heating unit types and fluid types. Source: Dimian et all 2008 p 321 [13].

Heating Unit Type	**Hot Fluid**	**Cold Fluid**	**U** $[\frac{W}{m^{2}°C}]$
Shell and Tube Heat Exchangers	Water	Water	800 - 1500
	Organic solvents	Organic solvents	100 - 300
	Light oils	Light oils	100 - 400
	Heavy oils	Heavy oils	50 - 300
	Reduced crude	Flashed crude	35 - 150
Heaters	Steam	Water	1500 - 4000
	Steam	Organic solvents	500 - 1000
	Steam	Light oils	300 - 900
	Steam	Heavy oils	60 - 450
	Steam	Gases	30 - 300
	Heat Transfer (hot) Oil	Heavy oils	50 - 300
	Heat Transfer (hot) Oil	Gases	20 - 200

	Flue gases	Steam	30 - 100
	Flue gases	Hydrocarbon vapours	30 -100

H. Aspen HYSYS Conceptual Design Figures (including design graphs, initial specified data, and HYSYS simulation costs of our selected design)

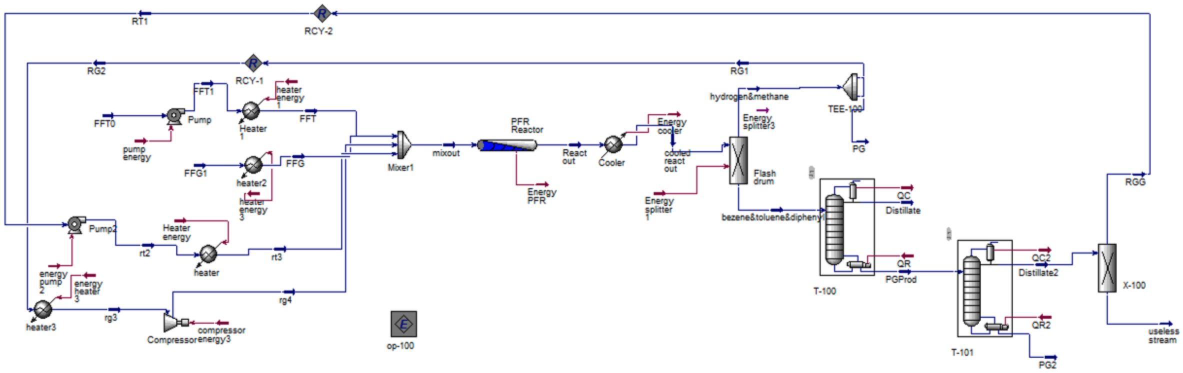


Fig H.1. Overview of Aspen Hysys conceptual design without PSA

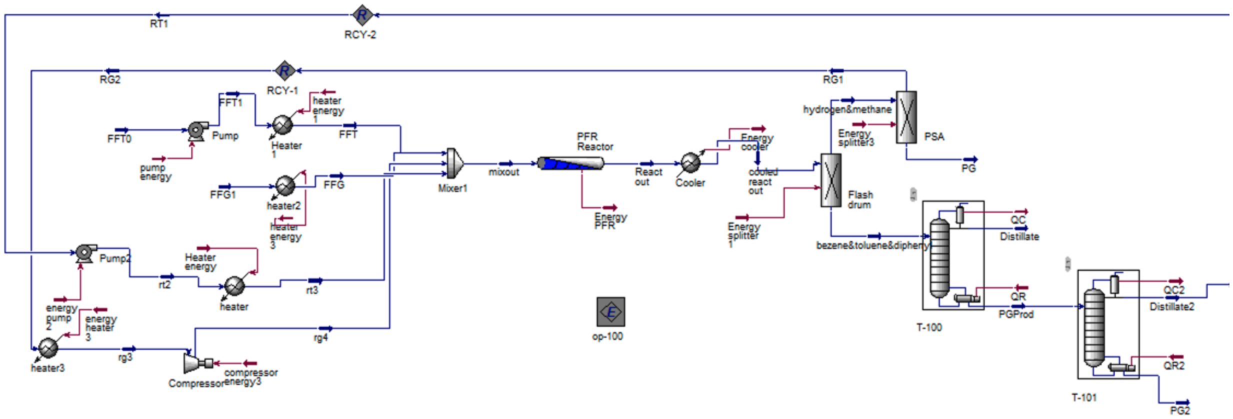
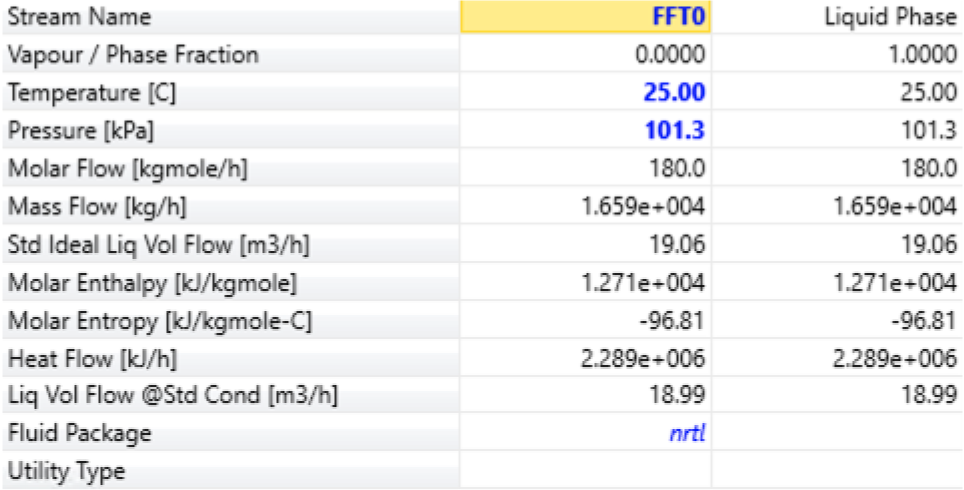
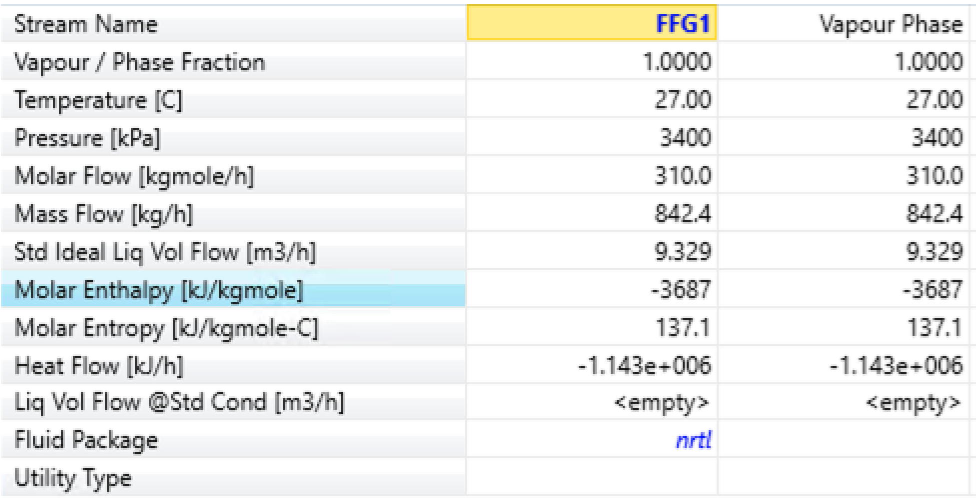


Fig H.2. Overview of Aspen Hysys conceptual design with PSA



Stream Name	FFT0	Liquid Phase
Vapour / Phase Fraction	0.0000	1.0000
Temperature [C]	25.00	25.00
Pressure [kPa]	101.3	101.3
Molar Flow [kgmole/h]	180.0	180.0
Mass Flow [kg/h]	1.659e+004	1.659e+004
Std Ideal Liq Vol Flow [m3/h]	19.06	19.06
Molar Enthalpy [kJ/kgmole]	1.271e+004	1.271e+004
Molar Entropy [kJ/kgmole-C]	-96.81	-96.81
Heat Flow [kJ/h]	2.289e+006	2.289e+006
Liq Vol Flow @Std Cond [m3/h]	18.99	18.99
Fluid Package	nrtl	
Utility Type		

Fig H.3. Initial specified inlet toluene flow rate of Aspen Hysys conceptual design with PSA

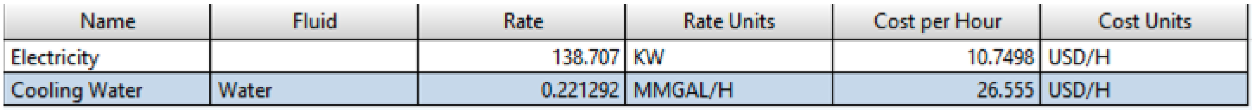


Stream Name	FFG1	Vapour Phase
Vapour / Phase Fraction	1.0000	1.0000
Temperature [C]	27.00	27.00
Pressure [kPa]	3400	3400
Molar Flow [kgmole/h]	310.0	310.0
Mass Flow [kg/h]	842.4	842.4
Std Ideal Liq Vol Flow [m3/h]	9.329	9.329
Molar Enthalpy [kJ/kgmole]	-3687	-3687
Molar Entropy [kJ/kgmole-C]	137.1	137.1
Heat Flow [kJ/h]	-1.143e+006	-1.143e+006
Liq Vol Flow @Std Cond [m3/h]	<empty>	<empty>
Fluid Package	nrtl	
Utility Type		

Fig H.4. Initial specified inlet mixed gas flow rate of Aspen Hysys conceptual design with PSA

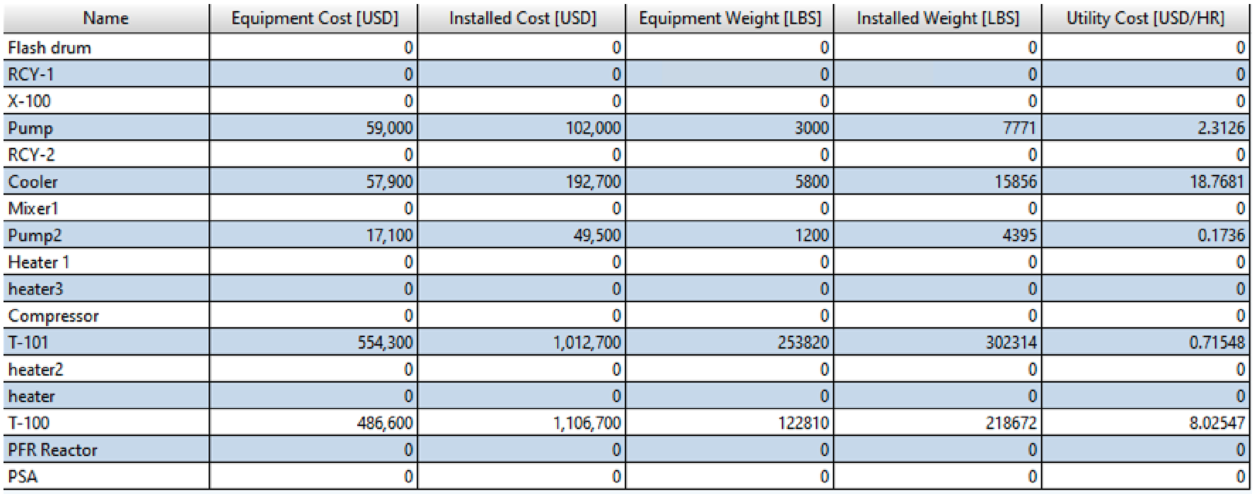
Total Capital Cost [USD]	5,688,030
Total Operating Cost [USD/Year]	1,766,880
Total Raw Materials Cost [USD/Year]	0
Total Product Sales [USD/Year]	0
Total Utilities Cost [USD/Year]	327,014
Desired Rate of Return [Percent/'Year]	20
P.O.Period [Year]	0
Equipment Cost [USD]	1,174,900
Total Installed Cost [USD]	2,463,600

Fig H.5. Total costs of Aspen Hysys conceptual design with PSA



Name	Fluid	Rate	Rate Units	Cost per Hour	Cost Units
Electricity		138.707	KW	10.7498	USD/H
Cooling Water	Water	0.221292	MMGAL/H	26.555	USD/H

Fig H.6. Utility costs of Aspen Hysys conceptual design with PSA



Name	Equipment Cost [USD]	Installed Cost [USD]	Equipment Weight [LBS]	Installed Weight [LBS]	Utility Cost [USD/HR]
Flash drum	0	0	0	0	0
RCY-1	0	0	0	0	0
X-100	0	0	0	0	0
Pump	59,000	102,000	3000	7771	2.3126
RCY-2	0	0	0	0	0
Cooler	57,900	192,700	5800	15856	18.7681
Mixer1	0	0	0	0	0
Pump2	17,100	49,500	1200	4395	0.1736
Heater 1	0	0	0	0	0
heater3	0	0	0	0	0
Compressor	0	0	0	0	0
T-101	554,300	1,012,700	253820	302314	0.71548
heater2	0	0	0	0	0
heater	0	0	0	0	0
T-100	486,600	1,106,700	122810	218672	8.02547
PFR Reactor	0	0	0	0	0
PSA	0	0	0	0	0

Fig H.7. Unit operation costs of Aspen Hysys conceptual design with PSA

I. Level 2 Economic Potential Equation

We defined the economic price of component i as E_i and the heat of combustion for component i as ΔH_i.

As a result, the economic potential is calculated below:

$$Economic\ Potential\ = P_B E_B + P_G y_{PH} \Delta H_{H_2} E_F + P_G (1 - y_{PH}) \Delta H_{CH4} E_F - F_{FT} E_{FT} - F_{FG} E_{FG} - E_{CO2}$$

J. Level 3 Economic Considerations

J.1 Level 3 Economic Potential Equation (Initially Considered)

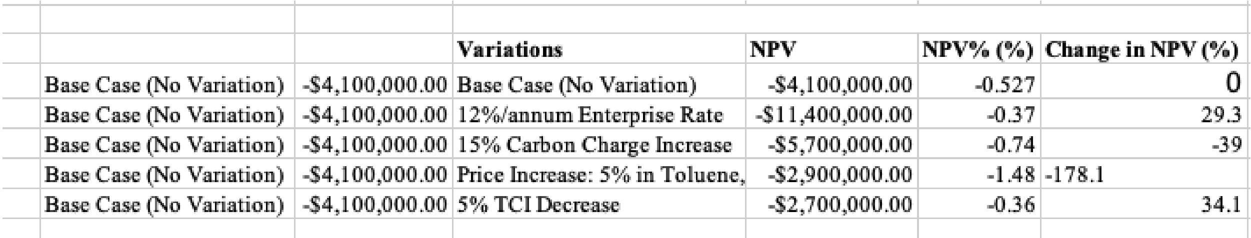
We defined the economic price of component i as E_i and the heat of combustion for component i as ΔH_i.

As a result, the economic potential is calculated below:

$$Economic\ Potential\ = P_B E_B + P_G y_{PH} \Delta H_{H_2} E_F + P_G (1 - y_{PH}) \Delta H_{CH4} E_F - F_{FT} E_{FT} - F_{FG} E_{FG} - E_{CO2}$$

J.2 Level 3 Sensitivity Analysis

J.2.1 Level 3 Sensitivity Calculations



		Variations	NPV	NPV% (%)	Change in NPV (%)
Base Case (No Variation)	-$4,100,000.00	Base Case (No Variation)	-$4,100,000.00	-0.527	0
Base Case (No Variation)	-$4,100,000.00	12%/annum Enterprise Rate	-$11,400,000.00	-0.37	29.3
Base Case (No Variation)	-$4,100,000.00	15% Carbon Charge Increase	-$5,700,000.00	-0.74	-39
Base Case (No Variation)	-$4,100,000.00	Price Increase: 5% in Toluene,	-$2,900,000.00	-1.48	-178.1
Base Case (No Variation)	-$4,100,000.00	5% TCI Decrease	-$2,700,000.00	-0.36	34.1

Fig J.1. Sensitivity calculation data

J.2.2 Level 3 Sensitivity Tornado Plot

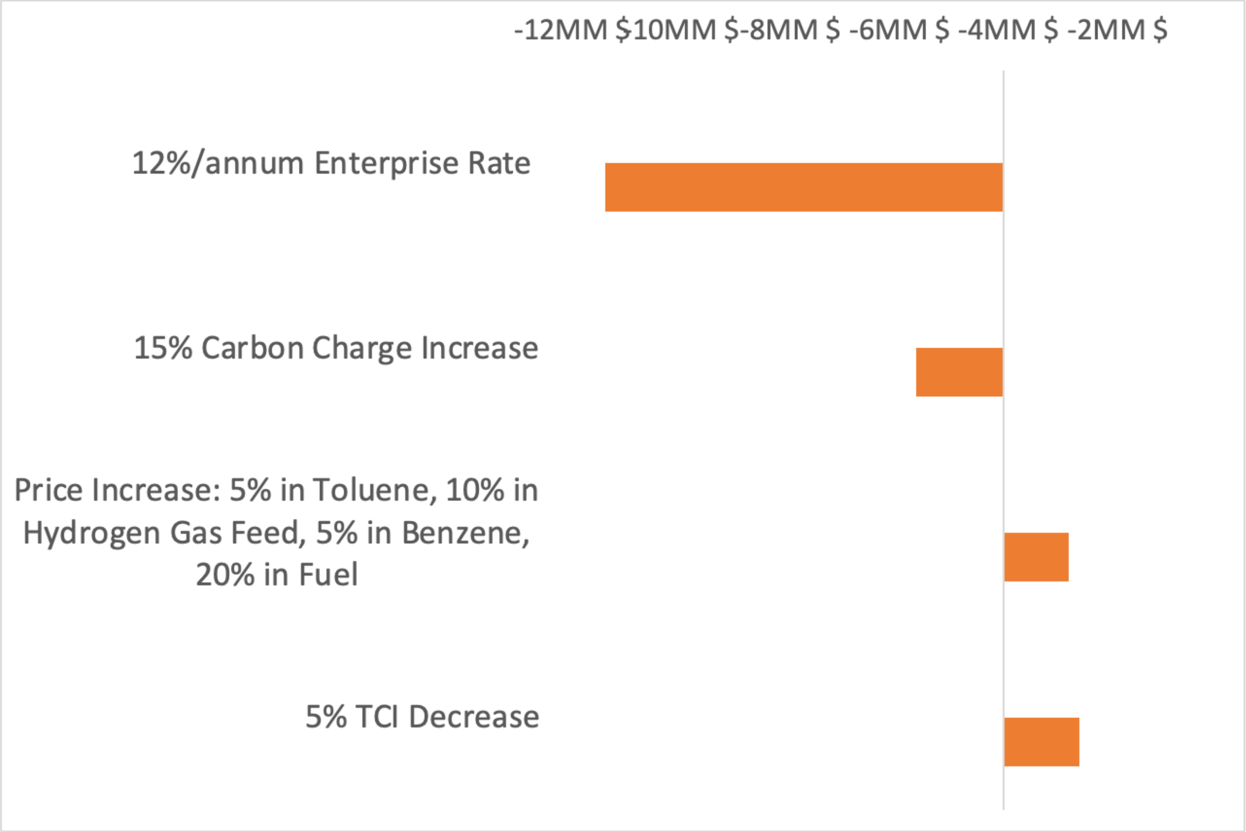
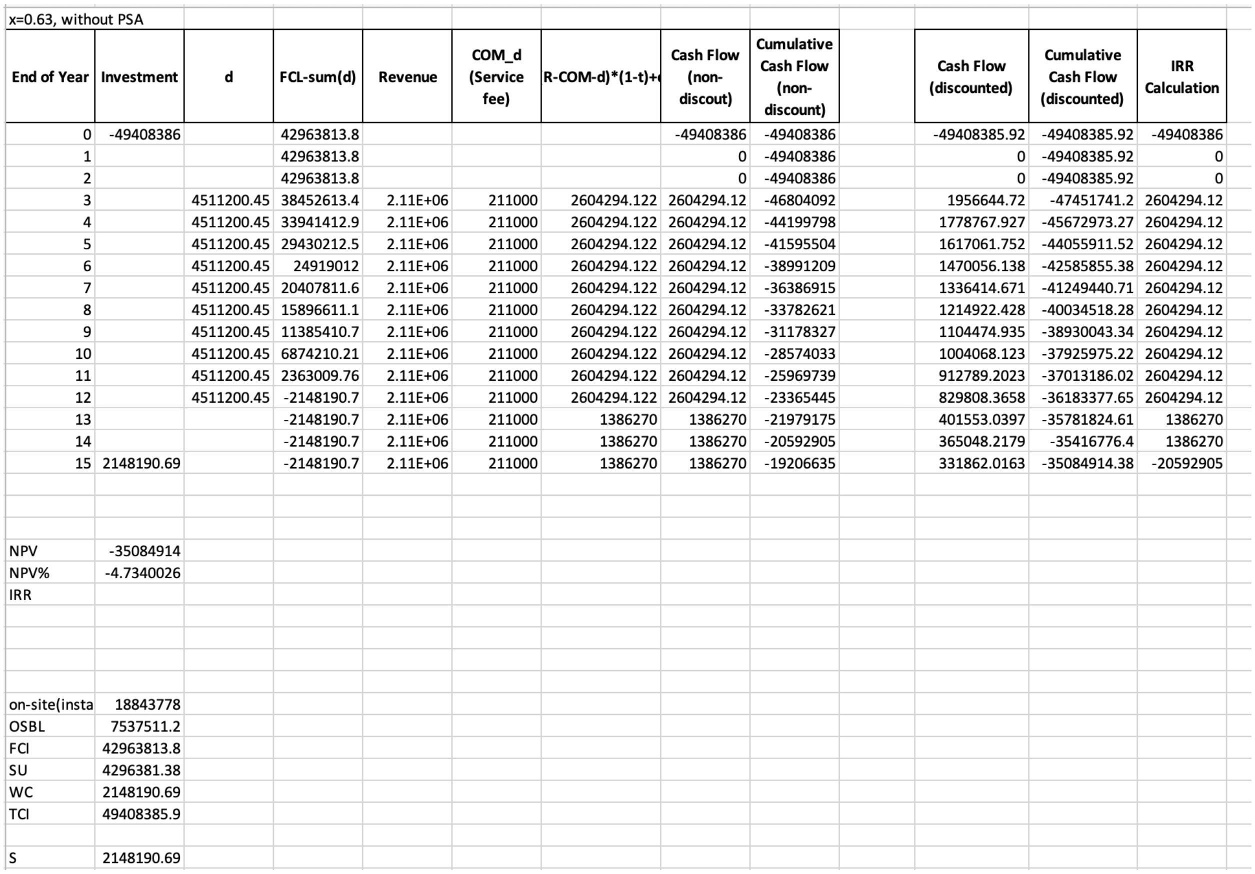


Fig J.2. Level 3 Sensitivity Analysis Tornado Plot (with 4 different variations)

K. Economic Calculations in Different Conversions and Design Decisions

K.1 Conversion x = 0.63, without PSA (Level 3)

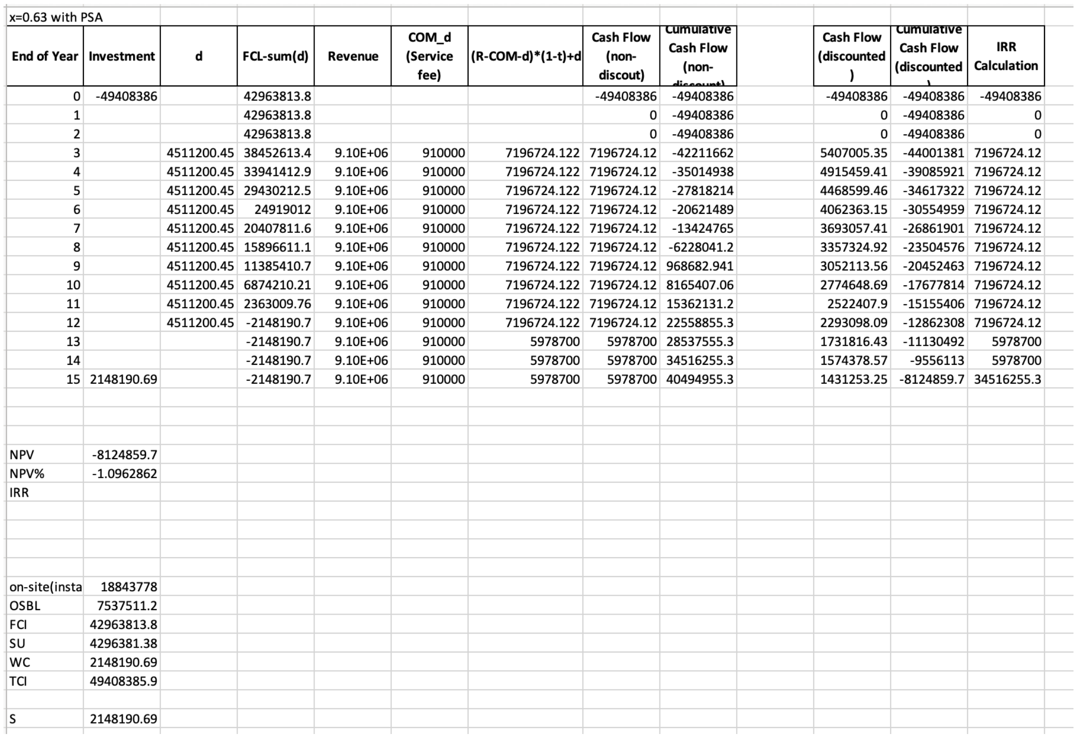


x=0.63, without PSA

End of Year	Investment	d	FCL-sum(d)	Revenue	COM_d (Service fee)	R-COM-d)*(1-t)+	Cash Flow (non-discout)	Cumulative Cash Flow (non-discount)	Cash Flow (discounted)	Cumulative Cash Flow (discounted)	IRR Calculation
0	-49408386		42963813.8				-49408386	-49408386	-49408385.92	-49408385.92	-49408386
1			42963813.8				0	-49408386	0	-49408385.92	0
2			42963813.8				0	-49408386	0	-49408385.92	0
3		4511200.45	38452613.4	2.11E+06	211000	2604294.122	2604294.12	-46804092	1956644.72	-47451741.2	2604294.12
4		4511200.45	33941412.9	2.11E+06	211000	2604294.122	2604294.12	-44199798	1778767.927	-45672973.27	2604294.12
5		4511200.45	29430212.5	2.11E+06	211000	2604294.122	2604294.12	-41595504	1617061.752	-44055911.52	2604294.12
6		4511200.45	24919012	2.11E+06	211000	2604294.122	2604294.12	-38991209	1470056.138	-42585855.38	2604294.12
7		4511200.45	20407811.6	2.11E+06	211000	2604294.122	2604294.12	-36386915	1336414.671	-41249440.71	2604294.12
8		4511200.45	15896611.1	2.11E+06	211000	2604294.122	2604294.12	-33782621	1214922.428	-40034518.28	2604294.12
9		4511200.45	11385410.7	2.11E+06	211000	2604294.122	2604294.12	-31178327	1104474.935	-38930043.34	2604294.12
10		4511200.45	6874210.21	2.11E+06	211000	2604294.122	2604294.12	-28574033	1004068.123	-37925975.22	2604294.12
11		4511200.45	2363009.76	2.11E+06	211000	2604294.122	2604294.12	-25969739	912789.2023	-37013186.02	2604294.12
12		4511200.45	-2148190.7	2.11E+06	211000	2604294.122	2604294.12	-23365445	829808.3658	-36183377.65	2604294.12
13			-2148190.7	2.11E+06	211000	1386270	1386270	-21979175	401553.0397	-35781824.61	1386270
14			-2148190.7	2.11E+06	211000	1386270	1386270	-20592905	365048.2179	-35416776.4	1386270
15	2148190.69		-2148190.7	2.11E+06	211000	1386270	1386270	-19206635	331862.0163	-35084914.38	-20592905

NPV	-35084914
NPV%	-4.7340026
IRR	
on-site(insta	18843778
OSBL	7537511.2
FCI	42963813.8
SU	4296381.38
WC	2148190.69
TCI	49408385.9
S	2148190.69

K.2 Conversion x = 0.63, with PSA (Level 3)

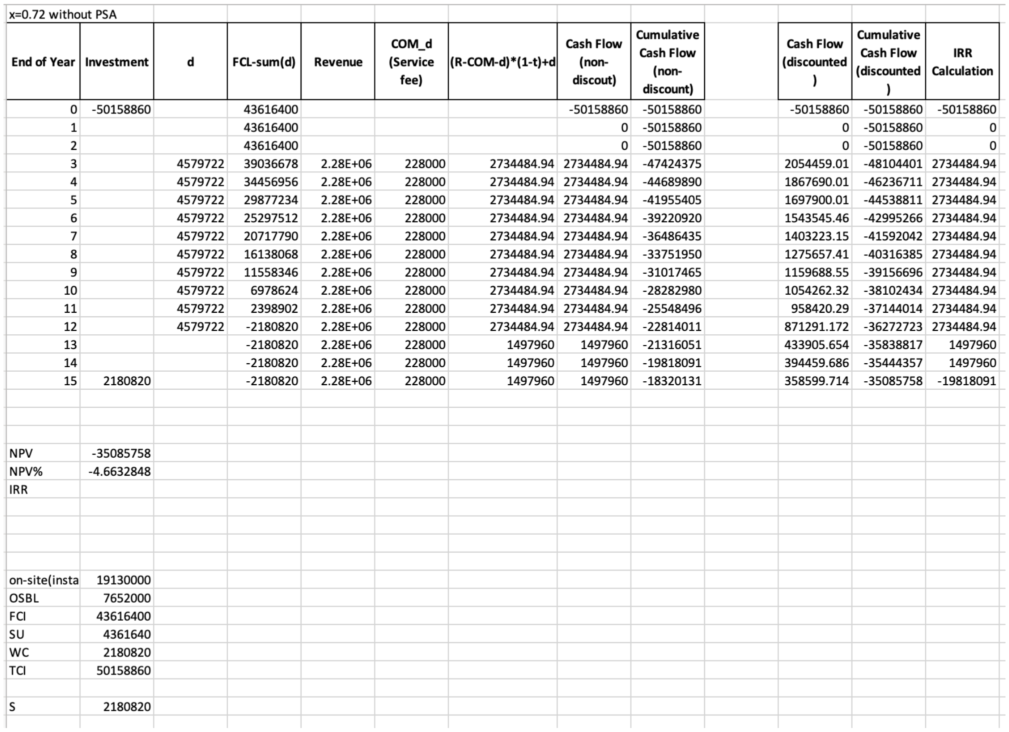


x=0.63 with PSA

End of Year	Investment	d	FCL-sum(d)	Revenue	COM_d (Service fee)	(R-COM-d)*(1-t)+d	Cash Flow (non-discout)	Cumulative Cash Flow (non-	Cash Flow (discounted)	Cumulative Cash Flow (discounted	IRR Calculation
0	-49408386		42963813.8				-49408386	-49408386	-49408386	-49408386	-49408386
1			42963813.8				0	-49408386	0	-49408386	0
2			42963813.8				0	-49408386	0	-49408386	0
3		4511200.45	38452613.4	9.10E+06	910000	7196724.122	7196724.12	-42211662	5407005.35	-44001381	7196724.12
4		4511200.45	33941412.9	9.10E+06	910000	7196724.122	7196724.12	-35014938	4915459.41	-39085921	7196724.12
5		4511200.45	29430212.5	9.10E+06	910000	7196724.122	7196724.12	-27818214	4468599.46	-34617322	7196724.12
6		4511200.45	24919012	9.10E+06	910000	7196724.122	7196724.12	-20621489	4062363.15	-30554959	7196724.12
7		4511200.45	20407811.6	9.10E+06	910000	7196724.122	7196724.12	-13424765	3693057.41	-26861901	7196724.12
8		4511200.45	15896611.1	9.10E+06	910000	7196724.122	7196724.12	-6228041.2	3357324.92	-23504576	7196724.12
9		4511200.45	11385410.7	9.10E+06	910000	7196724.122	7196724.12	968682.941	3052113.56	-20452463	7196724.12
10		4511200.45	6874210.21	9.10E+06	910000	7196724.122	7196724.12	8165407.06	2774648.69	-17677814	7196724.12
11		4511200.45	2363009.76	9.10E+06	910000	7196724.122	7196724.12	15362131.2	2522407.9	-15155406	7196724.12
12		4511200.45	-2148190.7	9.10E+06	910000	7196724.122	7196724.12	22558855.3	2293098.09	-12862308	7196724.12
13			-2148190.7	9.10E+06	910000	5978700	5978700	28537555.3	1731816.43	-11130492	5978700
14			-2148190.7	9.10E+06	910000	5978700	5978700	34516255.3	1574378.57	-9556113	5978700
15	2148190.69		-2148190.7	9.10E+06	910000	5978700	5978700	40494955.3	1431253.25	-8124859.7	34516255.3

NPV	-8124859.7
NPV%	-1.0962862
IRR	
on-site(insta	18843778
OSBL	7537511.2
FCI	42963813.8
SU	4296381.38
WC	2148190.69
TCI	49408385.9
S	2148190.69

K.3 Conversion x = 0.72, without PSA (Level 3)



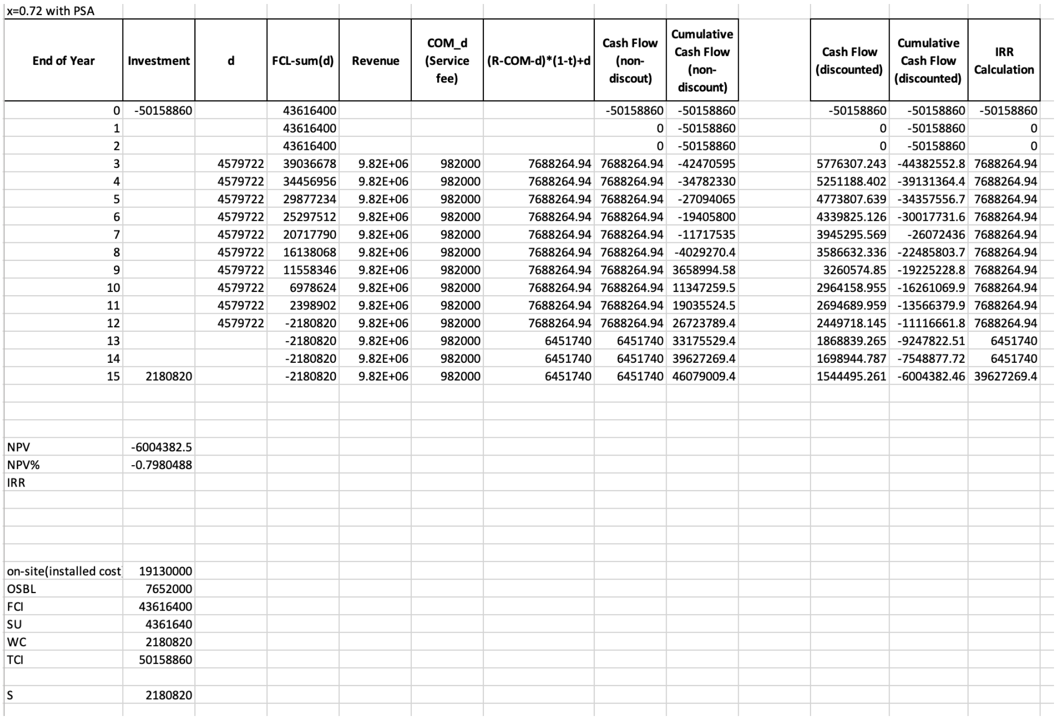
x=0.72 without PSA

End of Year	Investment	d	FCL-sum(d)	Revenue	COM_d (Service fee)	(R-COM-d)*(1-t)+d	Cash Flow (non-discout)	Cumulative Cash Flow (non-discount)		Cash Flow (discounted)	Cumulative Cash Flow (discounted)	IRR Calculation
0	-50158860		43616400				-50158860	-50158860		-50158860	-50158860	-50158860
1			43616400				0	-50158860		0	-50158860	0
2			43616400				0	-50158860		0	-50158860	0
3		4579722	39036678	2.28E+06	228000	2734484.94	2734484.94	-47424375		2054459.01	-48104401	2734484.94
4		4579722	34456956	2.28E+06	228000	2734484.94	2734484.94	-44689890		1867690.01	-46236711	2734484.94
5		4579722	29877234	2.28E+06	228000	2734484.94	2734484.94	-41955405		1697900.01	-44538811	2734484.94
6		4579722	25297512	2.28E+06	228000	2734484.94	2734484.94	-39220920		1543545.46	-42995266	2734484.94
7		4579722	20717790	2.28E+06	228000	2734484.94	2734484.94	-36486435		1403223.15	-41592042	2734484.94
8		4579722	16138068	2.28E+06	228000	2734484.94	2734484.94	-33751950		1275657.41	-40316385	2734484.94
9		4579722	11558346	2.28E+06	228000	2734484.94	2734484.94	-31017465		1159688.55	-39156696	2734484.94
10		4579722	6978624	2.28E+06	228000	2734484.94	2734484.94	-28282980		1054262.32	-38102434	2734484.94
11		4579722	2398902	2.28E+06	228000	2734484.94	2734484.94	-25548496		958420.29	-37144014	2734484.94
12		4579722	-2180820	2.28E+06	228000	2734484.94	2734484.94	-22814011		871291.172	-36272723	2734484.94
13			-2180820	2.28E+06	228000	1497960	1497960	-21316051		433905.654	-35838817	1497960
14			-2180820	2.28E+06	228000	1497960	1497960	-19818091		394459.686	-35444357	1497960
15	2180820		-2180820	2.28E+06	228000	1497960	1497960	-18320131		358599.714	-35085758	-19818091

NPV	-35085758
NPV%	-4.6632848
IRR	

on-site(insta	19130000
OSBL	7652000
FCI	43616400
SU	4361640
WC	2180820
TCI	50158860
S	2180820

K.4 Conversion x = 0.72, with PSA (Level 3)



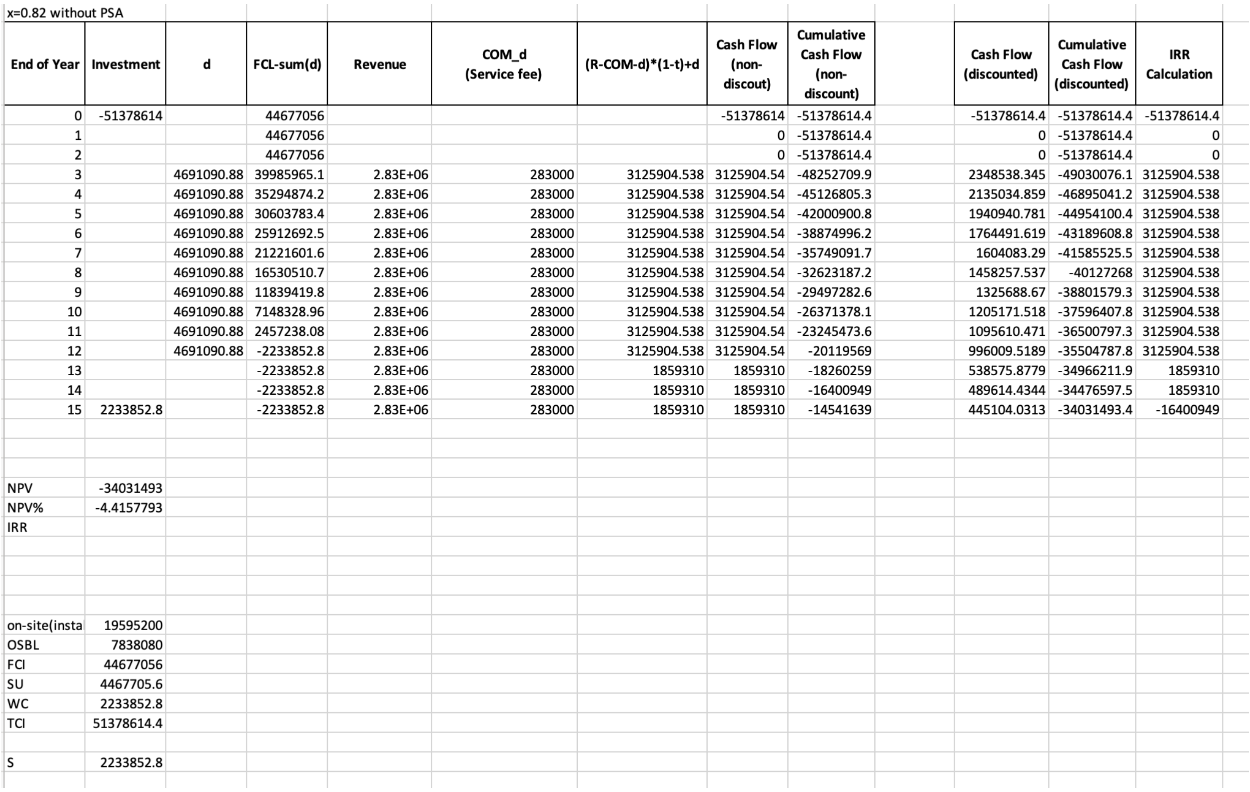
x=0.72 with PSA

End of Year	Investment	d	FCL-sum(d)	Revenue	COM_d (Service fee)	(R-COM-d)*(1-t)+d	Cash Flow (non-discout)	Cumulative Cash Flow (non-discount)		Cash Flow (discounted)	Cumulative Cash Flow (discounted)	IRR Calculation
0	-50158860		43616400				-50158860	-50158860		-50158860	-50158860	-50158860
1			43616400				0	-50158860		0	-50158860	0
2			43616400				0	-50158860		0	-50158860	0
3		4579722	39036678	9.82E+06	982000	7688264.94	7688264.94	-42470595		5776307.243	-44382552.8	7688264.94
4		4579722	34456956	9.82E+06	982000	7688264.94	7688264.94	-34782330		5251188.402	-39131364.4	7688264.94
5		4579722	29877234	9.82E+06	982000	7688264.94	7688264.94	-27094065		4773807.639	-34357556.7	7688264.94
6		4579722	25297512	9.82E+06	982000	7688264.94	7688264.94	-19405800		4339825.126	-30017731.6	7688264.94
7		4579722	20717790	9.82E+06	982000	7688264.94	7688264.94	-11717535		3945295.569	-26072436	7688264.94
8		4579722	16138068	9.82E+06	982000	7688264.94	7688264.94	-4029270.4		3586632.336	-22485803.7	7688264.94
9		4579722	11558346	9.82E+06	982000	7688264.94	7688264.94	3658994.58		3260574.85	-19225228.8	7688264.94
10		4579722	6978624	9.82E+06	982000	7688264.94	7688264.94	11347259.5		2964158.955	-16261069.9	7688264.94
11		4579722	2398902	9.82E+06	982000	7688264.94	7688264.94	19035524.5		2694689.959	-13566379.9	7688264.94
12		4579722	-2180820	9.82E+06	982000	7688264.94	7688264.94	26723789.4		2449718.145	-11116661.8	7688264.94
13			-2180820	9.82E+06	982000	6451740	6451740	33175529.4		1868839.265	-9247822.51	6451740
14			-2180820	9.82E+06	982000	6451740	6451740	39627269.4		1698944.787	-7548877.72	6451740
15	2180820		-2180820	9.82E+06	982000	6451740	6451740	46079009.4		1544495.261	-6004382.46	39627269.4

NPV	-6004382.5
NPV%	-0.7980488
IRR	

on-site(installed cost	19130000
OSBL	7652000
FCI	43616400
SU	4361640
WC	2180820
TCI	50158860
S	2180820

K.5 Conversion x = 0.82, without PSA (Level 3)



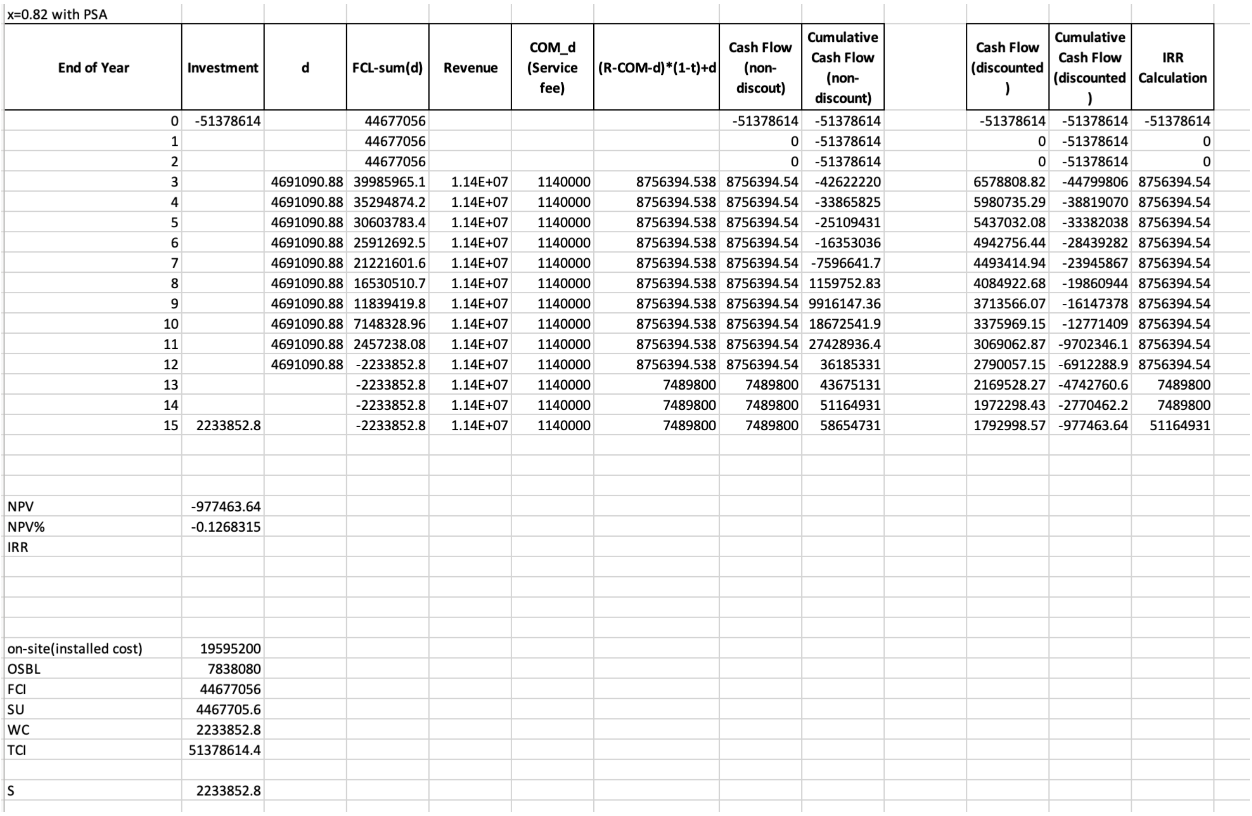
x=0.82 without PSA

End of Year	Investment	d	FCL-sum(d)	Revenue	COM_d (Service fee)	(R-COM-d)*(1-t)+d	Cash Flow (non-discout)	Cumulative Cash Flow (non-discount)		Cash Flow (discounted)	Cumulative Cash Flow (discounted)	IRR Calculation
0	-51378614		44677056				-51378614	-51378614.4		-51378614.4	-51378614.4	-51378614.4
1			44677056				0	-51378614.4		0	-51378614.4	0
2			44677056				0	-51378614.4		0	-51378614.4	0
3		4691090.88	39985965.1	2.83E+06	283000	3125904.538	3125904.54	-48252709.9		2348538.345	-49030076.1	3125904.538
4		4691090.88	35294874.2	2.83E+06	283000	3125904.538	3125904.54	-45126805.3		2135034.859	-46895041.2	3125904.538
5		4691090.88	30603783.4	2.83E+06	283000	3125904.538	3125904.54	-42000900.8		1940940.781	-44954100.4	3125904.538
6		4691090.88	25912692.5	2.83E+06	283000	3125904.538	3125904.54	-38874996.2		1764491.619	-43189608.8	3125904.538
7		4691090.88	21221601.6	2.83E+06	283000	3125904.538	3125904.54	-35749091.7		1604083.29	-41585525.5	3125904.538
8		4691090.88	16530510.7	2.83E+06	283000	3125904.538	3125904.54	-32623187.2		1458257.537	-40127268	3125904.538
9		4691090.88	11839419.8	2.83E+06	283000	3125904.538	3125904.54	-29497282.6		1325688.67	-38801579.3	3125904.538
10		4691090.88	7148328.96	2.83E+06	283000	3125904.538	3125904.54	-26371378.1		1205171.518	-37596407.8	3125904.538
11		4691090.88	2457238.08	2.83E+06	283000	3125904.538	3125904.54	-23245473.6		1095610.471	-36500797.3	3125904.538
12		4691090.88	-2233852.8	2.83E+06	283000	3125904.538	3125904.54	-20119569		996009.5189	-35504787.8	3125904.538
13			-2233852.8	2.83E+06	283000	1859310	1859310	-18260259		538575.8779	-34966211.9	1859310
14			-2233852.8	2.83E+06	283000	1859310	1859310	-16400949		489614.4344	-34476597.5	1859310
15	2233852.8		-2233852.8	2.83E+06	283000	1859310	1859310	-14541639		445104.0313	-34031493.4	-16400949

NPV	-34031493
NPV%	-4.4157793
IRR	

on-site(insta	19595200
OSBL	7838080
FCI	44677056
SU	4467705.6
WC	2233852.8
TCI	51378614.4
S	2233852.8

K.6 Conversion x = 0.82, with PSA (Level 3)



x=0.82 with PSA

End of Year	Investment	d	FCL-sum(d)	Revenue	COM_d (Service fee)	(R-COM-d)*(1-t)+d	Cash Flow (non-discout)	Cumulative Cash Flow (non-discount)		Cash Flow (discounted)	Cumulative Cash Flow (discounted)	IRR Calculation
0	-51378614		44677056				-51378614	-51378614		-51378614	-51378614	-51378614
1			44677056				0	-51378614		0	-51378614	0
2			44677056				0	-51378614		0	-51378614	0
3		4691090.88	39985965.1	1.14E+07	1140000	8756394.538	8756394.54	-42622220		6578808.82	-44799806	8756394.54
4		4691090.88	35294874.2	1.14E+07	1140000	8756394.538	8756394.54	-33865825		5980735.29	-38819070	8756394.54
5		4691090.88	30603783.4	1.14E+07	1140000	8756394.538	8756394.54	-25109431		5437032.08	-33382038	8756394.54
6		4691090.88	25912692.5	1.14E+07	1140000	8756394.538	8756394.54	-16353036		4942756.44	-28439282	8756394.54
7		4691090.88	21221601.6	1.14E+07	1140000	8756394.538	8756394.54	-7596641.7		4493414.94	-23945867	8756394.54
8		4691090.88	16530510.7	1.14E+07	1140000	8756394.538	8756394.54	1159752.83		4084922.68	-19860944	8756394.54
9		4691090.88	11839419.8	1.14E+07	1140000	8756394.538	8756394.54	9916147.36		3713566.07	-16147378	8756394.54
10		4691090.88	7148328.96	1.14E+07	1140000	8756394.538	8756394.54	18672541.9		3375969.15	-12771409	8756394.54
11		4691090.88	2457238.08	1.14E+07	1140000	8756394.538	8756394.54	27428936.4		3069062.87	-9702346.1	8756394.54
12		4691090.88	-2233852.8	1.14E+07	1140000	8756394.538	8756394.54	36185331		2790057.15	-6912288.9	8756394.54
13			-2233852.8	1.14E+07	1140000	7489800	7489800	43675131		2169528.27	-4742760.6	7489800
14			-2233852.8	1.14E+07	1140000	7489800	7489800	51164931		1972298.43	-2770462.2	7489800
15	2233852.8		-2233852.8	1.14E+07	1140000	7489800	7489800	58654731		1792998.57	-977463.64	51164931

NPV	-977463.64
NPV%	-0.1268315
IRR	

on-site(installed cost)	19595200
OSBL	7838080
FCI	44677056
SU	4467705.6
WC	2233852.8
TCI	51378614.4
S	2233852.8

K.7 Conversion x = 0.86, without PSA (Level 3)

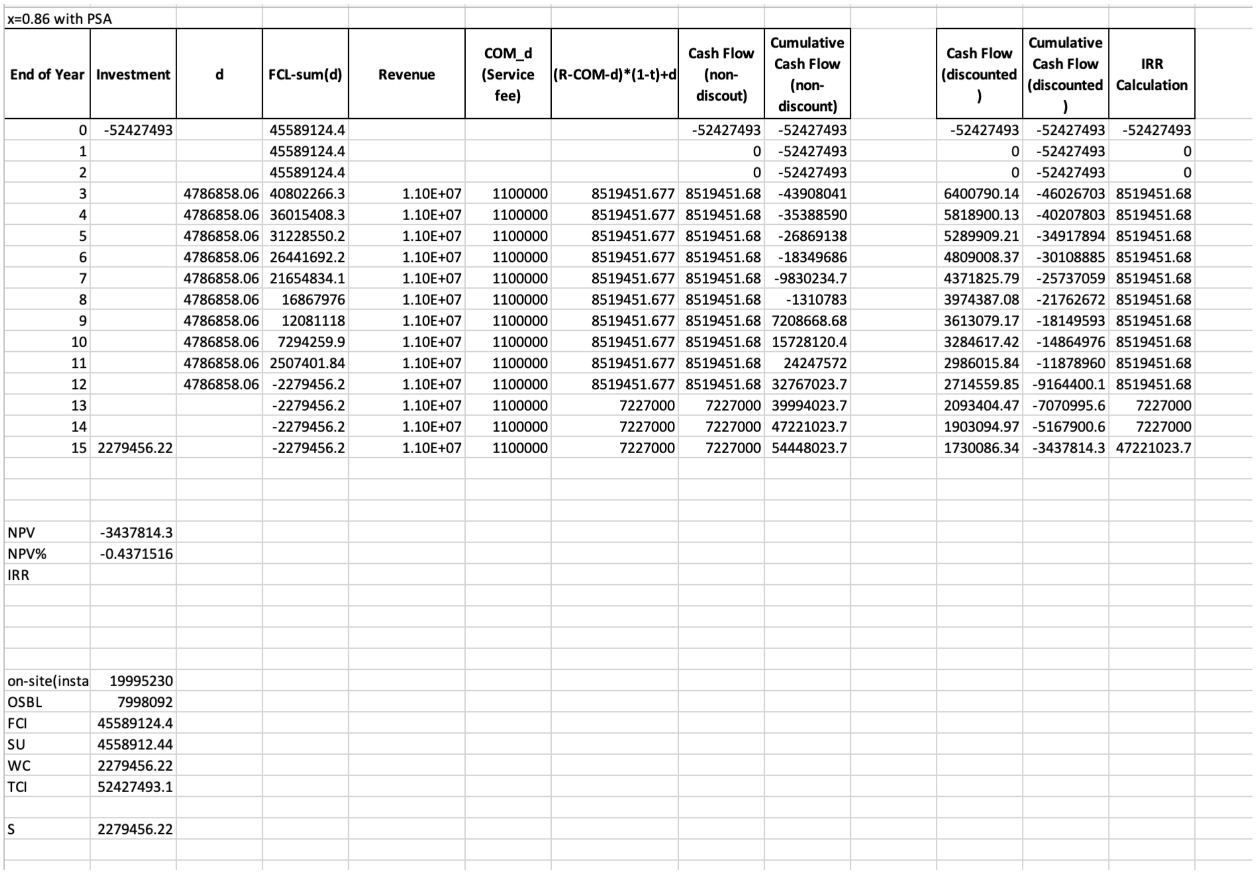
x=0.86 withoutPSA

End of Year	Investment	d	FCL-sum(d)	Revenue	COM_d (Service fee)	(R-COM-d)*(1-t)+d	Cash Flow (non-discout)	Cumulative Cash Flow (non-discount)		Cash Flow (discounted)	Cumulative Cash Flow (discounted)	IRR Calculation
0	-52427493		45589124.4				-52427493	-52427493		-52427493	-52427493	-52427493
1			45589124.4				0	-52427493		0	-52427493	0
2			45589124.4				0	-52427493		0	-52427493	0
3		4786858.06	40802266.3	2.74E+06	274000	3092631.677	3092631.68	-49334861		2323539.95	-50103953	3092631.68
4		4786858.06	36015408.3	2.74E+06	274000	3092631.677	3092631.68	-46242230		2112309.05	-47991644	3092631.68
5		4786858.06	31228550.2	2.74E+06	274000	3092631.677	3092631.68	-43149598		1920280.95	-46071363	3092631.68
6		4786858.06	26441692.2	2.74E+06	274000	3092631.677	3092631.68	-40056966		1745709.96	-44325653	3092631.68
7		4786858.06	21654834.1	2.74E+06	274000	3092631.677	3092631.68	-36964335		1587009.05	-42738644	3092631.68
8		4786858.06	16867976	2.74E+06	274000	3092631.677	3092631.68	-33871703		1442735.5	-41295909	3092631.68
9		4786858.06	12081118	2.74E+06	274000	3092631.677	3092631.68	-30779071		1311577.73	-39984331	3092631.68
10		4786858.06	7294259.9	2.74E+06	274000	3092631.677	3092631.68	-27686440		1192343.39	-38791987	3092631.68
11		4786858.06	2507401.84	2.74E+06	274000	3092631.677	3092631.68	-24593808		1083948.54	-37708039	3092631.68
12		4786858.06	-2279456.2	2.74E+06	274000	3092631.677	3092631.68	-21501176		985407.76	-36722631	3092631.68
13			-2279456.2	2.74E+06	274000	1800180	1800180	-19700996		521448.023	-36201183	1800180
14			-2279456.2	2.74E+06	274000	1800180	1800180	-17900816		474043.657	-35727140	1800180
15	2279456.22		-2279456.2	2.74E+06	274000	1800180	1800180	-16100636		430948.779	-35296191	-17900816

NPV	-35296191
NPV%	-4.4882546
IRR	

on-site(insta	19995230
OSBL	7998092
FCI	45589124.4
SU	4558912.44
WC	2279456.22
TCI	52427493.1
S	2279456.22

K.8 Conversion x = 0.86, with PSA (Level 3)

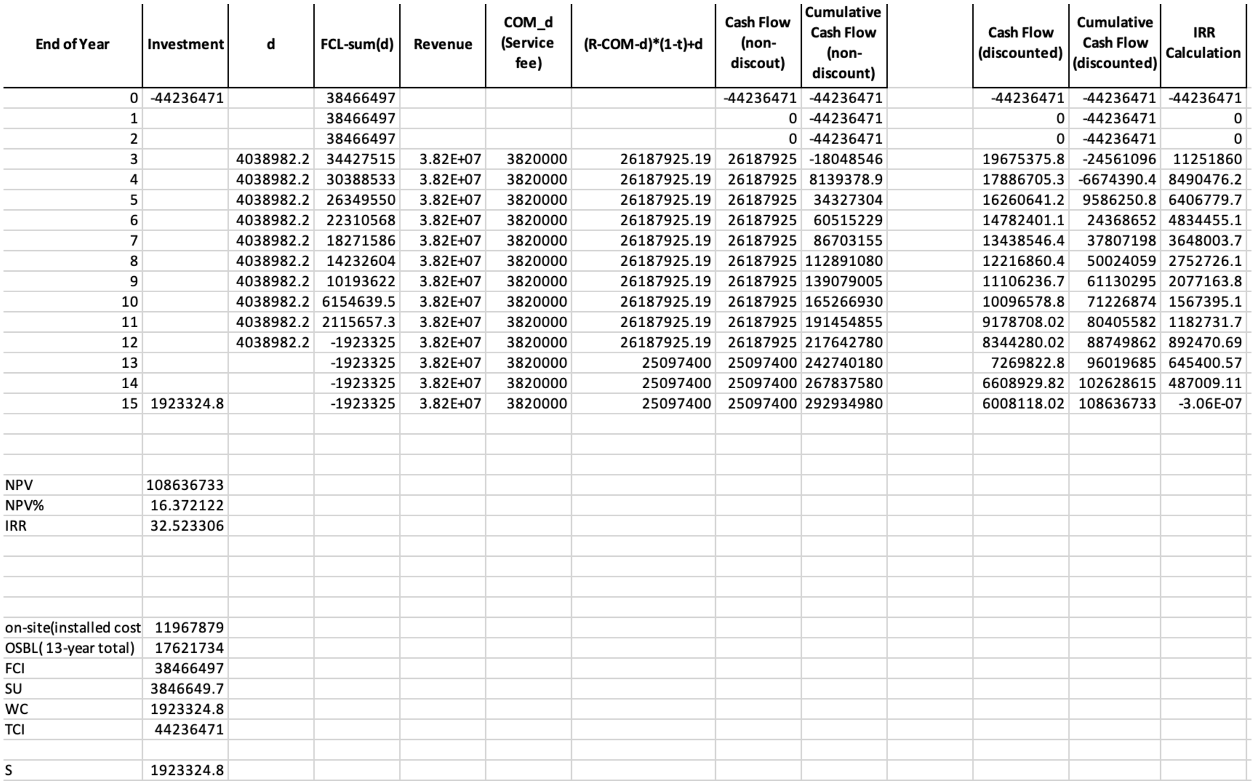


x=0.86 with PSA

End of Year	Investment	d	FCL-sum(d)	Revenue	COM_d (Service fee)	(R-COM-d)*(1-t)+d	Cash Flow (non-discout)	Cumulative Cash Flow (non-discount)	Cash Flow (discounted)	Cumulative Cash Flow (discounted)	IRR Calculation
0	-52427493		45589124.4				-52427493	-52427493	-52427493	-52427493	-52427493
1			45589124.4				0	-52427493	0	-52427493	0
2			45589124.4				0	-52427493	0	-52427493	0
3		4786858.06	40802266.3	1.10E+07	1100000	8519451.677	8519451.68	-43908041	6400790.14	-46026703	8519451.68
4		4786858.06	36015408.3	1.10E+07	1100000	8519451.677	8519451.68	-35388590	5818900.13	-40207803	8519451.68
5		4786858.06	31228550.2	1.10E+07	1100000	8519451.677	8519451.68	-26869138	5289909.21	-34917894	8519451.68
6		4786858.06	26441692.2	1.10E+07	1100000	8519451.677	8519451.68	-18349686	4809008.37	-30108885	8519451.68
7		4786858.06	21654834.1	1.10E+07	1100000	8519451.677	8519451.68	-9830234.7	4371825.79	-25737059	8519451.68
8		4786858.06	16867976	1.10E+07	1100000	8519451.677	8519451.68	-1310783	3974387.08	-21762672	8519451.68
9		4786858.06	12081118	1.10E+07	1100000	8519451.677	8519451.68	7208668.68	3613079.17	-18149593	8519451.68
10		4786858.06	7294259.9	1.10E+07	1100000	8519451.677	8519451.68	15728120.4	3284617.42	-14864976	8519451.68
11		4786858.06	2507401.84	1.10E+07	1100000	8519451.677	8519451.68	24247572	2986015.84	-11878960	8519451.68
12		4786858.06	-2279456.2	1.10E+07	1100000	8519451.677	8519451.68	32767023.7	2714559.85	-9164400.1	8519451.68
13			-2279456.2	1.10E+07	1100000	7227000	7227000	39994023.7	2093404.47	-7070995.6	7227000
14			-2279456.2	1.10E+07	1100000	7227000	7227000	47221023.7	1903094.97	-5167900.6	7227000
15	2279456.22		-2279456.2	1.10E+07	1100000	7227000	7227000	54448023.7	1730086.34	-3437814.3	47221023.7

NPV	-3437814.3
NPV%	-0.4371516
IRR	
on-site(insta	19995230
OSBL	7998092
FCI	45589124.4
SU	4558912.44
WC	2279456.22
TCI	52427493.1
S	2279456.22

K.9 Economic Calculations with Final PSA Design at Conversion x = 0.75



End of Year	Investment	d	FCL-sum(d)	Revenue	COM_d (Service fee)	(R-COM-d)*(1-t)+d	Cash Flow (non-discout)	Cumulative Cash Flow (non-discount)		Cash Flow (discounted)	Cumulative Cash Flow (discounted)	IRR Calculation
0	-44236471		38466497				-44236471	-44236471		-44236471	-44236471	-44236471
1			38466497				0	-44236471		0	-44236471	0
2			38466497				0	-44236471		0	-44236471	0
3		4038982.2	34427515	3.82E+07	3820000	26187925.19	26187925	-18048546		19675375.8	-24561096	11251860
4		4038982.2	30388533	3.82E+07	3820000	26187925.19	26187925	8139378.9		17886705.3	-6674390.4	8490476.2
5		4038982.2	26349550	3.82E+07	3820000	26187925.19	26187925	34327304		16260641.2	9586250.8	6406779.7
6		4038982.2	22310568	3.82E+07	3820000	26187925.19	26187925	60515229		14782401.1	24368652	4834455.1
7		4038982.2	18271586	3.82E+07	3820000	26187925.19	26187925	86703155		13438546.4	37807198	3648003.7
8		4038982.2	14232604	3.82E+07	3820000	26187925.19	26187925	112891080		12216860.4	50024059	2752726.1
9		4038982.2	10193622	3.82E+07	3820000	26187925.19	26187925	139079005		11106236.7	61130295	2077163.8
10		4038982.2	6154639.5	3.82E+07	3820000	26187925.19	26187925	165266930		10096578.8	71226874	1567395.1
11		4038982.2	2115657.3	3.82E+07	3820000	26187925.19	26187925	191454855		9178708.02	80405582	1182731.7
12		4038982.2	-1923325	3.82E+07	3820000	26187925.19	26187925	217642780		8344280.02	88749862	892470.69
13			-1923325	3.82E+07	3820000	25097400	25097400	242740180		7269822.8	96019685	645400.57
14			-1923325	3.82E+07	3820000	25097400	25097400	267837580		6608929.82	102628615	487009.11
15	1923324.8		-1923325	3.82E+07	3820000	25097400	25097400	292934980		6008118.02	108636733	-3.06E-07

NPV	108636733
NPV%	16.372122
IRR	32.523306
on-site(installed cost	11967879
OSBL(13-year total)	17621734
FCI	38466497
SU	3846649.7
WC	1923324.8
TCI	44236471
S	1923324.8

K.10 Economic Calculations (NPV) Equation

$$FCI = 1.3 * (ISBL + OSBL)$$

$$TCI = FCI + SU + WC = FCI + 0.1 * FCI + 0.05 * FCI$$

$$Depreciation = \frac{(FCI+SU-S)}{10}$$

$$Discounted\ Cash\ Flow = \frac{(Revenue-Service\ fee-Depreciation)*(1-Tax\ rate)+Depreciation}{(1+Enterprise\ rate)^{Year}}$$

L.1 MATLAB Codes for Solving PFR ODEs, Selectivity vs. Conversion, and Reactor Volume vs. Conversion in Different Reactor Temperature and Pressure Conditions in Level-3 Processes

```
Ptotal = 34*10^5; %unit Pa
R=8314; %unit Pa*L/(mol K)
%R=0.0821;
%Ptotal = 34;
% T=878; %unit K
T=828;
y0 = [146146 730730 0 0 0 876876];%initial condition on reactor outlet flowrate, unit mol/h
```

```
%PB = 146146; %unit mol/h, equal to 100kta
Vspan=[0 10000000]; %reactor volume from 0 to 210000
[V,F]=ode45(@(V,F) myode(V,F,R,T,Ptotal),Vspan,y0)
T=873;
Vspan2=[0 3100000]
[V1,F1]=ode45(@(V,F) myode(V,F,R,T,Ptotal),Vspan2,y0)
T=900;
Vspan3 =[0 1300000]
[V2,F2]=ode45(@(V,F) myode(V,F,R,T,Ptotal),Vspan3,y0)
% define x = (FT0-FT)/FT0
FT0 = 146146;  %assume a consatnt FT0
FT=F(:,1); % F matrix got from ode.m, FT correspnds to the first column
x = (FT0-FT)./(FT0);
FT1=F1(:,1);
x1 = (FT0-FT1)./(FT0);
FT2=F2(:,1);
x2 = (FT0-FT2)/(FT0);
Volume = V(:,1).*10^(-3); % V matrix got from ode.m, unit in m3
Volume1 = V1(:,1).*10^(-3);
Volume2 = V2(:,1).*10^(-3);
figure(1)
plot(x,Volume)
hold on
plot(x1,Volume1)
plot(x2,Volume2)
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Reactor Volume]
(m^3)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
lgd = legend('T = 555°C','T = 600°C','T = 627°C','location','northwest');
lgd.FontSize = 15;
ylim([0 2000]);
%define s=PB/(FT0-FT)
PB=F(:,3);
PB1=F1(:,3);
PB2=F2(:,3);
%FT01= ones(109,1);
%FT02 = FT01.*146146;
s = PB./(FT0-FT);
%s1=1-s;
s2 = PB1./(FT0-FT1);
```

```
%s4=1-s2;
s3 = PB2./(FT0-FT2);
%s5=1-s3;
figure(2)
plot(x,s)
hold on
plot(x1,s2)
plot(x2,s3)
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Selectivity]$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
lgd = legend('T = 555°C','T = 600°C','T = 627°C','location','northwest');
lgd.FontSize = 15;
function Y = myode(V,F,R,T,Ptotal)
Y = zeros(6,1);
kf1 = 1.188*10^14*exp(-52000/(1.987*T));
kf2 = 1.1647*10^(-5)*exp(-30190/(1.987*T));
Keq = 10^(-734.92/T-8.1046+3.1294*log10(T)-7.0804*10^(-4)*T+8.523*10^(-8)*T^2);
r1 = kf1*Ptotal^1.5*F(2)^(0.5)*F(1)/(F(6)^(1.5)*R^1.5*T^1.5); %reaction rate
r2 = kf2*Ptotal^2*(F(3)^2/F(6)^2-F(5)*F(2)/(F(6)^2*Keq));
Y(1)= -r1;
Y(2)= -r1+r2;
Y(3) = r1-2*r2;
Y(4) = r1;
Y(5) = r2;
Y(6) = 0;
end
```

L.2 MATLAB Codes for Stream Flow Rates Calculations in Level 3 Design without PSA

```
yfh = 0.95;
yph = 0.6;
MR = 5;
PB = 146146; %unit mol/h
%balances for streams (mole flow rate)
FFT = PB./s;
FT = PB./(s.*x); %level 3 FT balance
FH = MR*PB./(s.*x); % FH=MR*FT;
RT = PB.*(1-x)./(s.*x);%toluene recycle stream
FT1 = FT.*(1-x);  %conversion, FT1 is the reactor outlet toluene flow rate(separator inlet)
PD = PB*(1-s)./(2*s); % level 3 PD bal
FFG= (FFT-0.5.*(FFT-PB)+FFT*yph./(1-yph))/(yfh-(1-yfh)/(1-yph)); %google doc eqn (18)&(19)
PG = FFG*(1-yfh)+FFT./(1-yph);%google doc eqn (19)
FG = FFG+(MR*PB./(x.*s)-FFG*yfh)./yph;
RG = MR*PB./(x.*s)-FFG*yfh; %google doc eqn (22)
%mass flow rate
FFG_mass = FFG.*2.7*10^(-3); %95%H2 and 5% CH4
FFT_mass = FFT.*92.14*10^(-3);
PD_mass = PD.*154.21*10^(-3);
PB_mass = PB*78.11*10^(-3);
RT_mass = RT.*92.14*10^(-3);
RG_mass = RG.*(yph*2+(1-yph)*16)*10^(-3);
FG_mass = RG_mass+FFG_mass;
FT_mass = FT.*92.14*10^(-3);
FGT_mass=FG_mass+FT_mass; % define FGT as FG+FT, total flow rate to the reactor
%manual matlab graph#3 fresh feed flow rate vs conversion
figure(3)
plot(x,FFG_mass)
hold on
plot(x,FFT_mass)
hold off
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Fresh Feed Flow Rate]
(kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
lgd = legend('Fresh Feed Hydrogen and Methane','Fresh Feed Toluene','location','northwest');
lgd.FontSize = 15;
%manual matlab graph#4 production rate vs conversion
```

```
figure (4)
plot(x,PD_mass)
hold on
plot(x,yline(11415))
hold off
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Product Flow Rate]
(kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
lgd = legend('Product Diphenyl','Product Benzene','location','northwest');
lgd.FontSize = 15;
%manual matlab graph#5 limiting recycle rate vs conversion
figure (5)
plot(x,RT_mass)
ylim([0 150000]);
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Limiting Toluene Recycle Flow Rate]
(kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
%manual matlab graph#6 Total Flow rate vs conversion
figure(6)
plot(x,FGT_mass)
ylim([0 200000]);
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Total Flow Rate to Reactor]
(kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
%manual matlab graph#7&8 Total Flow rate to separation system vs conversion
FST = RG+PG+PB+PD+RT;
yb = PB./FST;
yd = PD./FST;
yt = RT./FST;
yh = (RG+PG).*yph./FST;
ych4 = (RG+PG-(RG+PG).*yph)./FST;
FST_mass= ((RG+PG).*(yh.*2+ych4.*16)+PB.*78.11+PD.*154.21+RT.*92.14)*10^(-3);
%manual matlab graph#7 Total Flow rate to separation system vs conversion
figure(7)
plot(x,FST_mass)
ylim([0 200000]);
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
```

```
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Total Flow Rate to Separator] (kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
%manual matlab graph#8 Mole fraction of each component entering the separation system vs conversion
figure(8)
plot(x,yb)
hold on
plot(x,yd)
plot(x,yt)
plot(x,yh)
plot(x,ych4)
hold off
ylim([0 1]);
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Mole Fraction Entering Separator]$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
lgd = legend('Benzene','Diphenyl','Toluene','Hydrogen','Methane','location','northwest');
lgd.FontSize = 15;
```

L.3 MATLAB Codes for Stream Flow Rates Calculations in Level 3 Design with PSA

```
yfh = 0.95;
MR = 5;
PB = 146146; %unit mol/h
%balances for streams
FFT = PB./s;
FT = PB./(s.*x); %level 3 FT balance
FH = MR*PB./(s.*x); % FH=MR*FT;
RT = PB.*(1-x)./(s.*x);%toluene recycle stream
PD = PB*(1-s)./(2*s); % level 3 PD bal
FFH = (MR*FT+9*PB*(1+s)./(2*s))./10;  %FFH+PH*0.9=MR*FT & FFH-PH = PB(1+s)/(2s)
PH = 10*FFH-10*PB*(1+s)./(2*s);
FFG = FFH./0.95;
RG = 0.9*PH; %90% H2 into PSA go to recycle
FG = FFG+RG;
PCH4 = FFT; %FT-RT=PCH4, T consumed = CH4 produced
yph = PH*0.1./(PCH4+PH*0.1);
FGT=FG+FT; % define FGT as FG+FT, total flow rate to the reactor
%mass flowrate
```

```
FFG_mass = FFG.*2.7*10^(-3); %95%H2 and 5% CH4
FFT_mass = FFT.*92.14*10^(-3);
PD_mass = PD.*154.21*10^(-3);
PB_mass = PB.*78.11*10^(-3);
RT_mass = RT.*92.14*10^(-3);
RG_mass = RG.*2*10^(-3);
FG_mass = RG_mass + FFG_mass;
FT_mass = FT.*92.14*10^(-3);
FGT_mass=FG_mass+FT_mass; % define FGT as FG+FT, total flow rate to the reactor
%manual matlab graph#3 fresh feed flow rate vs conversion
figure(3)
plot(x,FFG_mass)
hold on
plot(x,FFT_mass)
hold off
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Fresh Feed Flow Rate]
(kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
lgd = legend('Fresh Feed Hydrogen and Methane','Fresh Feed Toluene','location','northwest');
lgd.FontSize = 15;
ylim([0 70000]);
%manual matlab graph#4 production rate vs conversion
figure (4)
plot(x,PD_mass)
hold on
plot(x,yline(11415))
hold off
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Product Flow Rate]
(kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
lgd = legend('Product Diphenyl','Product Benzene','location','northwest');
lgd.FontSize = 15;
%manual matlab graph#5 limiting recycle rate vs conversion
figure (5)
plot(x,RT_mass)
ylim([0 150000]);
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Limiting Toluene Recycle Flow Rate]
(kg/hr)$','interpreter','latex');
```

```
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
%manual matlab graph#6 Total Flow rate vs conversion
figure(6)
plot(x,FGT_mass)
ylim([0 200000]);
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Total Flow Rate to Reactor]
(kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
%manual matlab graph#7&8 Total Flow rate to separation system vs conversion
FST = RG+PH+PCH4+PB+PD+RT;
yb = PB./FST;
yd = PD./FST;
yt = RT./FST;
yh = PH./FST;
ych4 = PCH4./FST;
FST_mass= ((PH.*2+PCH4.*16)+PB.*78.11+PD.*154.21+RT.*92.14)*10^(-3);
%manual matlab graph#7 Total Flow rate to separation system vs conversion
figure(7)
plot(x,FST_mass)
ylim([0 200000]);
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Total Flow Rate to Separator]
(kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
%manual matlab graph#8 Mole fraction of each component entering the separation system vs conversion
figure(8)
plot(x,yb)
hold on
plot(x,yd)
plot(x,yt)
plot(x,yh)
plot(x,ych4)
hold off
ylim([0 1]);
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Mole Fraction Entering
Separator]$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
lgd = legend('Benzene','Diphenyl','Toluene','Hydrogen','Methane','location','northwest');
lgd.FontSize = 15;
```

L.4 MATLAB Codes for Economic Potential Calculations

```
pb = 100*10^3; %mass flowrate of benzene in MT/yr
yfh = 0.95;
mb=78.11; %molar mass of butene
mt=92.14; %molar mass of toluene
md=154.21; %molar mass of diphenyl
mh=2; %molar mass of H2
mc=16.04; %molar mass of CH4
deltaH_d=5.92;  %heat of combustion in MMBtu/kmol
deltaH_h2=0.271;
deltaH_ch4=0.844;

yph=0.25;
s=0:0.01:1;

pg = ((mh*yph+mc*(1-yph))/mb)*pb./(s.*(1-yph));
pg1 = (1/mb)*(pb*10^3)./(s.*(1-yph)); %molar flow rate in kmol
pbt = pb*900; %total profit from benzene production, unit $/yr
pdt = (deltaH_d*3/mb)*pb*10^3*((1-s)./(2*s)); %total profit from diphenyl production, unit $/yr
pgt = (3*pg1)*(yph*deltaH_h2+(1-yph)*deltaH_ch4);
fftt = 600*(mt/mb)*pb./s;
fgt = 1400*((mh*yfh+mc*(1-yfh)))*(pg1*10^-3*yph+pb.*(1+s)./(mb*(2*s)))/yfh;

EP=(pbt+pdt+pgt-fftt-fgt)*10^-6; %EP, unit MM/yr


s2=0.9;
yph2=0:0.01:1;

pg2 = (mh*yph2+mc*(1-yph2))/mb.*pb./(s2*(1-yph2));
pg22 = (1/mb)*(pb*10^3)./(s2*(1-yph2));
pbt2 = pb*900; %total profit from benzne production, unit $/yr
pdt2 = (deltaH_d*3/mb)*pb*10^3*((1-s2)/(2*s2)); %total profit from diphenyl production, unit $/yr
pgt2 = (3*pg22).*(yph2*deltaH_h2+(1-yph2)*deltaH_ch4);
fftt2 = 600*(mt/mb)*pb/s2;
fgt2 = 1400*((mh*yfh+mc*(1-yfh)))*(10^-3*pg2.*yph2+pb*(1+s2)/(mb*2*s2))/yfh;

EP2=(pbt2+pdt2+pgt2-fftt2-fgt2)*10^-6;

figure
plot(s,EP)
```

```
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Selectivity]$','interpreter','latex'); yl = ylabel('$[Economic
Potential](mmdollars/year)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
figure
plot(yph2,EP2)
```

L.5 MATHEMATICA Codes for Economic Potential Calculations in Level-2 Design

```
In[1]:= Pb=100000
Out[1]= 100000
In[2]:= Eb=900
Out[2]= 900
In[35]:= FFG=Pb/((((yfh-Pb)/yph)-1)*(1-yph))
Out[35]= 100000/((-1+(-100000+yfh)/yph) (1-yph))
In[34]:= PG=(FFG*yfh-Pb)/yph
Out[34]= (-100000-(100000 yfh)/(-yfh+yph))/yph
In[36]:= Clear[EP]
In[37]:=
EP[yph_,yfh_]=Pb*Eb+PG*yph*1.416*10^8*4.25+PG*(1-yph)*5.563*10^7*4.25-119242*600-FFG*14
000-PG(1-yph)*40-(PG*(1-yph))*40
Out[37]= 18454800-1400000000/((-1+(-100000+yfh)/yph) (1-yph))+6.018*10^8 (-100000-(100000
yfh)/(-yfh+yph))+(2.36427*10^8 (1-yph) (-100000-(100000 yfh)/(-yfh+yph)))/yph
In[39]:= Plot3D[18454800-1400000000/((-1+(-100000+yfh)/yph) (1-yph))+6.018*10^8
(-100000-(100000 yfh)/(-yfh+yph))+(2.36427*10^8 (1-yph) (-100000-(100000
yfh)/(-yfh+yph)))/yph,{yfh,0,1},{yph,0,1}]
Out[39]=
In[32]:= Plot3D[(18454800+1400000000/(-yfh+yph)+6.018*10^8 (-100000-(100000
yfh)/(-yfh+yph))+(2.36427*10^8 (1-yph) (-100000-(100000
yfh)/(-yfh+yph)))/yph)/10^6,{yfh,0,1},{yph,0,1}]
```

L.6 Matlab Codes for Economic Potential Calculations in Level-3 Design without PSA and with PSA

```
% Substance Price
B = 900; % benzene $/MT
T = 600; % toluene $/MT
G = 1400; % gas feed(0.95H2+0.05CH4) $/MT
C = 40; % CO2 charge $/MT
Fuel = 4.25; %Fuel value (Diphenyl and Purge Stream) $/GJ
```

```
B1 = 900*1.05; % benzene $/MT
T1 = 600*1.05; % toluene $/MT
G1 = 1400*1.1; % gas feed(0.95H2+0.05CH4) $/MT
C1 = 40*1.15; % CO2 charge $/MT
Fuel1 = 4.25*1.2; %Fuel value (Diphenyl and Purge Stream) $/GJ
%{
yfh = 0.95;
yph = 0.7;
x = 0:0.1:1;  %nnnnnnnnnnnnnnnnnn
FT0 = 146146;
MR = 5;
PB = 146146;
%FT = FT0-x*FT0;
%index = find(F{:,1}==x);
%PB = F(index,1);
%s = PB/(FT0-FT);
s = 0.95;  %nnnnnnnnnnnnnnnnnnnn
PD = PB*(1-s)/(2*s);
RT = PB*(1-x)/(s*x);
FFT = PB/s;
FT = PB/(s*x); %level 3 FT balance
FH = MR*PB/(s*x); % FH=MR*FT;
FT1 = FT*(1-x);  %conversion, FT1 is the reactor outlet toluene flowrate(separtor inlet)
FFG= (FFT-0.5.*(FFT-PB)+FFT*yph./(1-yph))/(yfh-(1-yfh)/(1-yph)); %google doc eqn (18)&(19)
PG = FFG*(1-yfh)+FFT/(1-yph);%google doc eqn (19)
FG = FFG+(MR*PB/(x*s)-FFG*yfh)/yph;
RG = MR*PB/(x*s)-FFG*yfh;%google doc eqn (22)
FFG_mass = FFG.*2.7*10^(-3); %95%H2 and 5% CH4
FFT_mass = FFT.*92.14*10^(-3);
PD_mass = PD.*154.21*10^(-3);
PB_mass = PB*78.11*10^(-3);
RT_mass = RT.*92.14*10^(-3);
RG_mass = RG.*(yph*2+(1-yph)*16)*10^(-3);
FG_mass = RG_mass+FFG_mass;
FT_mass = FT.*92.14*10^(-3);
FGT_mass=FG_mass+FT_mass; % define FGT as FG+FT, total flow rate to the reactor
%}
```

```
% Without PSA
% FFT FFG PPG PB CO2
% produced from methane combustion as a fuel (0.0535*2795kmol/hr*44.01kg/kmol*8.76)
% 8.76 -> MT/yr
PT = 15240*8.76*600;
PGas = 1330*8.76*1400; %gas feed (-)
PB = 12920*8.76*900;
PPG = 489.6*11790*0.00876*4.25; %fuel out(+)
CO2 = 0.3875*489.6*44.01*8.76*40;
EP_max_W = PB+PPG-PT-PGas-CO2;
% With PSA
% FFT FFG PPG PB CO2
% produced from methane combustion as a fuel (0.0603*2606kmol/hr*44.01kg/kmol*8.76)
% 8.76 -> MT/yr
PT2 = 15000*8.76*600;
PG2 = 681*8.76*1400;
PB2 = 12690*8.76*900;
PPG2 = 247.6*47830*0.00876*4.25; %fuel out(+)
CO22 = 0.71*247.6*44.01*8.76*40;
EP_max_P = PB2+PPG2-PT2-PG2-CO22;
PT3 = 15000*8.76*600*1.05;
PG3 = 681*8.76*1400*1.1;
PB3 = 12690*8.76*900*1.05;
PPG3 = 247.6*47830*0.00876*4.25*1.2; %fuel out(+)
CO23 = 0.71*247.6*44.01*8.76*40;
EP_max_P3 = PB3+PPG3-PT3-PG3-CO23;
PT4 = 15000*8.76*600;
PG4 = 681*8.76*1400;
PB4 = 12690*8.76*900;
PPG4 = 247.6*47830*0.00876*4.25; %fuel out(+)
CO24 = 0.71*247.6*44.01*8.76*40*1.15;
EP_max_P4 = PB4+PPG4-PT4-PG4-CO24;
```

L.7 Matlab Codes for Equipment Cost Calculations in Level-3 Design

```
% Marshall and Swift Index
MS = 1650;
% ignored pump, mixer, splitter costs (assumption)
% direct-fired heaters
```

```
% purchased cost
a = MS./280.*5.07.*10.^3*10*8.^0.85.*(1+0+0.15);
% installed cost
b = MS./280.*5.07.*10.^3*10*8.^0.85.*(1.27+1+0+0.15);
% total cost
t = a+b;

% process furnaces
% purchased cost
a0 = MS./280.*5.52*10.^3*50.^0.85.*(1+0+0.15);
b0 = MS./280.*5.52*10.^3*50.^0.85.*(1.27+1+0+0.15);
t0 = a0+b0;

% compressors
% purchased cost
a1 = MS./280.*517.5*100.^0.82.*1.29;
% installed cost
b1 = MS./280.*517.5*100.^0.82.*(2.11+1.29);
% total cost
t1 = a1+b1;


% reactors
% purchased cost
a2 = MS./280.*101.9.*14.34^1.066*26.25^0.82*1.45*3.67;
% installed cost
b2 = MS./280.*101.9.*14.34^1.066*26.25^0.82*(2.18+1.45*3.67);
% total cost
t2 = a2+b2;

% cooler (from hysys)
t3 = 26300+129500;

% same except separator system (total equipment cost)
% Without PSA conceptual cost (no hysys included)
tt = t2+t3+2*t1+3*t0;

% With PSA conceptual cost (no hysys included)
tt1 = t2+t3+2*t1+3*t0;

% Without PSA
```

```
op = 2195430; % operating costs/yr from hysys
ecic = 2445300+3983200+t+192150; % equipment + installed cost

% With PSA
op1 = 3970720; % operating costs/yr from hysys
ecic1 = 2570600+4171600+t+192150; % equipment + installed cost
```

L.8 Matlab Codes for Without PSA Mole and Mass Balance and Separation Costs

```
yfh=0.95; %inlet hydrogen composition
yph=0.7; %outlet hydrogen combustion

x = 0.716438;  %conversion
FT0=146146; %initial toluene molar flow in [mol/hr]
MR= 5; %molar ratio
PB = 146146; %desired benzene molar flow rate in [mol/h]

s=0.280925;  %selectivity
R=8.314; %ideal gas constant in J/mol*K
T =873; %Temperature

PD = PB*(1-s)/(2*s); %Diphenyl outlet
RT = PB*(1-x)/(s*x); %Toluene Recycle
FFT = PB/s; %Fresh Toluene rate
FT = PB/(s*x); %level 3 FT balance
FH = MR*PB/(s*x); % FH=MR*FT;
FT1 = FT*(1-x);  %conversion, FT1 is the reactor outlet toluene flow rate(separator inlet)
FFG= (FFT-0.5.*(FFT-PB)+FFT*yph./(1-yph))/(yfh-(1-yfh)/(1-yph)); %google doc eqn (18)&(19)
PG = FFG*(1-yfh)+FFT/(1-yph);%google doc eqn (19)
FG = FFG+(MR*PB/(x*s)-FFG*yfh)/yph;
RG = MR*PB/(x*s)-FFG*yfh;%google doc eqn (22)

%mass flow rates
FFG_mass = FFG.*2.7*10^(-3); %95%H2 and 5% CH4
FFT_mass = FFT.*92.14*10^(-3);
PD_mass = PD.*154.21*10^(-3);
PB_mass = PB*78.11*10^(-3);
RT_mass = RT.*92.14*10^(-3);
RG_mass = RG.*(yph*2+(1-yph)*16)*10^(-3);
FG_mass = RG_mass+FFG_mass;
```

```
FT_mass = FT.*92.14*10^(-3);
FGT_mass=FG_mass+FT_mass; % define FGT as FG+FT, total flow rate to the reactor

%separation cost calculator
FST = RG+PG+PB+PD+RT; %Total outlet

yb = PB/FST; %molar ratio
yd = PD/FST; %diphenyl ratio
yt = RT/FST; %toluene ratio
yh = (RG+PG)*yph/FST; %hydrogen ratio
ych4 = (RG+PG-(RG+PG)*yph)/FST; %purge methane combustion
FST_mass= ((RG+PG)*(yh*2+ych4*16)+PB*78.11+PD*154.21+RT*92.14)*10^(-3); %Outlet mass


w=PB*R*T*1*log(1/yb)+PD*R*T*1*log(1/yd)+RT*R*T*1*log(1/yt)+(RG+PG)*R*T*(yph*log(yph/yh
)+(1-yph)*log((1-yph)/ych4));
Csep = lamda*e*w*8760 %1yr=8760hr
```

L.9 Matlab Codes for Without PSA Mol and Mass Balance and Separation Costs

```
yfh = 0.95; %inlet hydrogen composition
yph = 0.7;  %outlet hydrogen combustion
MR = 5; %molar ratio
PB = 146146; %desired benzene molar flow rate in [mol/h]

%balances for streams (mole flow rate)
FFT = PB./s;
FT = PB./(s.*x); %level 3 FT balance
FH = MR*PB./(s.*x); % FH=MR*FT;
RT = PB.*(1-x)./(s.*x);%toluene recycle stream
FT1 = FT.*(1-x);  %conversion, FT1 is the reactor outlet toluene flow rate(separator inlet)
PD = PB*(1-s)./(2*s); % level 3 PD bal

%FH = FH0-PD; % H2 bal:FH-PH-PD=0           zhe yi hang hao xiang mei yong
FFG= (FFT-0.5.*(FFT-PB)+FFT*yph./(1-yph))/(yfh-(1-yfh)/(1-yph)); %google doc eqn (18)&(19)
PG = FFG*(1-yfh)+FFT./(1-yph);%google doc eqn (19)
FG = FFG+(MR*PB./(x.*s)-FFG*yfh)./yph;
RG = MR*PB./(x.*s)-FFG*yfh; %google doc eqn (22)
%PG = FFG; %??????????????????????????????? overall bal H+CH4 in = H+CH4 out?
```

```
%mass flowrate
FFG_mass = FFG.*2.7*10^(-3); %95%H2 and 5% CH4
FFT_mass = FFT.*92.14*10^(-3);
PD_mass = PD.*154.21*10^(-3);
PB_mass = PB*78.11*10^(-3);
RT_mass = RT.*92.14*10^(-3);
RG_mass = RG.*(yph*2+(1-yph)*16)*10^(-3);
FG_mass = RG_mass+FFG_mass;
FT_mass = FT.*92.14*10^(-3);
FGT_mass=FG_mass+FT_mass; % define FGT as FG+FT, total flow rate to the reactor

%manual matlab graph#3 fresh feed flow rate vs conversion
figure(3)
plot(x,FFG_mass)
hold on
plot(x,FFT_mass)
hold off
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Fresh Feed Flow Rate] (kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
lgd = legend('Fresh Feed Oxygen and Methane','Fresh Feed Toluene','location','northwest');
lgd.FontSize = 15;

%manual matlab graph#4 production rate vs conversion
figure (4)
plot(x,PD_mass)
hold on
plot(x,yline(11415))
hold off
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Product Flow Rate] (kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
lgd = legend('Product Diphenyl','Product Benzene','location','northwest');
lgd.FontSize = 15;

%manual matlab graph#5 limiting recycle rate vs conversion
figure (5)
plot(x,RT_mass)
```

```
ylim([0 150000]);
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Limiting Toluene Recycle Flow Rate] (kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');

%manual matlab graph#6 Total Flow rate vs conversion
figure(6)
plot(x,FGT_mass)
ylim([0 200000]);
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Total Flow Rate to Reactor] (kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');

%manual matlab graph#7&8 Total Flow rate to separation system vs conversion

FST = RG+PG+PB+PD+RT;

yb = PB./FST;
yd = PD./FST;
yt = RT./FST;
yh = (RG+PG).*yph./FST;
ych4 = (RG+PG-(RG+PG).*yph)./FST;

FST_mass= ((RG+PG).*(yh.*2+ych4.*16)+PB.*78.11+PD.*154.21+RT.*92.14)*10^(-3);

%manual matlab graph#7 Total Flow rate to separation system vs conversion
figure(7)
plot(x,FST_mass)
ylim([0 200000]);
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Total Flow Rate to Separator] (kg/hr)$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');

%manual matlab graph#8 Mole fraction of each component entering the separation system vs conversion

figure(8)
plot(x,yb)
hold on
```

```
plot(x,yd)
plot(x,yt)
plot(x,yh)
plot(x,ych4)
hold off
ylim([0 1]);
a =gca; set(a,'Fontsize',15,'FontName','Times');%,'XTick',[0:0.1:0.8],'YTick',[-3:0.5:2]);
xl = xlabel('$[Conversion]$','interpreter','latex'); yl = ylabel('$[Mole Fraction Entering
Separator]$','interpreter','latex');
set(xl,'Fontsize',20,'FontName','Times');set(yl,'Fontsize',20,'FontName','Helvetica');
lgd = legend('Benzene','Diphenyl','Toluene','Hydrogen','Methane','location','northwest');
lgd.FontSize = 15;
```

L.10 Matlab Codes for PSA system and Distillation Column Calculations

```
%% The Langmur Model
T=303; %T in K
P=1:80; %P in ATM
%The k's
k1=4.89;
k2=-0.00905;
k3=0.000534;
k4=1795.9;
k5=0.396;
k6=187.4;
qmax=k1+k2*T;
B=k3*exp(k4/T);
n=k5+k6/T;
%Langmur Eqution
q=(qmax*B*P.^n)./(1+B*P.^n);
plot(P,q) %Absorbtion plot
%% PSA Size Calculation
%Feed Data
Fin=277.78; %Fin in mol/s
Pin=25; %Feed Presure In ATM
nH=0.6; %Hydrogen Molar Fraction in Feed
nCH4=0.4; %Methane Molar Fraction in Feed
%Recovery Data
Pout=2;  %Off Gas Presure In ATM
outH=0.9; %Recovery Rate
%Other Data
t=300; %Absortion time
```

```
f=0.95; %Load Fraction
FinH=Fin*nH; %Hydrogen Feed
FinCH4=Fin*nCH4; %Methane Feed
FoutH=FinH*outH; %Hydrogen Out
HOff=FinH-FoutH; %Hydrogen Off Gas
nHOFF=HOff/(FinCH4+HOff); %Hydrogen Off Gas Fraction
nCH4OFF=FinCH4/(FinCH4+HOff); %Methane Off Gas Fraction
PPinCH4=nCH4*Pin; %Methane Partial Pressure In
PPoutCH4=nCH4OFF*Pout; %Methane Partial Pressure Out
qh=(qmax*B*PPinCH4.^n)./(1+B*PPinCH4.^n);
qL=(qmax*B*PPoutCH4.^n)./(1+B*PPoutCH4.^n);
Mb=((FinCH4*t)/((qh-qL)*f)); %Total Adsorbent For One Bed in kg
TotalMB=Mb*10^-3*4; %Total Adsorbent Mass in MT
Vol=Mb/(795*0.8); %Volume of One Bed
D=(Vol/pi)^(1/3);
L=4*D;



F = 1.286*10^6;% mol/hr
T = 595.6+273.15; % in K
P = 2100; % in kPa
zt = 0.0339;
zh = 0.7131;
zb = 0.1065;
zm = 0.1364;
zd = 0.01;
q = 1;

BDVLE=readmatrix('benzene_diphenyl.txt');
x1 = BDVLE(:,1);
y1 = BDVLE(:,2);
TDVLE=readmatrix('toluene_diphenyl.txt');
x2 = TDVLE(:,1);
y2 = TDVLE(:,2);

a_BD = 21.59;
a_TD = 9.441;

R_min = a_TD*(zb+zt)/(zb*(a_BD-a_TD))+zd/(zb*(a_BD-1));
R = 1.5*R_min;
D = F*zb;
```

```
B = F*(zt+zd);
s = D/B*(R+q)-(1-q);
a_avg = (a_TD * a_BD)^(1/2);
Nmin = log((0.998*0.997)/((1-0.998)*(1-0.997)))/(log(a_avg));

syms N
eqn = (N-Nmin)/(N+1) == 0.75*(1-(R-R_min)/(R+1))^(0.5688);
Y = solve(eqn,N,'Real',true);
N =  46658679190790189/3066699211313907;
N_real = 1.5*N; % the real number of stages

V_B = s*B;
V_T = (R+1)*D;
L_B = B*(1+s);
L_T = R*D;

Lamda_D = 32.2; % molar latent heat of distillate (benzene) in kJ/mol
Lamda_B = (34.4+57.5)/2; % molar latent heat of bottom (toluene and diphenyl) in kJ/mol

% heat loads on the condenser and reboiler
Q_C = Lamda_D*V_T; % kJ/hr
Q_R = Lamda_B*V_B; % kJ/hr

% column diameter
p_toluene = 897; % liquid toluene density in kg/m^3
p_toluene2 = 0.016; % gas toluene density in kg/m^3
p_benzene = 890; % liquid benzene density in kg/m^3
p_benzene2 = 0.16;% gas benzene density in kg/m^3
p_diphenyl = 323; % diphenyl density in kg/m^3
p_diphenyl2 = 80;
MW_Vtop = 0.07811; % vapor molar weight(kg/mol), mostly benzene
MW_Vbot = 0.09214*zt/(zt+zd)+0.15421*zd/(zt+zd);

p_vt = p_benzene2;
p_lt = p_benzene;
p_vb = p_toluene2*zt/(zt+zd)+p_diphenyl2*zd/(zt+zd);
p_lb = p_toluene*zt/(zt+zd)+p_diphenyl*zd/(zt+zd);
Mvb = 2; %æ”¹
Mlb = 4;
```

```
ft = (L_T/V_T)*(p_vt/p_lt)^0.5; %flow parameter at top, D&M Eqn 6.7
fb = (L_B/V_B)*(p_vb/p_lt)^0.5*(Mvb/Mlb)^1.5; %flow parameter at bottom
ct = 439/(1+2.5*ft^1.2); %capaccity parameter at the top, choose tray spacing 24 in, c unit in m/h
cb = 439/(1+2.5*fb^1.2);
Ft_flood = 0.8*(p_lt-p_vt)^0.5*ct; %at top, D&M eqn 6.10
Fb_flood = 0.8*(p_lb-p_vb)^0.5*cb;

At = MW_Vtop/(0.6*Ft_flood*p_vt^0.5)*V_T;
AB = MW_Vbot/(0.6*Fb_flood*p_vb^0.5)*V_B;
Dt = 2*sqrt(At/3.14);
DB = 2*sqrt(AB/3.14);

% column height
H_t = 0.6; % meters
H = 3*H_t +H_t*N_real;

% reboiler and condenser heat exchange
A_C = Q_C*1000/(1600*318.15*3600); % at 45 C
A_R = Q_R*1000/(1600*318.15*3600); % at 45 C

% second column
a_TD2 = 9.441;
R_min2 = 1*1/(0.77*(a_TD2-1));

R2 = 1.5*R_min2;

D2 = F*(zt+zd)*0.77; % mol/hr
B2 = F*(zt+zd)*0.23;
%72110*0.1791; % mol/hr
s2 = D2/B2*(R2+q)-(1-q);
a_avg2 = a_TD2;
Nmin2 = log((0.998*0.997)/((1-0.998)*(1-0.997)))/(log(a_avg2));
syms N2
eqn = (N2-Nmin2)/(N2+1) == 0.75*(1-(R2-R_min2)/(R2+1))^(0.5688);
Y2 = solve(eqn,N2,'Real',true);
N2 = 27365578415648071/1247651968848981;
N_real2 = 2*N2; % the real number of stages

V_B2 = s2*B2;
V_T2 = (R2+1)*D2;
L_B2 = B2*(1+s2);
```

```
L_T2 = R2*D2;

Lamda_D2 = 34.4; % molar latent heat of distillate (toluene) in kJ/mol
Lamda_B2 = 57.5; % molar latent heat of bottom (diphenyl) in kJ/mol

% heat loads on the condenser and reboiler
Q_C2 = Lamda_D2*V_T2; % kJ/hr
Q_R2 = Lamda_B2*V_B2; % kJ/hr


p_vt2 = p_toluene2;
p_lt2 = p_toluene;
ft2 = (L_T2/V_T2)*(p_vt2/p_lt2)^0.5; %flow parameter at top, D&M Eqn 6.7
ct2 = 439/(1+2.5*ft2^1.2); %capaccity parameter at the top, choose tray spacing 24 in, c unit in m/h
Ft_flood2 = 0.8*(p_lt2-p_vt2)^0.5*ct2; %at top, D&M eqn 6.10

MW_Vtop2 = 0.09214;
At2 = MW_Vtop2/(0.6*Ft_flood2*p_vt2^0.5)*V_T;
Dt2 = 2*sqrt(At2/3.14);


% column height
H_t2 = 0.5; % meters
H2 = 3*H_t2 +H_t2*N_real2;

% reboiler and condenser heat exchange

A_C2 = Q_C2*1000/(1600*318.15*3600); % at 45 C
A_R2 = Q_R2*1000/(1600*318.15*3600); % at 45 C
```

M. HAZOP Analysis

M.1 PFR HAZOP

Item	Study Node	Process Parameters	Guide Word	Possible Causes	Existing Safeguards	Action Required
1A	Reactor	Flow	No	● Clog in the feed pipes ● Leak in the feed pipes ● Leak in the reactor vessel ● Clog in reactor vessel ● Feed compressor/pump loss of power ● Feed compressor/pump leak or failure ● Feed compressor/pump clog ● Critical power failure ● PSA Failure	● Performing regular leak assessments. ● Performing regular electrical/wiring assessments. ● Regular quality assessments on the reactor product to assess any possible contaminate ● Insulating the pipes ● Using an corrosive resistant materials	● Stop all reaction operations ● Contact Emergency Services ● Use the secondary containment flair to discard all products ● Seal all pipes leaving and coming from the reactor ● Once the reactor clear performs an leak/clog assessment ● Perform an electrical assessment ● Restart the plant with the standard restart procedure. When restart the plant an unit safety analysis should be conducted
1B			High	● Too much reactants in the feed pipe ● PSA failure	● Preprocess storge of all reactants ● Controlled Flow addition of fluids to the reactant using valves and process control	● Lower the flow rate of the feed ● Monitor for a possible sign of a pressure jump. If pressure increases too much, stop all reaction operations
1C			Lower	● Clog in the feed pipes ● Leak in the feed pipes	● Performing regular leak assessments	● Perform a leak/clog assessment

				• Leak in the Reactor vessel • Clog in Reactor Vessel • Feed Compressor/pump loss of power • Feed Compressor/pump leak Feed Compressor/pump clog • Having too little feed	• Regular quality assessments on the reactor products to assess any possible contaminate • Insulating the pipes • Using corrosive resistant materials	• If flow rate in the feed pipes and in the feed is too low or there is rapid pressure drop, end all reactor operations Contact Emergency Services. Use the secondary containment flair to discard all products
1D			Part of	• Clog in the feed pipes • Leak in the feed pipes • Change in feed purity • Corrosion in the feed pipes • Feed contamination • PSA failure	• Performing semi regular feed quality testing • Performing corrosion assessments.	• In the case of a change in reactor composition it is important to maintain safe temperature and pressure levels. It may be useful to move to a different operating condition. • If the reactor composition is not manageable, stop all reaction operations
1E			Reverse	• Feed compressor/pump leak or failure • Feed compressor/pump power failure	• Performing regular leak assessments. • Using corrosive resistant materials • Performing regular electrical/wiring assessments	• Stop all reaction operations • Seal all pipes leaving and coming from the reactor • Perform an electrical assessment

1D			Other Than	Clog in the feed pipes Leak in the feed pipes Change in feed purity Corrosion in the feed pipes Feed contamination	Performing semi regular feed quality testings Performing corrosion assessments	Stop all reaction operations Contact Emergency Services Use the secondary containment flair to discard all products Seal all pipes leaving and coming from the reactor Once the reactor clear performs an contaminant assessment
2A		Temperature	Higher	Clogging of the heating jacket Heating jacket leak or block Reactor contamination Reactor pressure drop Failure in temperature process control Failure in pressure process control	Performing regular leak assessments. Having an secondary jacket cooling Having secondary temperature process control Using soft water in the heating jackets	Activate the secondary cooling jacket If continues stop all reaction operations Contact Emergency Services Use the secondary containment flair to discard all products Access the process control
2B			Lower	Increase Reactor Pressure Reactor Leak Feed contamination Failure in Temperature process control Failure in Pressure process control PSA failure	Using corrosive resistant materials Having secondary temperature process control	Lower the heating jacket duty Lower the reaction pressure with the containment flair

2C			Sooner	• Drop-in feed rate due to valve failure or leak • Failure in temperature process control	• Having secondary temperature process control • Performing regular leak assessments	• Use the secondary process control instruments to adjust the heating jacket • If needed use the emergency secondary cooling jacket
			Later	• Increase in the feed rate • Feed contamination	• Performing semi regular feed quality testing • Performing corrosion assessments	• Lower the heating jacket duty by lowering the amount of water is sent to the system
3A		Pressure	Higher	• Drop in temperature • Clog in reactor • Increase in the flow rate • Failure in temperature process control • Failure in pressure process control • Clog in reactor product stream	• Having secondary pressure process control • Having an safety valves for the feeds entering and leaving the process	• Use the secondary containment flair to discard some of the products • Lower the feed pump level • Lower the temperature of the reactor by lowering the duty of the heating jacket
3B			Lower	• Having an leak in the feed or reactor • Failure in temperature process control • Failure in pressure process control • Feed pump power failure • Feed pump mechanical failure	• Performing regular leak assessments. • Having secondary pressure process control • Insulating the pipes • Using corrosive resistant materials • Enclosing the reactor to the	• Switch to the secondary pump mechanism • If the pressure drops rapidly stop all reaction operations • Contact emergency services • Use the secondary containment flair to discard all products

					surrounding using cement - Having a secondary pump mechanism	- Seal all pipes leaving and coming from the reactor - Once the reactor clear performs an leak/clog assessment
3C			Sooner	- Clog in the reactor product stream - Increased Feed	- Performing semi regular feed quality testing - Performing corrosion assessments. - Having safety valves and secondary pressure relief mechanism	- Use the secondary containment flair to discard some of the products - Lower the heating duty on the jacket
3D			Later	- Feed pump power failure - Feed pump mechanical failure	- Having an secondary pump mechanism	- Switch to the secondary pump mechanism - If the pressure drops rapidly stop all reaction operations - Contact Emergency Services - Use the secondary containment flair to discard all products - Seal all pipes leaving and coming from the reactor - Once the reactor clear performs an leak/clog assessment
4A		Concentration	No	- Lack of flow - Clog in the feed pipes	- Performing regular leak assessments	- Stop all reaction operations

				• Leak in the feed pipes • Leak in the reactor vessel • Clog in reactor vessel • Feed compressor/pump loss of power • Feed compressor/pump leak or failure • Feed compressor/pump clog • Critical power Failure	• Performing regular electrical/wiring assessments. • Regular quality easements on the reactor product to assess any possible contaminate • Insulating the pipes • Using an corrosive resistant materials	• Contact Emergency Services • Restart the plant with the standard restart procedure. When restart the plant an unit safety analysis should be conducted
4B			Higher	• Too much feed • PSA failure	• Doing regular feed quality testing • Having recycle quality testing • Having an secondary process control on the PSA	• Close the gas recycle valve and bypass the PSA and send all the gas to the furnace • Switch to secondary gas pumps
4C			Lower	• Leak in the feed pipes • PSA failure	• Performing regular leak assessments. • Having secondary pressure process control • Insulating the pipes • Using corrosive resistant materials • Doing regular feed quality testing	• Perform a leak/clog assessment. • If flow rate in the feed pipes and in the feed is too low or there is a rapid pressure drop, end all reactor operations Contact Emergency Services. Use the secondary containment flair to discard all products • Close the gas recycle valve and bypass the PSA and send all the gas to the furnace

						• Switch to secondary gas pumps
4E			Other Then	• Feed contamination	• Doing regular feed quality testing	• Continue to work as usual with monitoring temperature and pressure of the reactor • If temperature and pressure of the reactor go outside the safe operating conditions or of product, quality drops too low which ends all reactor operations • Restart the plant with the standard restart procedure. When restart the plant an unit safety analysis should be conducted • Consider switching feed suppliers

M.2 Distillation Column-1 HAZOP and MSDS

Item	Study Node	Process Parameters	Guide Word	Possible Causes	Existing Safeguards	Action Required
5A	Distillation Column-1	Flow	No	• Clog in the feed pipes • Leak in the feed pipes • Leak in the Distillation Column • Clog in Distillation Column • Critical Power Failure • Valve failure	• Preforming regular leak assessments. • Regular quality easements on the reactor product to assess any possible contaminate • Insulating the pipes • Having secondary safety valves	• Stop all distillation operations • Contact Emergency Services • Once the plant is clear clear performs an leak/clog assessment • Restart the plant with the standard restart procedure. When restart the plant an unit safety analysis should be conducted • Do an safety quality analysis on the flash drum
5B			High	• Flash drum failure • Flash drum too cold • Flash drum pressure leak • Reactor Temperature Too Low	• Preforming regular leak assessments. • Secondary process control on all unit ops	• Depending on the feed composition lower the reflux rate of the feed. • Monitor for an possible sign of an liquid height jump. If flooding in the reactor is too high stop reactor operations.
5C			Lower	• Clog in the feed pipes • Leak in the feed pipes • Leak in the distillation vessel •	• Preforming regular leak assessments. • Regular quality easements on the reactor product to assess any possible contaminate • Insulating the pipes	• Perform an leak/clog assessment. • If flow rate in the feed pipes and in the feed is too low or there is too much weeping lower the rate on the reboiler.

					- Using corrosive resistant martials	
5D			Part of	- Clog in the feed pipes - Leak in the feed pipes - Change in feed purity - Corrosion in the feed pipes - Feed Contamination - Flash Drum failure	- Performing semi regular feed quality testing - Preforming corrosion assessments. - Having an secondary process control on the reactor	- Depending on the nature of the containment it may be useful to stop all reaction operations if the particle is small and the change of the feed is dependent quality wise it may be useful to recalibrate the boiler and reflux drum and increase or decrease the reflux and or boil up ratio.
6A		Temperature	Higher	- Feed contamination - Feed pressure drop - Flash drum clog - Reboiler clog or leak - Failure in Temperature process control - Failure in Pressure process control - Flash Drum Failure - Tray failure	- Performing regular quality and safety on the flash drum and reboiler. - Having secondary temperature process control	- Decrease the steam rate to the reboiler and or increase the cooling water to the condenser. - Decrease the distillation pressure - If continues and or extreme weeping is observed stop all reaction operations - Contact Emergency Services discard all products - Access the process control for an top down safety assement

6B			Lower	• Increase Distillation Column Pressure • Distillation Column Leak • Feed contamination • Failure in Temperature process control • Failure in Pressure process control • Tray clogging or failure	• Using corrosive resistant martials • Having secondary temperature process control	• Increase the pressure of the distillation column. • Increase the steam rate to the reboiler and or decrease the cooling water to the condenser. • If continues and or extreme flooding is observed stop all reaction operations • Contact Emergency Services discard all products
7A		Pressure	Higher	• Increase in temperature due to reboiler failure and or reflux drum • Clog in the dilatation column • Failure in Temperature process control • Failure in Pressure process control • Flash drum failure	• Having an safety valves for the feeds entering and leaving the process • Performing regular quality and safety on the flash drum and reboiler.	• Change the operating conditions of the reboilers and or condenser • Change the flash drum operating conditions • If the problem prosaists end distillation operations and perform and top down safety analysis
7B			Lower	• Having an leek in the feed or distillation drum • Failure in the falsh drum • Decrease in temperature due to reboiler failure and or reflux drum • Failure in Temperature process control • Failure in Pressure process control	• Preforming regular leak assessments. • Having secondary pressure process control • Insulating the pipes • Using corrosive resistant martials • Having an secondary pump mechanism	• Switch to the secondary pump mechanism • Perform an safety assessment on the flash drum. • If the pressure drops rapidly stop all distillation operations • Contact Emergency Services

					• Having seconder pressure process control	• Use the secondary containment flair to discard all products • Seal all pipes leaving and coming from the distillation column.

Team Member Work Statement

Michael Xing

I did most of the data analysis, writings, Hysys designs, and everything associated with this project.

Selina Liu

Revised the balances on process design, wrote Matlab code, made NPV calculation spreadsheet and sencitvity analysis. Wrote the report.

Yunus Ross

Wrote the Statement of process chemistrand process diagrams and program files for the level 2. Helped to create the MATLAB level 2 flow sheet and economic balance Made the HAZOP analysis for PFR-1. Did the safety research and calculations.

Print Name and Sign: _____________Langqi Xing____________________ Date: _____04/27/2022____

Print Name and Sign ____________Selina Liu_____________________ Date: ___04/27/2022______

Priname and Sign _____________Yunus Ross____________________ Date: ___04/27/2022______

Rating of Team Members for Design Project

Please rate each group member’s contributions in the categories below:
1-2 - unsatisfactory, 3 - acceptable/adequate, 4 – very good, 5 - excellent
Each member fills out one form and signs the bottom.

Name :	1) ____Michael Xing______	2) ___Yunus Ross_______	3) _______Selina Liu_________
Quality of work presented	__5___	___4__	___5__
Quantity of work performed	___5__	___4__	__5___
Effort	__5___	__5___	__5___
Punctuality (meetings and deadlines)	___5__	__5___	__5___
Knowledge of design methods	___5__	__5___	__5___
Class attendance	__5___	__5___	__5___
Communication	__5___	__5___	__5___

Do you feel that each member of the group deserves the same grade? If not, who does not and why?

Yes, each member of the group deserves the same grade.

It’s important to note that differences in performance will not necessarily affect individual grades; however, large discrepancies may result in differences in grades.

Additional comments:

Print Name and Sign: ________________Langqi Xing_____________________ Date:
______04/27/2022_____

Rating of Team Members for Design Project

Please rate each group member’s contributions in the categories below:
1-2 - unsatisfactory, 3 - acceptable/adequate, 4 – very good, 5 - excellent
Each member fills out one form and signs the bottom.

Name : 1) ____Langqi Xing______ 2) ___Yunus Ross_______ 3) _______Selina Liu_________

Quality of work presented	__5___	___4__	___5__
Quantity of work performed	___5__	___4__	__5___
Effort	__5___	__5___	__5___
Punctuality (meetings and deadlines)	___5__	__5___	__5___
Knowledge of design methods	___5__	__5___	__5___
Class attendance	__5___	__5___	__5___
Communication	__5___	__5___	__5___

Do you feel that each member of the group deserves the same grade? If not, who does not and why?

Yes, each member of the group deserves the same grade.

It’s important to note that differences in performance will not necessarily affect individual grades; however, large discrepancies may result in differences in grades.

Additional comments:

Print Name and Sign: _______________Selina Liu____________________ Date:
______04/27/2022____

Rating of Team Members for Design Project

Please rate each group member’s contributions in the categories below:
1-2 - unsatisfactory, 3 - acceptable/adequate, 4 – very good, 5 - excellent
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Name :	1) ____Michael Xing______	2) ___Yunus Ross_______	3) _______Selina Liu_________
Quality of work presented	__5___	___5__	___5__
Quantity of work performed	___5__	___4__	__5___
Effort	__5___	__5___	__5___
Punctuality (meetings and deadlines)	___5__	__5___	__5___
Knowledge of design methods	___5__	__4___	__5___
Class attendance	__5___	__5___	__5___
Communication	__4___	__5___	__4___

Do you feel that each member of the group deserves the same grade? If not, who does not and why?

Yes, each member of the group deserves the same grade.

It’s important to note that differences in performance will not necessarily affect individual grades; however, large discrepancies may result in differences in grades.

Additional comments:

Print Name and Sign: ________________Yunus Ross_____________________ Date:
______04/27/2022_____