A DESIGN APPROACH FOR ON-PURPOSE PROPYLENE PRODUCTION WITH SAFETY AND SUSTAINABILITY CONSIDERATIONS

A Thesis

by

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ABSTRACT

The advent of Shale Gas and the increasing spread between the supply and demand curves for propylene present an opportunity for adopting alternative pathways to produce propylene. This study aims to investigate a sustainable process design approach to on-purpose propylene production. An FEL-1 level analysis was performed on the various technologies used to produce on-purpose propylene and it was determined that propane dehydrogenation (PDH) was the most profitable route. A hierarchical approach to sustainable process design is proposed and implemented in a case study with propane dehydrogenation (PDH) as the process under consideration. A base case design was developed and avenues for reduction in overall energy and water consumption, as well as reduction in carbon and VOC emissions, were analyzed. Process integration and intensification techniques were applied to reduce dependence on external utilities and to lower the overall capital investment. Waste heat recovery and off gas recycle were additional options used to intensify the overall energy consumption of the process. Emissions from the process were calculated from the EPA's guidelines. Economic and environmental metrics models were then developed to study the impact of the integration and intensification techniques. Up to 70% reductions in CO2 emissions were achieved as a result of this approach to sustainable design. The Sustainability Weighted Return on Investment (SWROI) metric was evaluated for all cases. In addition, an inherent safety analysis was performed of the flowsheets developed and the PRI and PSI indices were estimated to identify potentially high-risk streams. Multi-objective decision making for the optimum design was facilitated by the sustainability and safety metrics augmented with the traditional economic criteria.

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NOMENCLATURE

PDH	Propane Dehydrogenation
OPP	On-purpose Propylene
FCC	Fluidized Catalytic Cracking
NGL's	Natural Gas Liquids
MTO	Methanol to Olefins
MTP	Methanol to Propylene
MTA	Metric Tons per Annum
MISR	Metric for Inspecting Sales and Reactants
HEN	Heat Exchanger Network
MER	Minimum Energy Requirements
CC	Composite Curve
GCC	Grand Composite Curve
CCR	Continuous Catalyst Regeneration
SHP	Selective Hydrogenation Process
PSA	Pressure Swing Adsorption
PP Splitter	Propylene-Propane Splitter
HPC	Heat Pump Compressor
OGR	Off-Gas Recycle
WHR	Waste Heat Recovery
DCFROR	Discounted Cash Flow Rate of Return
MACRS	Modified Accelerated Cost Recovery System

IRR	Internal Rate of Return
ROI	Return on Investment
NPV	Net Present Value
EPA	Environmental Protection Agency
SWROI	Sustainability Weighted Return on Investment
SASWROIM	Safety and Sustainability Weighted Return on Investment Metric
ASP	Annual Sustainability Profit
ASSP	Annual Safety and Sustainability Profit
AEP	Annual Economic Profit
LFL	Lower Flammability Limit
UFL	Upper Flammability Limit
QRA	Quantitative Risk Assessment
PIIS	Prototype Index for Inherent Safety
ISI	Inherent Safety Index
PRI	Process Route Index
PSI	Process Stream Index

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1. INTRODUCTION

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Fossil resources have seen an incredible shift in resource consumption, utilization, and treatment strategies in recent years as shale oil and gas have emerged as one of the most lucrative energy options for the United States. Shale based natural gas in the US Gulf Coast has spurred recent increase in industrial activities and is projected to continue growing in the near future. While it is important to continue the growth for the US manufacturing jobs, it is also crucial that the sustainability of processes is taken into account while designing and operating these new processes. Annual production from shale gas has increased from 1,293 billion cubic feet (Bcf) in 2007, to 15,213 billion cubic feet in 2015, accounting for approximately 44% of the total United States natural gas production(Al-Douri et al., 2017). The Energy Information Administration projects that shale gas is going to make-up roughly two-thirds of total U.S. Natural Gas production by 2040, thereby accounting for a quarter of the U.S. energy production (U.S.EIA, 2017b). It is estimated that over the next two decades US will have cumulative production of 459 trillion cubic feet (Tcf) of shale gas which can be used to produce a wide variety of value-added chemicals and fuels (Al-Douri et al., 2017, Siirola, 2014, Zhang and El-Halwagi, 2017) with major shifts in manufacturing routes, supply chains, and environmental impact (Hasaneen and El-Halwagi, 2017, Gao and You, 2015).

Shale gas typically has more Natural Gas Liquids (NGLs) and introduces new clean feedstock in the form of ethane, propane, butanes and higher hydrocarbons in the market. Such

NGLs offer attractive pathways to produce olefins (Ortiz-Espinoza et al., 2017b, Thiruvenkataswamy et al., 2016, He and You, 2016, Yang and You, 2017). In particular, the production of propylene will be highly impacted by the increasing supply of shale gas.

Propylene has traditionally been produced as a by-product of ethylene from steam cracking, or as a by-product of gasoline in fluid catalytic cracking (FCC) in refineries. Together, these technologies accounted for 90% of the propylene market until 2012 (ICIS, 2012). Recently, the availability of low cost ethane in the United States has shifted the steam cracker feed from naphtha to ethane primarily due to higher yields in ethylene obtained by using ethane (ICIS, 2012). The production of propylene from FCC depends on the gasoline prices. If prices are high, the propylene produced is used to make octane-boosting alkylate. On the other hand, if the demand is low, refiners cut operations and propylene output falls. This implies that the propylene supply was dictated more by the developments in the gasoline and ethylene markets, than the demand for propylene.

The demand for propylene is expected to grow from 109 million tons in 2014, to about 165 million tons by 2030, roughly 12-14% greater than the amount of propylene that can be produced by the conventional technologies (Mackenzie, 2014). This gap between demand and supply can be filled by the new ‘on-purpose’ propylene technologies (OPP) which utilize feedstocks derived from shale gas. Examples include Propane Dehydrogenation (PDH), Methanol-to-Propylene/Olefins (MTP/MTO), and Olefin Metathesis. The choice of the optimal production route depends on various factors such as feedstock availability, market conditions, price volatility, technology maturity, sustainability, and safety (Guillen-Cuevas et al., 2018, Roy et al., 2016).

Process systems engineering tools offer an attractive framework for incorporating sustainability in the conceptual design and optimization of process technologies. Several reviews and textbooks cover the principles, techniques, and applications of systems approaches to the inclusion of sustainability in the creation and assessment of process flowsheets. Examples include the use of process integration (Sengupta and El-Halwagi, 2017, El-Halwagi and Yee Foo, 2000, El-Halwagi, 1997, El-Halwagi, 2017a, Foo et al., 2012, Sikdar, 2001) , green chemistry and engineering (Allen and Shonnard, 2001, Anastas and Zimmerman, 2003), sustainable design of processes, products, and supply chain, and sustainability metrics. Focus has also been given to the sustainable design aspects in engineering for the creation of products (You, 2015, Ruiz-Mercado and Cabezas, 2016). Sikdar highlighted the need of sustainability evaluation of processes and systems through the use of sustainability metrics (Sikdar, 2003). Material efficiency, water conservation, energy efficiency and greenhouse gas emissions are some of the metrics that have been used to compare various processes for sustainability (Sikdar et al., 2017). A complete analysis of sustainability of processes is often not possible due to several conflicting goals, measurement and our inability to compare all options (Mukherjee et al., 2015). Recently, El-Halwagi has introduced the Sustainably Weighted Return on Investment (SWROI) metric (El-Halwagi, 2017e) which augments sustainability criteria in the conventional calculation of financial return on investment. The use of aggregated metrics, such as the SWROI, can help the decision makers to easily determine and interpret the sustainability tradeoffs of a process and in terms of traditional indicators such as ROI. It should be mentioned that sustainable process design is different from product sustainability where the entire life cycle of a product is taken into account and each life cycle stage is evaluated, which is not the focus of this paper.

In this paper, several propylene-production pathways are studied, assessed, and screened based on multiple criteria. First, high-level screening is carried out to provide preliminary screening. The promising pathways are simulated with sufficient details to enable conceptual design and techno-economic analysis. Process integration is carried out to enhance the performance of each pathway. Economic, environmental, and safety metrics are used in the assessment. This case study for on-purpose propylene production process is used to systematically develop a method to assess sustainability and safety of the process during the initial design phases.

2. PROBLEM STATEMENT

Reprinted (adapted) with permission from AGARWAL, A., SENGUPTA, D. & EL-HALWAGI, M. 2018. Sustainable Process Design Approach for On-Purpose Propylene Production and Intensification. ACS Sustainable Chemistry & Engineering, 6, 2407-2421. Copyright (2018) American Chemical Society.

It has been clear that the market for propylene is facing a supply gap owing to the shift in feedstock of naphtha crackers to ethane and volatility in the prices of gasoline. This work looks to address this supply gap by analyzing alternatives ways to produce propylene. In addition, the rising concerns of climate change have made it necessary to design processes which are sustainable and have a lower carbon footprint. This study aims to design a sustainable on-purpose propylene production facility. For the purpose of this work, the United States Gulf Coast is chosen as the desired location because of the proximity to cheap feedstock sources. A techno-economic analysis is carried out to answer the following questions:

1) What is the most promising economic route for propylene production?
2) What does the process flowsheet look like for this route?
3) What are the key sustainability metrics associated with this process?
4) What process changes can be made to improve the sustainability performance of the process?
5) How do these changes affect the economics and overall sustainability of the process?
6) Which is the desired process flowsheet based on economic and sustainability criteria?
7) Do new metrics for sustainability in economic terms (SWROI) help in making better selection of processes?

8) How do the changes made due to process integration and intensification affect the inherent safety of the process?

A base case design with a capacity of 600,000 metric tons per annum (MTA) propylene production is designed. The available feedstocks considered are propane, ethane/ethylene, butylene, and methanol depending on the type of OPP technology used.

3. METHODOLOGY

Reprinted (adapted) with permission from AGARWAL, A., SENGUPTA, D. & EL-HALWAGI, M. 2018. Sustainable Process Design Approach for On-Purpose Propylene Production and Intensification. ACS Sustainable Chemistry & Engineering, 6, 2407-2421. Copyright (2018) American Chemical Society.

The proposed method for the assessment and screening of the various propylene-production pathways uses a hierarchical approach that starts with limited data and calculations to perform a preliminary screening, then, proceeds with more detailed analysis for the promising alternatives. Techno-economic assessment and sustainability analysis is carried out and integrated with the economic criteria. ***Figure 1*** shows a summary of these steps.

Process data inventory is created in the first step by collecting information on the various process alternatives, their feedstocks, the chemical pathways to produce the desired product, and the feedstock and product market prices.

Stoichiometric-economic targeting is performed to quickly eliminate certain process options based on overall profitability of a process. This uses the data from the process data inventory. The metric for inspecting sales and reactants "MISR" (El-Halwagi, 2017b) is used as the indicator in this case as shown in Equation 1. If the value of the MISR is less than one, the pathway is discarded. For pathways with MISR > 1, the process in considered to be potentially viable which warrants a more detailed techno-economic analysis to assess the profitability criteria of the process. As a rule of thumb, higher values of MISR are typically more desirable.

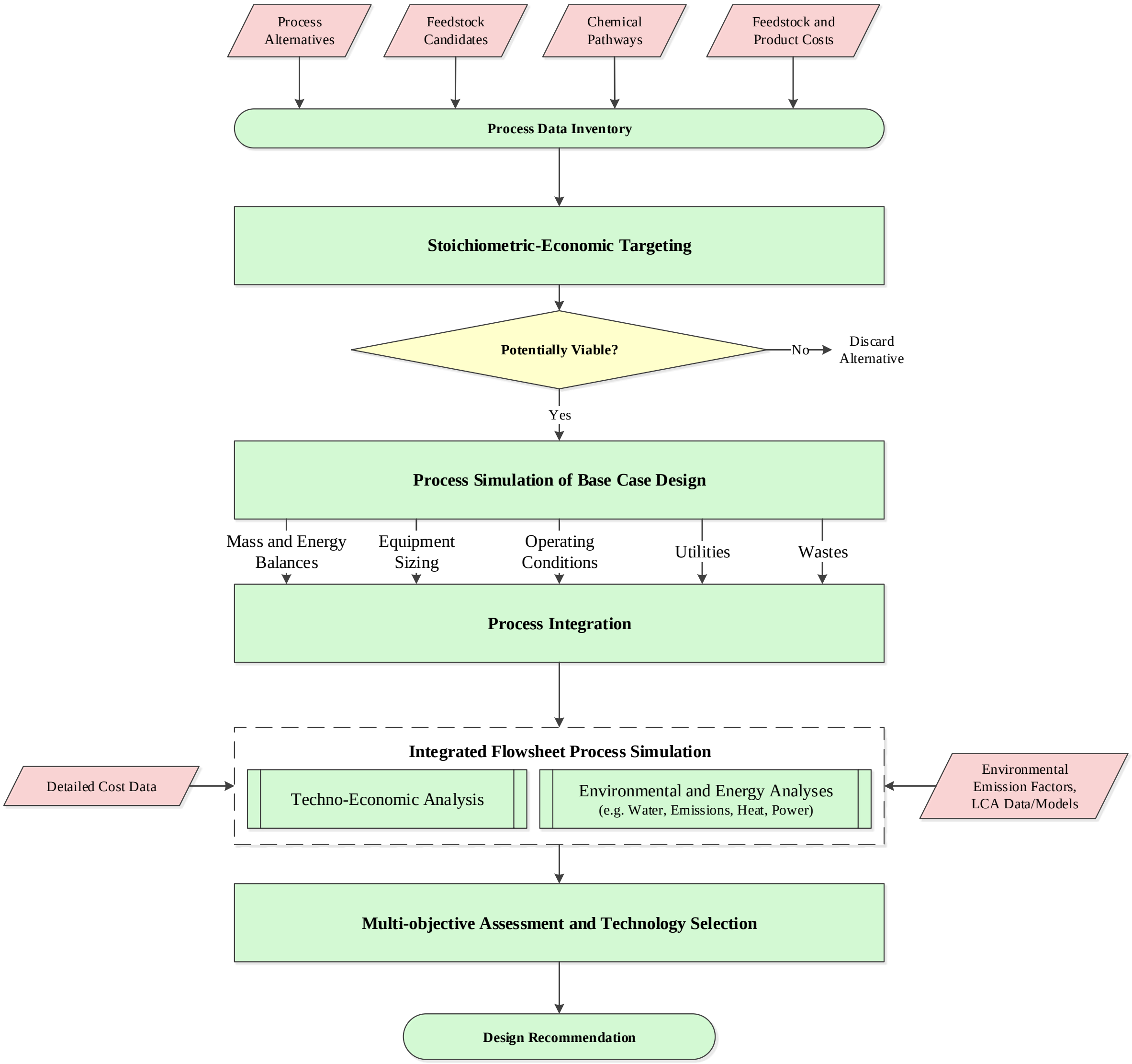

Figure 1: Proposed Hierarchical Approach for Process Sustainability Assessment Methodology

$$MISR = \frac{\sum_{p=1}^{N_{products}} Annual\ \ production\ \ rate\ of\ \ product\ \ p \times Purchase\ price\ of\ \ product\ \ p}{\sum_{r=1}^{N_{reactants}} Annual\ \ feed\ rate\ of\ \ reactant\ r \times Purchase\ price\ of\ \ reactant\ r} \tag{1}$$

Economically Viable process choice is guided by the value of MISR. Significantly higher MISR values will be more desirable to further analyze. However, if the MISR values are close for two or more processes, they should all be considered for further evaluation. Process alternatives having MISR less than 1 signifies that it costs more to purchase raw materials than earned by selling the finished products. Hence no process modification will be good enough to overcome this barrier, particularly if better MISR values are obtained from other process options.

Simulation of Base Case Design of the process options having high MISR is developed as the next step. A base case design is used to identify the process flow from raw material to the final product. This is also the step when two or more processes having similar MISR need to be expanded in scope of analysis, such as comparing for technologies that give better productivity, yield etc. The objective in the base case design step is to establish the potential unit operations to be utilized in the flow-scheme and construct a detailed process flowsheet. Traditional process synthesis steps ensure that the base case provides the individual and total mass and energy balances for the process and technology choice. Other important information that can be computed from the base case include equipment sizing, utilities and types, optimal operating conditions, and environmental waste streams.

Process Integration step follows the base case design using the flow information for mass and energy streams. Mass and energy integration can be performed using tools like the thermal pinch analysis for heat integration which deals with the optimal structure of heat exchange between process streams, as well as optimal use of utilities18. The analysis identifies targets for minimum hot and cold utility consumptions (referred to as Minimum Energy Requirements "MER"). Composite curves (CC) may be used to represent the counter-current heat flow among the streams that have been selected for heat transfer. The Grand Composite Curves (GCC) plots the excess heat of the hot and cold streams across temperature intervals which determines the selection and placement of utilities. Finally, a Heat Exchanger Network

(HEN) can be synthesized and optimized for MER and maximum heat recovery by eliminating redundant elements and finding the trade-off between utility consumption, heat exchange area, and number of units.

Integrated Flowsheet Process Simulation is created from the results of process integration. These flowsheets typically show reduced material and energy consumption, and the overall environmental footprint, however this may lead to increase or decrease in capital costs for the process. Rigorous techno-economic analysis and environmental analyses are carried out with characterization for available emission streams.

4. CASE STUDY

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4.1 On-Purpose Propylene Technologies

The case study considers the following technologies: Propane Dehydrogenation (PDH), Metathesis, Methanol-to-Olefins and Methanol-to-Propylene (MTO/MTP) since they are the most established technology routes to directly produce propylene (Jasper and El-Halwagi, 2015, Izadi, 2011). These are also the processes that have been commercially established through facilities around the world. In the PDH process, propane is converted to propylene over a bed of catalyst at high temperatures and low pressures. MTO/MTP process converts methanol into olefins, and it can be controlled to produce more propylene than ethylene. The MTO process converts methanol to olefins over a fluidized catalyst bed operating between 350-550 ^{o}C (Izadi, 2011). In China, the abundance of coal has accelerated the widespread adoption of this route through coal gasification technologies. Olefin metathesis uses the ethylene (C2) and butylene (C4) to produce two C3 molecules. The key determinants in the feasibility of this technology are the spread in prices between ethylene and propylene, and the availability of butylenes.

For a preliminary assessment of the candidate technologies, a stoichiometric-economic targeting is performed using the MISR metric from Equation 1. The annual production rate of 600,000 metric tons per annum was used in this calculation, using stoichiometric ratios of the reactants. The prices of feedstock and products is given in ***Table 1***. The calculated values of the

MISR are reported in Table 2. As can be seen from Table 2, PDH shows the highest potential for profitability. In the MTO process, it is considered that the propylene to ethylene ratio is 1.8 (Funk et al., 2013) to maximize propylene production. For the considered costs of raw materials and values of products, both metathesis and MTO have MISR values less than one and, therefore, will not be considered for further analysis.

Table 1: Feedstock and Product Prices for MISR Calculation

Feedstock/Product	Price
Propane	\$0.48/kg[a]
Propylene	\$0.95/kg[b]
Ethylene	\$0.65/kg[c]
Butylene	\$1.18/kg[d]
Methanol	\$396/MT[e]

[a]U.S.EIA (2017a); [b]Platts (2017b); [c]ICIS (2017b); [d]Platts (2017a); [e]MethanexCorporation (2017)

Table 2: Metric for Inspecting Sales and Reactants (MISR) for competing Propylene Production Processes

On-Purpose Propylene Process	MISR
Propane Dehydrogenation	2.07
Olefin Metathesis	0.95
Methanol to Olefins	0.98

It is worth noting that these results are only valid for the considered prices of raw materials and products. For instance, if the methanol price decreases from \$396/MT to \$300/MT (ICIS, 2017a) (e.g., in China due to the relatively low cost of producing methanol from coal), the value of MISR increases to 1.29 rendering the process potentially viable. Similarly, olefin metathesis process has an MISR=1 if the price of C4 raffinate drops from \$1179/MT to \$1100/MT. Based on this preliminary analysis, it was decided to choose PDH as the primary chemical production route of choice. Table 2 represents MISR values for different technologies based on 100% selectivity. It is worth noting that the selectivity of Propane Dehydrogenation is 90% (Gregor and Wei, 2005) which gives the MISR of PDH as 1.86. This is still greater than 1 and more profitable when compared to the Olefin Metathesis and MTO technology options.

4.2 Base Case Model and Simulation

Figure 2 is a schematic representation of the PDH flowsheet. In this process, propane is passed over a hot bed of catalyst where it reacts to produce propylene and hydrogen. Honeywell UOP's OLEFLEX^{TM} and CB&I Lummus' CATOFIN^{TM} technologies dominate the market in this sector (Nawaz, 2015). UOP's Oleflex process is used in 16 of the 23 operating PDH units in the world and UOP had been awarded 34 of the last 39 dehydrogenation worldwide since 2011 (Banach, 2016). In this paper, the OLEFLEX^{TM} process was chosen for simulation for its wider acceptability in the world.

Nawaz (2015) gave an overview of the process flow for the OLEFLEX^{TM} process. Figure 2 extracts key features from the OLEFLEX^{TM} technology but is not intended to replicate or claimed to represent the OLEFLEX^{TM} process. Computer-aided simulation using Aspen HYSYS was carried out for a process producing 600,000 MTA (metric ton per annum) of propylene.

The flowsheet can be broadly divided into the following sections: depropanizer column, reactor, reactor effluent cooling and compression, cold box, SHP reactor, deethanizer column, and the propylene-propane splitter column. Fresh propane feed is mixed with recycled propane and enters the depropanizer column. The depropanizer column is designed to separate C4+ material coming in the fresh feed and formed in the dehydrogenation reactors. The pressure of the column is kept high enough such that cooling water can be used as the condensing media. The propane rich steam from depropanizer overhead enters the cold box where its auto-refrigeration property is utilized to cool the reactor effluent stream. The cold-box is modeled based on the patented (O'Brien, 2001) design which does not require any external refrigeration.

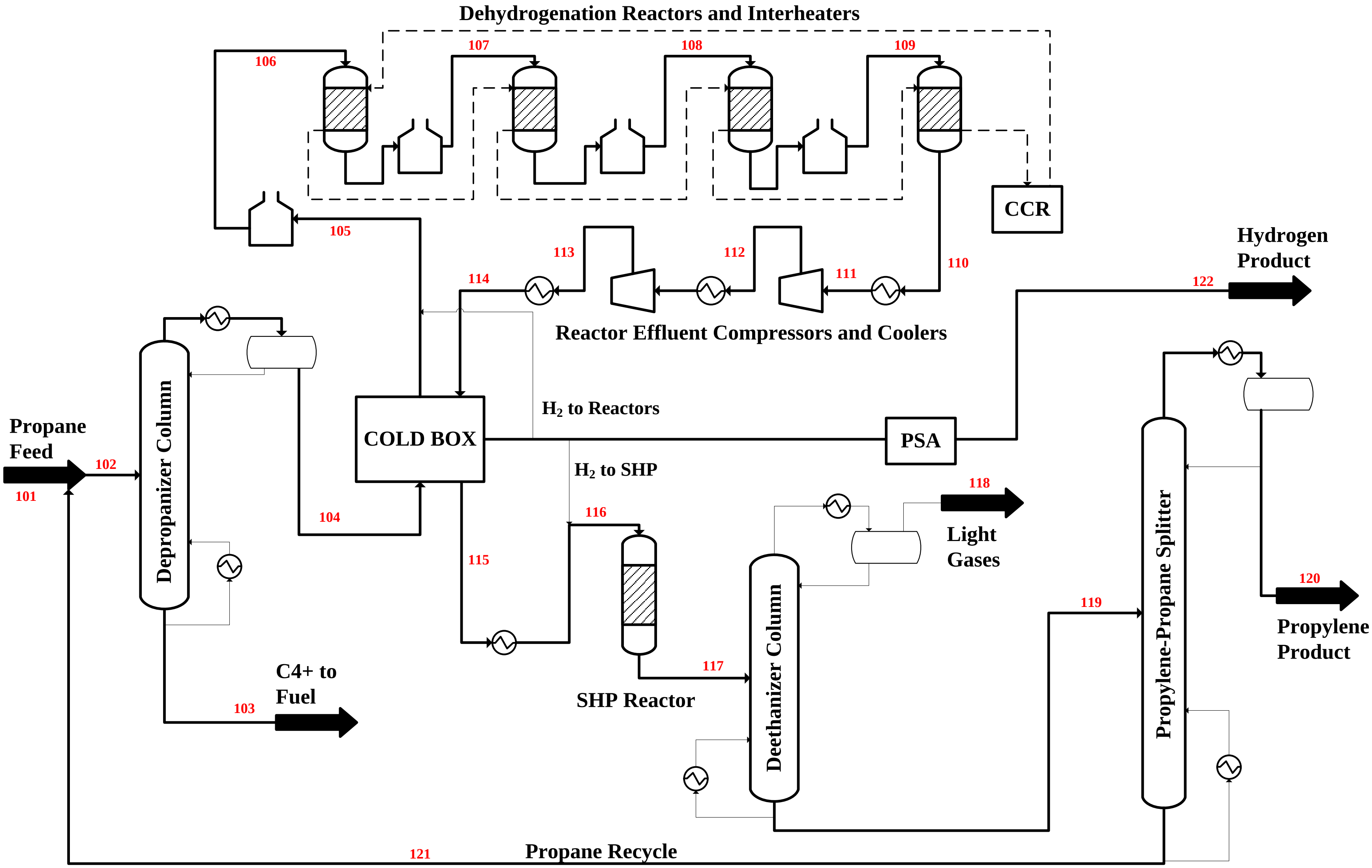

Figure 2: Simplified Process Flow Diagram for the Base Case

Coming out of the cold box, the propane feed stream is mixed with hydrogen stream and enters the fired-heater. The fired heater takes the feed temperature to 580-620 ^{o}C (Farjoo et al., 2011) before it enters the reactor system.

The reaction occurs over a fluidized catalyst bed in a radial flow reactor to minimize the pressure drop across the beds (Vora, 2012). A continuous catalyst regenerator (CCR) is used to continuously regenerate the catalyst by burning off the coke formed. The overall reaction selectivity towards propylene is 90% (mole) and the once-through conversion is 40% (mole) (Gregor and Wei, 2005). The remaining 10% of propane is converted in side reactions to produce light gases (methane, ethane, ethylene) (Farjoo et al., 2011) due to cracking, some diolefins (methyl-acetylene and propadiene), and some heavy key components (benzene, toluene, xylene) (Mole et al., 1985).

The reaction is highly endothermic in nature (ΔH = 124.3 kJ/mol) leading to considerable temperature drop in each reactor. Inter-stage heaters are placed to increase the temperature of each reactor effluent stream to the subsequent reactor inlet temperature. This makes the reactor section of the propane dehydrogenation process extremely energy intensive. The reactor effluent is a mix of propylene, unconverted propane, light gases such as methane, ethane and ethylene, diolefins, and some heavier hydrocarbon components formed in the reactor. The reactor effluent is cooled and then compressed in the multistage compressors and coolers. The compressed gas is then sent to the Cold Box where hydrogen is separated from the hydrocarbon stream. In order to liquefy the hydrocarbon material and separate out the hydrogen, the cold box uses a series of isentropic expansion, separation and subcooling (O'Brien, 2001). The auto-refrigeration across the expanders is a function of the pressure reduction.

Table 3: Stream Summary for the Base Case

	Unit	101	102	103	104	105	106	107	108	109	110	111
Vapor Fraction		0	0	0	0	1	1	1	1	1	1	1
Temperature	*K*	313.1	302.5	328.4	316.1	302.2	873.1	883.2	893.2	893.2	840.8	306.5
Pressure	*kPa*	6894.8	1514.8	1647.8	1772.0	475.7	379.2	296.5	215.8	137.9	124.1	96.5
Molar Flow	*kgmole/h*	1950	4827	6	4822	7291	7291	7736	8181	8615	9044	9044
Mass Flow	*kg/h*	85049	211822	274	211548	218391	218391	218390	218390	218390	218390	218394
Mole Fractions												
Hydrogen		0.0000	0.0000	0.0000	0.0000	0.3219	0.3219	0.3555	0.3859	0.4129	0.4376	0.4375
Methane		0.0027	0.0011	0.0000	0.0011	0.0161	0.0161	0.0208	0.0244	0.0272	0.0292	0.0292
Ethylene		0.0001	0.0000	0.0000	0.0000	0.0007	0.0007	0.0035	0.0057	0.0075	0.0090	0.0090
Ethane		0.0290	0.0117	0.0000	0.0117	0.0082	0.0082	0.0105	0.0123	0.0136	0.0146	0.0146
Propene		0.0000	0.0133	0.0000	0.0133	0.0089	0.0089	0.0628	0.1107	0.1526	0.1901	0.1901
Propane		0.9675	0.9735	0.9069	0.9737	0.6440	0.6440	0.5468	0.4607	0.3855	0.3187	0.3187
Propadiene		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0002	0.0002
m-Acetylene		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0002	0.0002
i-Butane		0.0006	0.0003	0.0856	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
n-Butane		0.0000	0.0000	0.0047	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene		0.0000	0.0000	0.0024	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0002	0.0002
Toluene		0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001

	Unit	112	113	114	115	116	117	118	119	120	121	122
Vapor Fraction		1	1	1	0	0	0	1	0.595	0	0	1
Temperature	*K*	403.9	395.4	306.5	310.0	333.0	334.0	220.0	293.8	284.3	296.1	308.4
Pressure	*kPa*	404.7	1404.4	1376.9	4238.2	4203.7	4100.3	446.1	928.7	894.2	1514.8	777.0
Molar Flow	*kgmole/h*	9044	9044	9044	4854	4871	4867	265	4606	1730	2878	1564
Mass Flow	*kg/h*	218394	218394	218394	206227	206262	206262	6663	199601	72828	126772	3152
Mole Fractions												
Hydrogen		0.4375	0.4375	0.4375	0.0002	0.0039	0.0030	0.0546	0.0000	0.0000	0.0000	1.0000
Methane		0.0292	0.0292	0.0292	0.0114	0.0113	0.0113	0.2079	0.0000	0.0000	0.0000	0.0000
Ethylene		0.0090	0.0090	0.0090	0.0146	0.0145	0.0145	0.2669	0.0000	0.0000	0.0000	0.0000
Ethane		0.0146	0.0146	0.0146	0.0257	0.0256	0.0256	0.4689	0.0001	0.0001	0.0000	0.0000
Propene		0.1901	0.1901	0.1901	0.3534	0.3521	0.3533	0.0015	0.3854	0.9947	0.0223	0.0000
Propane		0.3187	0.3187	0.3187	0.5930	0.5908	0.5914	0.0003	0.6141	0.0052	0.9776	0.0000
Propadiene		0.0002	0.0002	0.0002	0.0005	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
m-Acetylene		0.0002	0.0002	0.0002	0.0005	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
i-Butane		0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0000	0.0001	0.0000	0.0001	0.0000
n-Butane		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene		0.0002	0.0002	0.0002	0.0005	0.0005	0.0005	0.0000	0.0002	0.0000	0.0000	0.0000
Toluene		0.0001	0.0001	0.0001	0.0002	0.0002	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000

Hence, a high-pressure reactor effluent stream results in lower temperature across the expander, thereby making hydrogen separation easier. Hydrogen produced is partially sent to the dehydrogenation and Selective Hydrogenation Process (SHP) reactors and the net hydrogen is sent to the Pressure Swing Adsorption (PSA) unit for meeting pipeline quality specifications. Liquid from the cold box is sent to the SHP reactor to convert the diolefins formed in the side reactions to propylene. From SHP, the liquid is fed to the Deethanizer column to get rid of the C2- components. The Deethanizer bottoms are sent to the Propylene-Propane Splitter which produces the final propylene product.

The propylene-propane splitter is a super-fractionator due to the difficulty in the separation between the two components. The column bottoms from the PP Splitter contain the unconverted propane which is recycled back to the Depropanizer column. ***Table 3*** provides summary of the stream data from the base case simulation. The stream numbers are shown in ***Figure 2***.

4.3 Energy Analysis

The Aspen HYSYS simulation provided information on equipment involved, utility consumption, and the quality of energy required. The reactor section, compression and cooling section, and the product separation section are the big energy consumers in the process. The utilities used in the process include cooling water, low pressure (LP) steam, natural gas for firing in the heaters, and purchased electricity. The electricity could also be generated onsite, but not considered in this process analysis. A nominal 6.5 cents/kW-hr electricity rate has been assumed. A split up of the energy consumption in terms of the duty required and their respective costs of the utilities consumed is shown in ***Table 4***.

Table 4: Distribution of Utility Costs in Base Case

Utility Type	Unit Cost	Duty (MW)	Cost (MM$/yr)	% of Total Utility	Major Consumer in Process
Cooling Water	$0.023/m^3	358	8.4	10.7%	PP Splitter Condenser and Reactor Effluent Coolers (83%)
LP Steam	$10.7/kg	237.4	35.5	45%	PP Splitter Reboiler (80%)
Natural Gas	$10.1/MW-hr	159.3	15.7	19.9%	Fired Heaters (100%)
Electricity	$0.065/KW-hr	35.6	19.2	24.4%	Reactor Effluent Compressors (95%)
Total Utility		**790.3**	**78.8**	**100%**	

From ***Table 4***, LP Steam contributes 45% of the total annual utility costs. The reboiler for the PP Splitter consumes about 80% of the overall LP Steam. The separation between propane and propylene is extremely difficult due to the small difference between the relative volatility of the two components. This separation requires unusually large reflux and boil-up ratios leading to the massive reboiler and condenser energy requirements. The electricity consumption constitutes about 24% of the utility costs. The reactor effluent compressors are the major consumers of this electricity where the fluids exiting the reactor section are compressed from nearly 35 kPa to about 1500 kPa. The fired heaters are responsible for the entire natural gas firing requirement to get the feed to the reactor inlet temperatures. In the base case, the fired heater preceding Reactor 1 contributes to two-thirds of the fired heater duty as it heats the combined feed to from 29 ^{o}C to 600 ^{o}C. The total fixed capital investment for the base case scenario is approximately $585MM and given in ***Table 4***. Exchangers and the distillation columns combined contribute to roughly two-thirds of this value.

4.4 Process Integration

A thermal pinch analysis was performed on the base case to estimate the possibility for recovering heat within the process streams. The composite curves are shown in ***Figure 3***. The pinch temperature is found at 70.4 ^{o}C, and it can be seen from the composite curve that there is a large potential for integration above and below the pinch. The minimum hot and cold utility requirements are 278.5 MW (950 MMBtu/hr) and 230.7 MW (787 MMBtu/hr) respectively for a minimum temperature approach of 14^{o}C (25^{o}F). This minimum temperature approach is consistent with the rule of thumb values for petrochemical processes (March, 1998). The hot utility values are due to the large heating requirements of the fired heater and the PP splitter's reboiler.

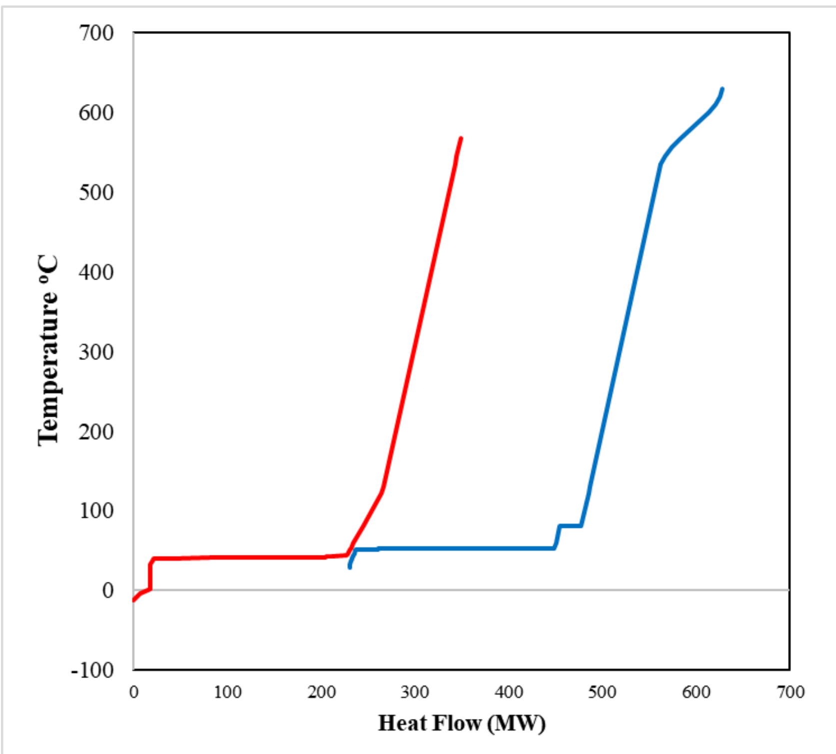

Figure 3: Pinch Analysis (Hot and Cold Composite Curves) for Base Case Design

The large cold utility requirements are due to the reactor effluent cooler, and the PP Splitter condenser. There is potential for heat exchange in the temperature range 40 ^oC - 550 ^oC which is constituted by heating and cooling requirements of the reactor feed and effluent streams. The composite curves can be further analyzed to systematically derive the optimum heat exchanger network which provides lowest energy consumption options from external utilities.

4.4.1 Integrated Case

Given the enormous costs of utilities in the base case, and results from the thermal pinch analysis indicating that heat exchanges are possible, an integrated case is developed to reduce the energy consumption from external sources by utilizing some of the process heat. ***Figure 4*** shows the process flow diagram after heat integration was implemented.

Table 5: Comparison of Utility costs for Base Case, Integrated Case, and Integrated + Intensified Case

Utility Type	Base Case Utility Cost (MM$/yr.)	Integrated Case Utility Cost (MM$/yr.)	Integrated and Intensified Case Utility Cost (MM$/yr.)
Cooling Water	8.4	3.6	1.2
LP steam	35.5	31.9	4.0
Natural Gas Firing	15.7	7.1	7.1
Electricity	19.2	19.2	27.1
Total Utility	**78.8**	**61.8**	**39.4**

The red, blue and green exchangers are the additions to the process which utilize the energy present in the reactor effluent streams to pre-heat the feed to the reactor, and partially provide energy to the Depropanizer and Deethanizer reboilers. The duty of the fired heater preceding Reactor 1 comes down from 106 MW (362.6 MMBtu/hr.) to 19 MW (64.8 MMBtu/hr.).

In order to achieve the process-process heat exchange, four additional heat exchangers must be added to the process. While this will lead to significant capital investment, the reduction in the sizes of the fired heater upstream of reactor 1, and the coolers in the reactor effluent cooling and compression section, offsets this value. Additionally, the combined reactor effluent cooling duty reduces from 126 MW (432 MMBtu/hr) to 15.5 MW (52.9 MMBtu/hr) as the reactor effluent is cooled by the reactor feed. There is $11.5MM additional capital invested with a payback period of 8 months for the four exchangers which results in utility reductions of almost $37MM/yr. when compared to the base case. ***Table 6*** shows the summary of stream data for the “Integrated Case” simulation.

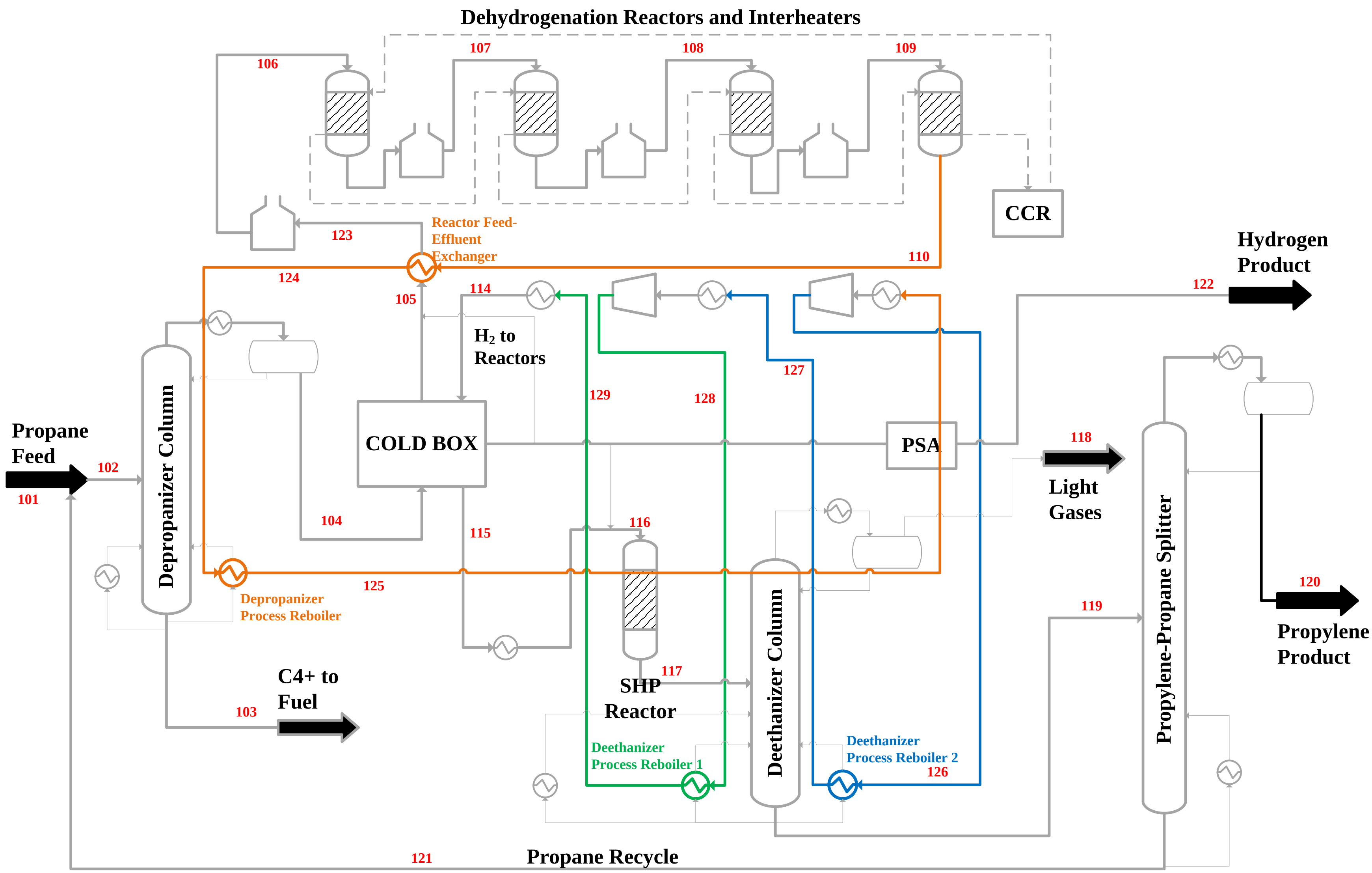

Figure 4: Simplified Process Flow Diagram for the Integrated Case

Table 6: Stream Summary for the Integrated Case

	Unit	101	102	103	104	105	106	107	108	109	110	114	115	116
Vapor Fraction		0	0	0	0	1	1	1	1	1	1	1	1	1
Temperature	*K*	313.2	302.5	324.1	316.1	302.2	873.1	883.2	893.2	893.2	840.8	403.9	395.4	306.5
Pressure	*kPa*	6894.8	1514.8	1641.0	1772.0	475.7	379.2	296.5	215.8	137.9	124.1	404.7	1404.4	1376.9
Molar Flow	*kgmole/h*	1950	4827	6	4822	7291	7291	7736	8181	8615	9044	9044	9044	9044
Mass Flow	*kg/h*	85049	211822	274	211548	218391	218391	218390	218390	218390	218390	218394	218394	218394
Mole Fractions														
Hydrogen		0.0000	0.0000	0.0000	0.0000	0.3219	0.3219	0.3555	0.3859	0.4129	0.4376	0.4375	0.4375	0.4375
Methane		0.0027	0.0011	0.0000	0.0011	0.0161	0.0161	0.0208	0.0244	0.0272	0.0292	0.0292	0.0292	0.0292
Ethylene		0.0001	0.0000	0.0000	0.0000	0.0007	0.0007	0.0035	0.0057	0.0075	0.0090	0.0090	0.0090	0.0090
Ethane		0.0290	0.0117	0.0000	0.0117	0.0082	0.0082	0.0105	0.0123	0.0136	0.0146	0.0146	0.0146	0.0146
Propene		0.0000	0.0133	0.0000	0.0133	0.0089	0.0089	0.0628	0.1107	0.1526	0.1901	0.1901	0.1901	0.1901
Propane		0.9675	0.9735	0.9069	0.9737	0.6440	0.6440	0.5468	0.4607	0.3855	0.3187	0.3187	0.3187	0.3187
Propadiene		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0002	0.0002	0.0002	0.0002
m-Acetylene		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0002	0.0002	0.0002	0.0002
i-Butane		0.0006	0.0003	0.0856	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
n-Butane		0.0000	0.0000	0.0047	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene		0.0000	0.0000	0.0024	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0002	0.0002	0.0002	0.0002
Toluene		0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0001	0.0001

	Unit	117	118	119	120	121	122	123	124	125	126	127	128	129
Vapor Fraction		0	0	0	1	0.595	0	0	1	1	1	1	1	1
Temperature	*K*	310.0	333.0	334.0	220.0	293.8	284.3	296.1	398.3	324.8	398.3	324.8	395.4	353.6
Pressure	*kPa*	4238.2	4203.7	4100.3	446.1	928.7	894.2	1514.8	110.3	96.5	110.3	96.5	1404.4	1390.6
Molar Flow	*kgmole/h*	4854	4871	4867	265	4606	1730	2878	9044	9044	9044	9044	9044	9044
Mass Flow	*kg/h*	206227	206262	206262	6663	199601	72828	126772	218394	218394	218394	218394	218394	218394
Mole Fractions														
Hydrogen		0.0002	0.0039	0.0030	0.0546	0.0000	0.0000	0.0000	0.4375	0.4375	0.4375	0.4375	0.4375	0.4375
Methane		0.0114	0.0113	0.0113	0.2079	0.0000	0.0000	0.0000	0.0292	0.0292	0.0292	0.0292	0.0292	0.0292
Ethylene		0.0146	0.0145	0.0145	0.2669	0.0000	0.0000	0.0000	0.0090	0.0090	0.0090	0.0090	0.0090	0.0090
Ethane		0.0257	0.0256	0.0256	0.4689	0.0001	0.0001	0.0000	0.0146	0.0146	0.0146	0.0146	0.0146	0.0146
Propene		0.3534	0.3521	0.3533	0.0015	0.3854	0.9947	0.0223	0.1901	0.1901	0.1901	0.1901	0.1901	0.1901
Propane		0.5930	0.5908	0.5914	0.0003	0.6141	0.0052	0.9776	0.3187	0.3187	0.3187	0.3187	0.3187	0.3187
Propadiene		0.0005	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002
m-Acetylene		0.0005	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002
i-Butane		0.0001	0.0001	0.0001	0.0000	0.0001	0.0000	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
n-Butane		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene		0.0005	0.0005	0.0005	0.0000	0.0002	0.0000	0.0000	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002
Toluene		0.0002	0.0002	0.0002	0.0000	0.0001	0.0000	0.0000	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001

4.4.2 Integrated Case with Intensification

After heat integration, the cost of LP Steam makes up for more than 50% of the total annualized utility costs (Table 4). If a reduction in the large steam consumption of the PP Splitter reboiler can be achieved, it would result in tremendous energy savings. This is confirmed by analyzing the Grand Composite Curves generated from the pinch analysis of the base case and integrated and intensified case scenarios shown in ***Figure 5***.

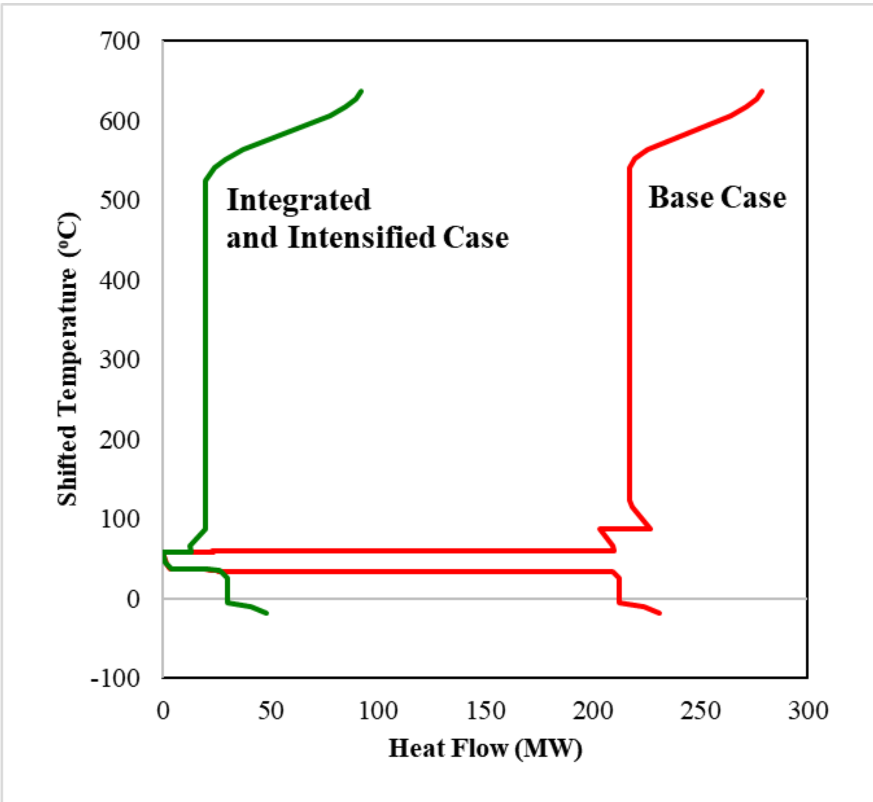

Figure 5: Comparison of Grand Composite Curves of Base Case and Integrated Case with Intensification

A large energy requirement can be observed around the 60°C mark on either side of the pinch. This loop on the GCC presents the opportunity of introducing a heat pump (Dumont et al., 2010, El-Halwagi, 2017d). There are many types of heat pumps used in the industry, such as electrically driven heat pumps and absorption driven heat pumps. However, in distillation, the most common type of heat pump utilized is the compression system (HPC)

The overhead vapor is first compressed in the heat pump compressor and the discharge is used to reboil the column bottoms liquid. In the PP Splitter, the difference between the boiling points of propane and propylene is very small. This makes it an ideal candidate for HPC as the compression ratio required to attain adequate temperature approach in the reboiler-condenser would be small. This would limit the electricity consumption in the compressor and make the process more viable.

Annakou and Mizsey (1995) discuss various heat pump compression schemes that can be employed in the PP Splitter design. A double compressor scheme has been used in this study where the first stage discharge is used to reboil the column bottoms, while the second stage discharge is condensed in a water-cooled condenser to provide operational flexibility in the process in the event of any upsets. ***Figure 6*****:** Process Flow Diagram for Integrated and Intensified Case with the addition of the Heat Pump Compression (HPC) system shows the simplified process flow diagram with the HPC installed along with the integrated scheme discussed previously.

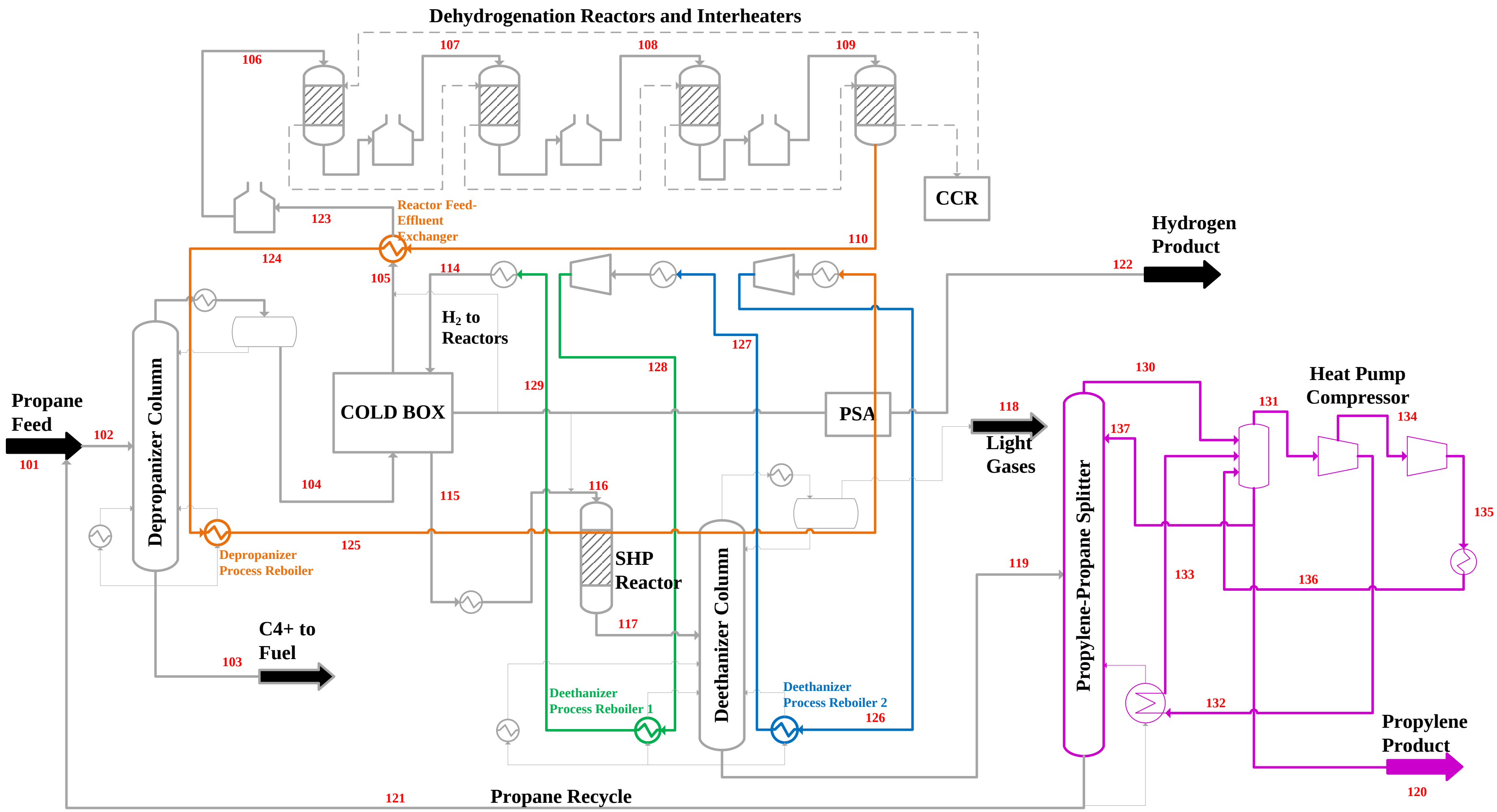

Figure 6: Process Flow Diagram for Integrated and Intensified Case with the addition of the Heat Pump Compression (HPC) system

Table 7: Stream Summary for the Integrated and Intensified Case

	101	102	103	104	105	106	107	108	109	110	114	115	116	117	118	119
Vapor Fraction	0	0	0	0	1	1	1	1	1	1	1	1	1	0	0	0
Temperature	313.2	302.5	324.1	316.1	302.2	873.1	883.2	893.2	893.2	840.8	403.9	395.4	306.5	310.0	333.0	334.0
Pressure	6894.8	1514.8	1641.0	1772.0	475.7	379.2	296.5	215.8	137.9	124.1	404.7	1404.4	1376.9	4238.2	4203.7	4100.3
Molar Flow	1950	4827	6	4822	7291	7291	7736	8181	8615	9044	9044	9044	9044	4854	4871	4867
Mass Flow	85049	211822	274	211548	218391	218391	218390	218390	218390	218390	218394	218394	218394	206227	206262	206262
Mole Fractions																
Hydrogen	0.0000	0.0000	0.0000	0.0000	0.3219	0.3219	0.3555	0.3859	0.4129	0.4376	0.4375	0.4375	0.4375	0.0002	0.0039	0.0030
Methane	0.0027	0.0011	0.0000	0.0011	0.0161	0.0161	0.0208	0.0244	0.0272	0.0292	0.0292	0.0292	0.0292	0.0114	0.0113	0.0113
Ethylene	0.0001	0.0000	0.0000	0.0000	0.0007	0.0007	0.0035	0.0057	0.0075	0.0090	0.0090	0.0090	0.0090	0.0146	0.0145	0.0145
Ethane	0.0290	0.0117	0.0000	0.0117	0.0082	0.0082	0.0105	0.0123	0.0136	0.0146	0.0146	0.0146	0.0146	0.0257	0.0256	0.0256
Propene	0.0000	0.0133	0.0000	0.0133	0.0089	0.0089	0.0628	0.1107	0.1526	0.1901	0.1901	0.1901	0.1901	0.3534	0.3521	0.3533
Propane	0.9675	0.9735	0.9069	0.9737	0.6440	0.6440	0.5468	0.4607	0.3855	0.3187	0.3187	0.3187	0.3187	0.5930	0.5908	0.5914
Propadiene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0002	0.0002	0.0002	0.0002	0.0005	0.0005	0.0000
M-Acetylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0002	0.0002	0.0002	0.0002	0.0005	0.0005	0.0000
i-Butane	0.0006	0.0003	0.0856	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
n-Butane	0.0000	0.0000	0.0047	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene	0.0000	0.0000	0.0024	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0002	0.0002	0.0002	0.0002	0.0005	0.0005	0.0005
Toluene	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0001	0.0001	0.0002	0.0002	0.0002

	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136
Vapor Fraction	0.595	0	0	1	1	1	1	1	1	1.000	1.000	1.000	0.000	1.000	1.000	0.000
Temperature	293.8	284.3	296.1	398.3	324.8	398.3	324.8	395.4	353.6	284.9	284.0	312.2	302.1	312.2	318.9	306.5
Pressure	928.7	894.2	1514.8	110.3	96.5	110.3	96.5	1404.4	1390.6	811.5	790.8	1289.2	1268.5	1289.2	1444.1	1409.6
Molar Flow	4606	1730	2878	9044	9044	9044	9044	9044	9044	37956	38375	36925	36925	1450	1450	1450
Mass Flow	199601	72828	126772	218394	218394	218394	218394	218394	218394	1597439	1615089	1554050	1554050	61039	61039	61039
Mole Fractions																
Hydrogen	0.0000	0.0000	0.0000	0.4375	0.4375	0.4375	0.4375	0.4375	0.4375	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.0000	0.0000	0.0292	0.0292	0.0292	0.0292	0.0292	0.0292	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethylene	0.0000	0.0000	0.0000	0.0090	0.0090	0.0090	0.0090	0.0090	0.0090	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0001	0.0001	0.0000	0.0146	0.0146	0.0146	0.0146	0.0146	0.0146	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003
Propene	0.3854	0.9947	0.0223	0.1901	0.1901	0.1901	0.1901	0.1901	0.1901	0.9950	0.9950	0.9950	0.9950	0.9950	0.9950	0.9950
Propane	0.6141	0.0052	0.9776	0.3187	0.3187	0.3187	0.3187	0.3187	0.3187	0.0047	0.0047	0.0047	0.0047	0.0047	0.0047	0.0047
Propadiene	0.0000	0.0000	0.0000	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
M-Acetylene	0.0000	0.0000	0.0000	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
i-Butane	0.0001	0.0000	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Butane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene	0.0002	0.0000	0.0000	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Toluene	0.0001	0.0000	0.0000	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

The heat pump compressor has the additional benefit of operating the PP Splitter at a lower pressure. The conventional design would require a high pressure to utilize cooling water as its condensing media. However, with the HPC, the column can be operated at lower pressures enhancing the relative volatility between the components (propane and propylene) and making separation easier.

Table 8: Comparison of Capital Costs in Base Case with the Integrated and Intensified Case

Equipment Type	**Base Case Capital Cost** ($MM, 2016)	**Integrated and Intensified Case Capital Cost** ($MM, 2016)
Columns	90	71
Vessels	14	14
Reactors	46	46
Exchangers	100	54
Pumps	1	0.5
Compressors	34	54
Fired Heaters	19	11
Refrigeration Equipment	17	17
Total Installed Capital Cost	**321**	**268**
Outside Battery Limits (OSBL) 30% (as a percentage of Total Installed Cost)[a]		
Detailed Engineering and Construction 30 % (as percentage of Total Installed Cost + OSBL)[a]		
Contingency 10% (as a percentage of Total Installed Cost + OSBL)[a]		
Total Fixed Capital Investment	**585**	**488**

[a]Towler and Sinnott (2013)

The conventional design required 220 stages to achieve the same separation that the heat pump compressor design can achieve in 160 stages. This also reduces the size of the distillation column and significantly lowered the capital investment requirement. There is overwhelming literature evidence to corroborate the application of heat pump systems to PP splitters in order to reduce capital and operating expenditure. Studies done by Quadri (1981), Supranto et al. (1986), and Olujic et al. (2006) discuss various configurations of the Heat Pump Compressor for the PP splitter but come up with similar conclusions for capital and operational cost savings. ***Table 7*** shows the summary of the stream data for the Integrated and Intensified case simulation. ***Table 8*** shows the capital costs of running the integrated case with the HPC system and compares it with base case.

While there is an increase in the electricity consumption, due to the addition of the heat pump, the overall utility costs have gone down considerably due to the elimination of the LP steam and cooling water costs in the PP Splitter's reboiler and condenser respectively. The overall utility costs are reduced to $39.9 MM which is almost 50% lower than the base case scenario. Additionally, the total fixed capital investment is reduced by 17% to $488MM due to the elimination of the large condenser/reboilers of the PP Splitter column, as well as the reduction in the size of the column due to lower pressure operation. It eliminates the requirement of steam in the overall process flowsheet and substantially reduces the cooling water requirement as well. A comparison of the capital and utility costs for all three scenarios for the design are shown in ***Figure 7*** and ***Figure 8*** and respectively.

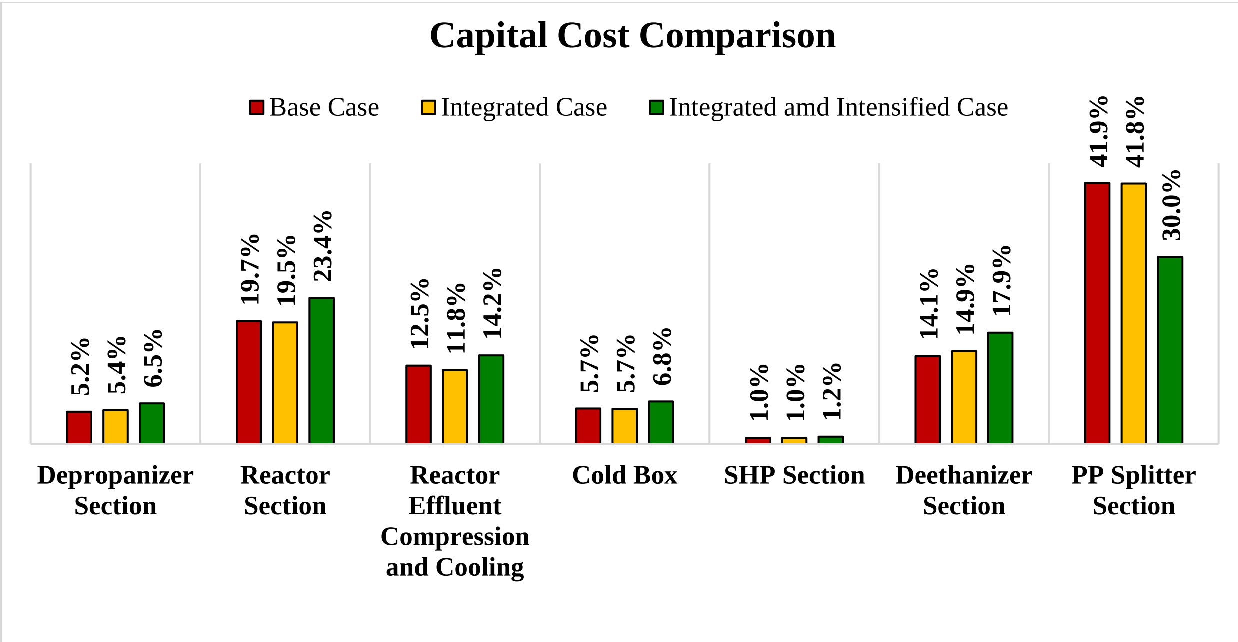

Figure 7: Comparison of Capital Costs for Base Case, Integrated Case, and Integrated Case with Intensification

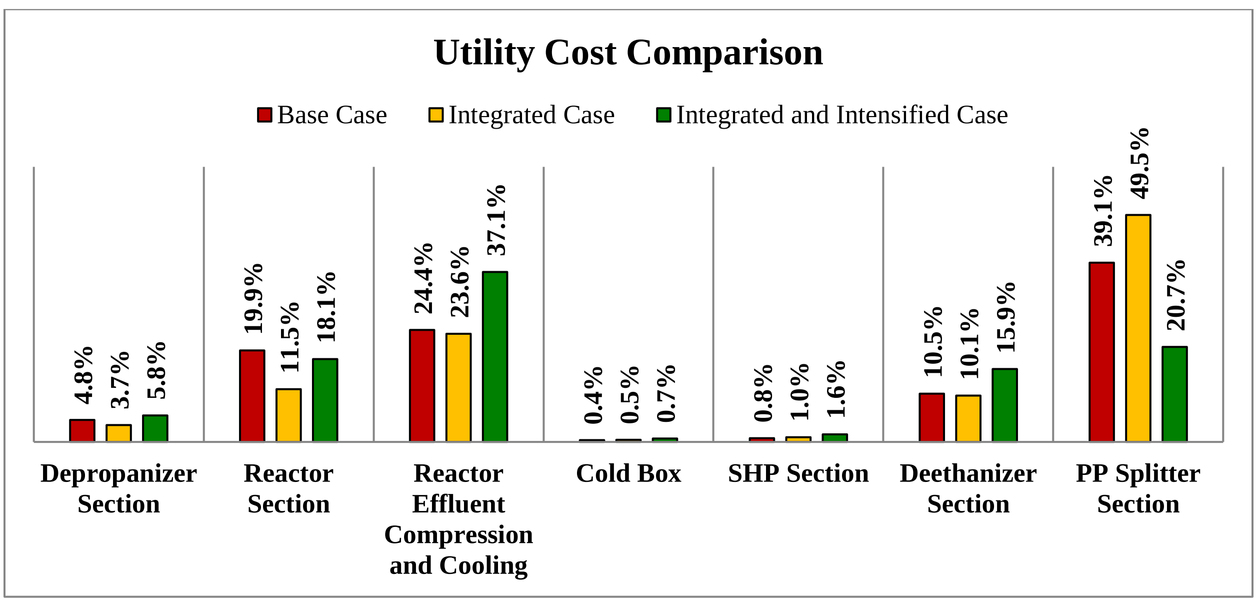

Figure 8: Comparison of Utility Costs for Base Case, Integrated Case, and Integrated Case with Intensification

The composite curves for the Integrated and Intensified Case implemented is shown in ***Figure 9***. The updated pinch temperature is at 70 ^oC with the minimum hot and cold utility requirements reduced to 92.2 MW and 48.4 MW respectively. The overlap area between the hot composite and cold composite curves is less than 15 MW. It may not be economically feasible to recover this overlap between the hot and cold streams as it would require large number of heat exchangers. Most of the hot utility requirement is above 100 ^oC which is supplied by the fired heaters in the reactor section. Significant cold utility requirement is at sub-zero temperatures for which refrigeration is required.

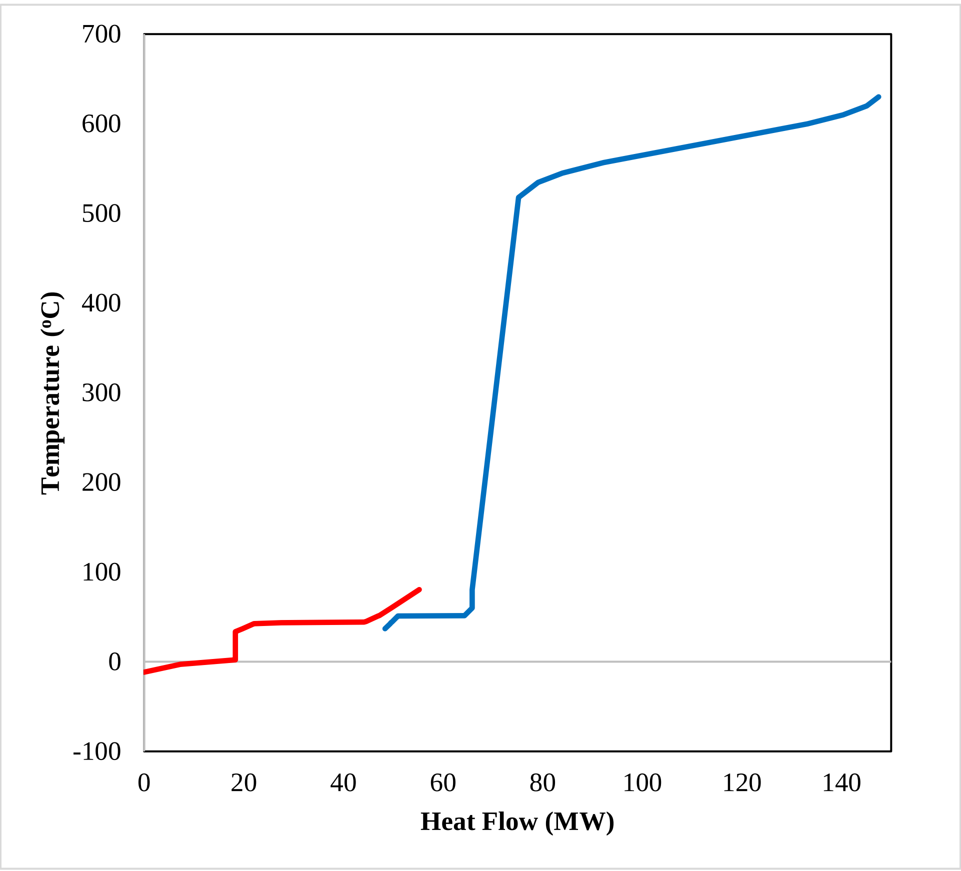

Figure 9: Composite Curves for Integrated and Intensified Case

4.5 Water Analysis

The water use in the process and subsequent economic cost for cooling water utility and LP Steam was minimized in the process by both integration and intensification options. This has been demonstrated in Table 4. The cost for a water recovery and reuse system can be considered outside the boundary limits of the current process considerations for further cost and resource use reduction. The PP Splitter condenser and reboiler in the base case, accounts for over 70% of the water consumption in the process in terms of cooling water and LP Steam requirements, respectively. Therefore, it can be safely assumed that due to the process intensification changes implemented, significant water reduction has already been achieved, as both the condenser and the reboiler have been replaced by a single process-process exchanger. The remaining water requirement in the process is minimal. A rigorous water treatment and recovery system would be a viable addition if there are other high-water consumers and discharges in the vicinity of the propylene plant to share the additional capital investment for the recovery system.

4.6 Emissions Analysis

It is critical to evaluate the environmental impact of the changes made in design for sustainability. One way to estimate that is to calculate the carbon footprint of these processes. Three major greenhouse gas emission sources have been identified in the PDH process:

- Natural gas combustion
- Electricity consumption
- Burning/flaring of waste streams

The Environmental Protection Agency (EPA) first published the AP-42 report in 1972, with updated being made periodically since, to quantify air emissions based on factors for different sources of emissions (U.S.EPA, 2016). Chapter-1.4 (U.S.EPA, 2017b) of AP-42 provides the emissions due to natural gas combustion. Estimating the annual consumption of natural gas in the process for combustion purposes can be used in conjunction with AP-42 emission factors to calculate the amount of greenhouse gas emissions as given in Table 9**.** The emission factor ratings determine the reliability of the estimate with "A" denoting most reliable estimate, which has been developed based on many observations, and widely accepted test procedures. On the other hand, "E" denotes a factor based on a single observation of questionable quality, or one extrapolated from another factor for a similar process.

Table 9: AP-42 Emission Factors for Natural Gas Combustion (Industrial Heaters) (U.S.EPA, 2016)

Pollutant	**Emission Factor (lb/10^6scf)**	**Emission Factor Rating**
CO_2	120,000	A
N_2O (Low NOx Burner)	0.64	E
SO_2	0.6	A
TOC	11	B
Methane	2.3	B
VOC	5.5	C

The eGRID2014v2 Annual Output Emission Rates (U.S.EPA, 2017a) lists the greenhouse gas emissions resulting from electricity consumption categorized based on sub-regional grids within United States. Since the electricity requirement in the process is known, the emissions resulting from them can also be estimated. In this paper, it is assumed that all electricity is purchased and the emission factors from the Texas Grid (ERCOT) are used as the basis for electricity generation emissions as given in

Finally, burning waste streams from the process will also result in greenhouse gas emissions. The offgas from deethanizer, flash gas from the cold box, and C4+ stream from depropanizer bottoms are the three waste streams identified in the process. In order to estimate the emissions from these streams, it is assumed that a complete combustion resulting in CO_2 emissions for the carbon species will occur in the flare system.

Table 10: Emission Factors for Electricity Generation (U.S.EPA, 2017a)

Electricity Source	**CO_2 (lb/MWhr)**	**Methane (lb/GWhr)**	**N_2O (lb/GWhr)**
ERCOT (Texas) Grid	1142.8	81.8	11.6
US Avg.	1122.9	110.9	16.0
SRMW (SERC Midwest)	1772.0	208.8	30.4

4.6.1 Waste Heat Recovery (WHR)

In addition to the conventional process integration and intensification techniques, low grade energy recovery in processes can be effectively utilized to increase the overall efficiency of the process. There are technologies and systems available to recover heat from industrial clean gases at high temperature (>650 ^oC), medium temperature (230 – 650 ^oC), and low temperature (<230 ^oC). About 60% of the unrecovered waste heat is of low quality (at temperatures <230 ^oC) (Sengupta, 2017). In the current process under consideration, the reaction of propane to propylene is endothermic in nature. Due to this, we have four fired heaters which heat the process gas to roughly 600 ^oC to maintain catalyst activity and increase conversion. The flue gas coming out of the radiation sections of these fired heaters is a good source of medium temperature heat. Ibrahim and Al-Qassimi(Ibrahim and Al-Qassimi, 2010) discuss the heat recovery calculation in the convection section and show that about 35% of the radiant section duty can be recovered in the convection section. For our calculations, a conservative value of 30% of the radiant section duty recovery is assumed without going into the details of fired heater design. A common application for utilizing this energy is steam generation (Sengupta, 2017). This steam generated can then be used in heating up the reboilers for depropanizer, deethanizer, and PP Splitter (for the Base Case and Integrated Case scenarios).

4.6.2 Off-Gas Recovery (OGR)

Another step which can be taken to minimize the carbon footprint, is utilizing the potential waste streams. It is observed that the Low Heating Value (LHV) of the deethanizer offgas stream is 1207 MJ/kgmol (Std.) which is more than 30% higher than the heating value of Natural Gas (915 MJ/kgmol (Std.)). Therefore, this stream can be used as fuel gas and reduce the consumption of Natural Gas. Given that the flow rate of this stream is 265 kgmol/hr, a maximum of 89 MW of duty can be extracted from this stream at 100% efficiency. Factoring in for the efficiency of burning fuel (85%), a significant portion of energy in the stream can be integrated with the process which leads to reduction in overall natural gas requirement.

The reduction in emissions resulting from waste heat recovery and offgas recycle options were analyzed and tabulated in ***Table 11***. 70% reduction in total emissions compared to the base case is achieved by implementing WHR and OGR with process integration and intensification. If a carbon tax of $25/ton of CO_2 is levied, this can translate to roughly $17.4 MM worth savings every year going from the base case design to the Integrated and Intensified case with waste heat recovery and Offgas recovery implemented.

Table 11: Comparison of Emissions with Waste Heat Recovery and Offgas Recovery for various scenarious

Pollutant	Base Case			Integrated Case			Integrated + Intensified Case		
	Base Case	**Base Case + WHR**	**Base Case + WHR + OGR**	**Integrated Case**	**Integrated Case with WHR**	**Integrated case +WHR + OGR**	**Integrated + Intensified Case**	**Integrated + Intensified Case + WHR**	**Integrated + Intensified case + WHR+ OGR**
	tons/yr			tons/yr			tons/yr		
CO2	1,013,054	911,646	748,282	820,723	776,074	612,710	531,606	480,676	317,312
Methane	21.94	20.00	20.00	18.25	17.40	17.40	15.99	15.01	15.01
SO2	3.57	3.07	3.07	2.61	2.39	2.39	0.85	0.60	0.60
TOC	65.50	56.20	56.20	47.87	43.77	43.77	15.63	10.96	10.96
VOC	32.75	28.10	28.10	23.93	21.89	21.89	7.81	5.48	5.48
N2O	4.98	4.44	4.44	3.95	3.72	3.72	2.71	2.44	2.44
Total Emissions	**1,013,182**	**911,758**	**748,394**	**820,819**	**776,164**	**612,800**	**531,649**	**480,711**	**317,347**
Cost of CO2 Emissions @$25/ton ($MM/yr.)	**25.33**	**22.79**	**18.71**	**20.52**	**19.40**	**15.32**	**13.29**	**12.02**	**7.93**

4.7 Economic Analysis

A Discounted Cash Flow Rate of Return (DCFROR) analysis (Towler and Sinnott, 2013) is done to develop more detailed economic indicators. The Return on Investment (ROI), Internal Rate of Return (IRR) and Net Present Value (NPV) are estimated over a 20-year period. The Modified Accelerated Cost Recovery System (MACRS) model over a 7-year recovery period is assumed for calculating depreciation and the tax rate is assumed to be 40%. Table 12 shows the economic indicators for all three cases.

Table 12: Economic Indicators for Base Case, Integrated Case, and Integrated Case with Intensification

Economic Criteria	Base Case	Integrated Case	Integrated and Intensified Case
Simple Pay-back (yrs)	5.82	5.34	4.06
Return on Investment (15yrs)	15%	17%	25%
NPV (15 yrs) [$MM]	240.7	314.6	489.5
IRR (15 yrs)	14%	16%	22%

4.8 Sustainability Analysis

El-Halwagi (2017c) introduced the Sustainability Weighted Return on Investment (SWROI) metric which is an extension of the Return on Investment concept with the augmented sustainability metrics and process integration targeting approaches. Considering a set a process alternatives: p = 1, 2, 3…., $N_{projects}$. For the p^{th} project, a new term called the Annual Sustainability Profit (ASP) is given in Equation 2.

$$ASP_P = AEP_P[\,1 + \sum_{i=1}^{N_{indicators}} w_i \left(\frac{Indicator_{p,i}}{Indicator_i^{Target}}\right)] \quad (1)$$

Where *i* is an index for the different sustainability indicators (other than net annual economic profit with *i* = 1, 2, 3…, $N_{indicators}$). AEP_p is the Annual Economic Profit. The weighing factor w_i is a ratio representing the relative importance of the i^{th} sustainability indicator compared to the annual net economic profit. The term $(\mathrm{Indicator}_{p,I})$ represents the value of the i^{th} sustainability indicator associated with the $p^{th\ project}$ and the term $(\mathrm{Indicator}_i^{\mathrm{Target}})$ corresponds to the target of the i^{th} sustainability indicator (obtained from process integration benchmarking or taken as the largest value from all project). The ratio $\left(\frac{Indicator_{p,i}}{Indicator_i^{Target}}\right)$ then represents the fractional contribution of project *p* towards meeting the desired/targeted performance for the i^{th} sustainability metric. The SWROI of a project *p* is then defined as given in Equation 3.

$$SWROI_P = \frac{ASP_p}{TCI_P} \quad (2)$$

Where TCP_p is the Total Capital Investment for project *p*.

Table 13 shows the detailed sustainability analysis of the options considered. The impact of WHR and OGR is evaluated on all three case studies listed above.

Table 13: Sustainability Weighted Analysis for all scenarios considered

Description	10 yr. Avg. Taxable Income MM$/yr	Total Capital Investment MM$	Water Reduction (Steam + CW) 10^6 kg/hr	Electrical Energy Savings (Power) MW	Fuel Savings (NG Firing in Fired Heaters) MW	CO2 emission Reductions 10^3 tons/yr.	VOC Reduction tons/yr.	ROI (10 yrs.)	SWROI
Weight Factors	-	-	**0.1**	**0.1**	**0.07**	**0.25**	**0.05**		
Targets	-	-	**45.08**	**36**	**159**	**1013**	**32.7**		
Base Case + WHR	67	643	0	0	0	101.4	4.6	10.38%	10.71%
Base Case + WHR + OGR	67	643	0	0	0	264.8	4.6	10.38%	11.13%
Integrated Case	79	645	25.6	0	87	192.3	8.8	12.29%	14.21%
Integrated Case + WHR	79	645	25.6	0	87	237	10.9	12.29%	14.38%
Integrated Case + WHR + OGR	79	645	25.6	0	87	400.3	10.9	12.29%	14.88%
Integrated + Intensified Case	104	536	38.7	-14.5	87	481.4	24.9	19.45%	24.12%
Integrated + Intensified Case + WHR	104	536	38.7	-14.5	87	532.4	27.3	19.45%	24.43%
Integrated + Intensified Case + WHR + OGR	104	536	38.7	-14.5	87	695.7	27.3	19.45%	**25.21%**

The different sustainability criteria are listed. The results for these criteria are used in Eqs. (2) and (3) to evaluate the sustainability weighted return on investment. The targets for this analysis are set based on the maximum realizable potential for reduction of the individual metrics. This can be deduced from the process integration studies done above for all categories except CO_2 emissions. For CO_2, it is theoretically possible to reduce and eliminate completely if capital investment is available. The weights are assigned based on the relative contribution to the overall profit. Since water, electricity, and fuel savings have been accounted for in terms of lower operating cost, they have been allotted lower weights. CO_2 emissions have not been accounted for in the profit equation in any step of our study which gives it a higher weight factor. It is worth noting that the electrical energy savings for the integrated and intensified case are negative because the addition of a compressor leads to an increase in the electricity consumption. It also marginally adds on to the water footprint as it is assumed that steam would be consumed to generate electricity that runs the compressor, but the overall result is a reduction in water footprint due to the elimination of large condensers and reboilers on the PP Splitter.

It can be seen that the Integrated and Intensified Case with the waste heat recovery and off gas recycle has the highest SWROI value and is the most attractive overall design, both from an economic and sustainability point of view. From the above analysis, the trend is an increasing SWROI as the integration and intensification options are implemented. However, this may not always be the case, as often there could be a tradeoff between the overall reductions achieved and the total capital invested.

4.10 Safety Analysis

In the previously developed flowsheets, an economic, energy, and sustainability analysis is performed, and various metrics have been derived. One aspect of primary importance is generally left for analysis once the design has been completed and that has to do with process safety. To ensure the inclusion of safety during the design stages, the inherent safety of the process can be evaluated.

There are several metrics proposed for the evaluation of inherent safety of a process which take into account the chemical and process parameters that are available at the early stages. One such approach is the Quantitative Risk Assessment (QRA), in which a process is analyzed for the failure frequency and then combined with the consequence analysis to provide a measure of the overall risk. When considering complete flowsheets, QRA becomes rather complex and arduous. Other metrics like the Process Route Index (PRI) (Leong and Shariff, 2009) and the Process Stream Index (PSI) have been developed in order to capture the comprehensive risks posed by multi-component streams while minimizing scope for human error.

PRI can be used to rank different process flowsheets based on their inherent safety levels, while PSI serves to rank individual process streams within a process according their risk levels. Both are defined as a function of the stream parameters such as flammability, temperature, pressure, and density. The PRI was benchmarked by Leong and Shariff (2009) against the Prototype Index for Inherent Safety (PIIS) (Edwards and Lawrence, 1993), the Inherent Safety Index (ISI) (Heikkilä, 1999), and the i-Safe Index (Palaniappan et al., 2004). In addition, PRI can distinguish between process flowsheets that were ranked at the same level of Inherent Safety by the ISI (Ortiz-Espinoza et al., 2017a). Both PRI and the PSI indices have the limitation that they only rank processes or streams relative to one another, therefore do not provide a quantitative measure of risk. While QRA is a more comprehensive approach, the combined use of PRI and PSI provides a useful tool for an initial comparative assessment of inherent safety.

4.10.1 Process Route Index (PRI)

The basis for the PRI index is a set of process parameters related to the potential damage that can cause an explosion (Leong and Shariff, 2009). The distance due to explosion is given by Crowl and Louvar (2002) where the process parameters that influence consequences fir to explosion include the total mass of flammable material in the cloud, and the lower heat of combustion. Additionally, the combustibility of the material plays an important role in determining the explosion hazard. Heikkilä (1999), Edwards and Lawrence (1993) showed that combustibility can be defined as the difference between the Lower Flammability Limit (LFL) and Upper Flammability Limit (UFL) of a given substance. The term “mass” can be converted into basic process parameters (pressure and density) which can be directly extracted from any process simulator. The logic behind this being that the mass of fluid released during a leak is a function of the density of the fluid and the pressure differential between the system and surroundings. Therefore, PRI can be defined as (Leong and Shariff, 2009):

$$\mathbf{PRI} = \mathbf{f}(\mathbf{density}, \mathbf{pressure}, \mathbf{energy}, \mathbf{combustibility}) \tag{4}$$

The combustibility of the mixture is calculated based on the difference between the upper and lower flammability limits. These can be corrected for temperatures using the equations (5) and (6) as given in Crowl and Louvar (2002). The lower flammability limit is not affected by changes in pressure, but the upper flammability limit has to be corrected for pressure using the equation (7) (Crowl and Louvar, 2002).

$$\mathrm{LFL_T} = \mathrm{LFL_{25}}\left[1 - \frac{0.75(\mathrm{T}-25)}{\Delta \mathrm{H_c}}\right] \tag{5}$$

$$\mathrm{UFL_T} = \mathrm{UFL_{25}}\left[1 + \frac{0.75(\mathrm{T}-25)}{\Delta \mathrm{H_c}}\right] \tag{6}$$

$$\mathrm{UFL_T} = \mathrm{UFL} + 20.6(\log(P) + 1) \tag{7}$$

Where, $\mathrm{LFL_T}$=Lower Flammability Limit (T(°C)), $\mathrm{UFL_T}$=Upper Flammability Limit (T(°C)), $\Delta \mathrm{H_c}$= heat of combustion for component (kcal/mol), P = Pressure (MPa). Since PRI represents the overall process route, it is acceptable to take an average of all the properties in equation (4) resulting in:

$$\mathbf{PRI} = [(\mathbf{average\ mass\ heating\ value}) \times (\mathbf{average\ fluid\ density}) \times (\mathbf{average\ pressure}) \times (\mathbf{average}\ \Delta \mathbf{FL_{mix}})]/\mathbf{10^{\wedge}8} \tag{8}$$

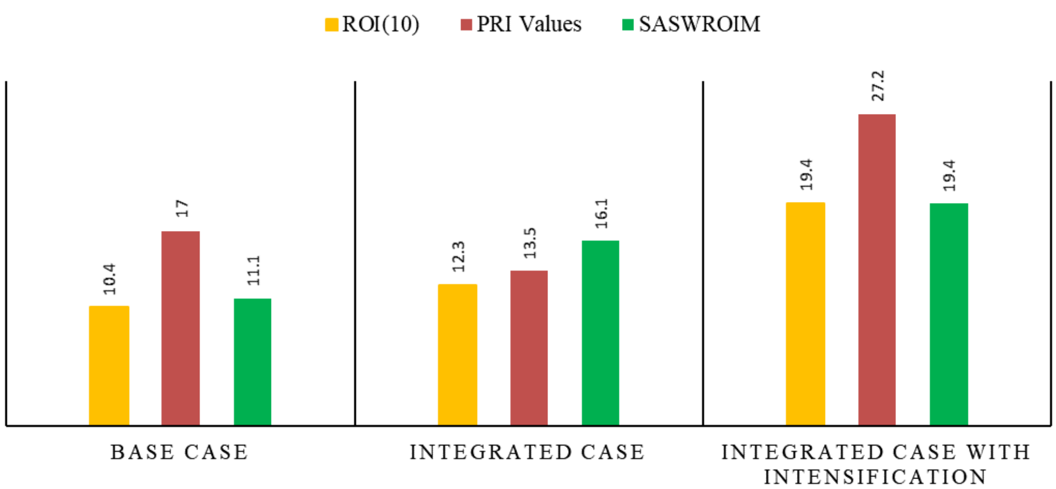

Figure 10: Chart showing PRI Values, ROI, and SWROI for all three cases considered

PRI values were calculated for all the three cases and ***Figure 10*** shows the comparison of these values for the three flowsheets under consideration. It is interesting to note that the integrated and intensified case is the one resulting in the lowest PRI number, meaning it is the safest route among the three processes compared.

4.10.2 SASWROIM - Safety and Sustainability Weighted ROI Metric

Analogous to the SWROIM metric describe above, a safety and sustainability weighted return on investment metric can be introduced which incorporates safety metrics along with the sustainability factors. Once the traditional economic return on investment (ROI) has been calculated for the base case design, a set of safety and sustainability indicators are identified. A comprehensive assessment of these factors yields the values indexed as $Indicator_{Base,i}$. The associated target values for these indicators are designated $Indicator_{Target,i}$. Strategic benchmarking techniques based on best achievable practices, can be utilized to determine the values of these targets (Guillen-Cuevas et al., 2018).

Several process and design alternatives can be generated using process synthesis, analysis, integration, and intensification activities. Representing each of these alternatives by an index *p*, with p = 1,2,3…$N_{projects}$, a new term called the Annual Safety and Sustainability Profit (ASSP) can be introduced for the p^{th} project which is defined as:

$$\mathrm{ASSP_P} = \mathrm{AEP_P}[1 + \sum_{i=1}^{N_{indicators}} w_i \left(\frac{\mathrm{Indicator_{Base,i}} - \mathrm{Indicator_{p,i}}}{\mathrm{Indicator_{Base,i}} - \mathrm{Indicator_i^{Target}}}\right)] \tag{9}$$

The SASWROIM can then defined as:

$$\mathrm{SASWROI_P} = \frac{\mathrm{ASSP_p}}{\mathrm{TCI_P}} \tag{10}$$

In Equation (9), w_i is the weighing factor in the form of a ratio representing the relative importance of the sustainability and safety factors compared to the economic profits. $Indicator_{p,i}$ is the value of the i^{th} safety or sustainability factor associated with the p^{th} design option. The denominator $Indicator_{Base,i} - Indicator_{Target,i}$ is the improvement (where the difference is positive) or deterioration (where the difference is negative) associated with the p^{th} design. Therefore, the ratio $\left(\frac{\mathrm{Indicator_{Base,i}} - \mathrm{Indicator_{p,i}}}{\mathrm{Indicator_{Base,i}} - \mathrm{Indicator_i^{Target}}}\right)$ represents the fractional contribution of the p^{th} design option toward the target performance associated with the i^{th} safety or sustainability metric. The term $ASSP_P$ is the generalized form for the quantification of the overall profit as well as possible safety and sustainability benefits of the project. This term is enhanced when there is an improvement in safety or sustainability compared to the base case design, and its value is reduced when the alternative design option results in deterioration of the safety or sustainability relevant performance indicators when compared to those associated with the base case project. The final SASWROIM is then defined in equation (10).

Table 14 below tabulates the SASROIM values for the three flowsheets (Base Case, Integrated Case, Integrated Case with Intensification) that we have considered in our case study. As can be seen, the Integrated Case with Intensification has a PRI value of 27.2 which is the highest among the three design options. This translates to a relatively unsafe design as compared to the other two scenarios. However, the resulting sustainability benefits of performing intensification in the PP Splitter design, offset the deteriorated safety performance resulting due to the introduction of high pressure streams in the process. Overall, the Integrated Case with Intensification gets a SASWROIM value of 19.4% which is considerably higher than that of the remaining design options considered.

Table 14: Tabulation of the SASWROIM values for various process flowsheets

Description	10 yr. Avg. Taxable Income MM$/yr	Total Capital Investment MM$	ROI(10)	SWROI	PRI Values	SASWROIM
Weight Factors					***0.25***	
Targets					***8.5***	
Base Case	67	643	10.38%	11.13%	17	**11.13%**
Integrated Case	79	645	12.29%	14.88%	13.5	**16.15%**
Integrated Case with Intensification	104	536	19.45%	25.21%	27.2	**19.38%**

4.10.3 Process Stream Index (PSI)

As we saw in the above case, the Integrated Case with Intensification has the highest SASWROIM value but ranks at the bottom in terms of its relative safety metric. Hence, in order to identify the most vulnerable parts of the process flowsheet, we can use the Process Safety Index (PSI) which was introduced by Shariff et al. (2012). Similar to the PRI, PSI is used to determine the inherent risk severity of individual streams within the process. The PSI can then be used to prioritize the inherent safety of individual stream against the overall streams in the simulation (Shariff et al., 2012). This relative ranking is developed for all parameters affecting the explosion hazard as discussed previously.

$$I_e = \frac{\text{heating value of individual stream}}{\text{average heating value of all streams}} \tag{11}$$

$$I_p = \frac{\text{pressure value of individual stream}}{\text{average pressure value of all streams}} \tag{12}$$

$$I_r = \frac{\text{density of individual stream}}{\text{average density of all streams}} \tag{13}$$

$$I_{FL} = \frac{\Delta FL \text{ of individual stream}}{\text{average } \Delta FL \text{ of all streams}} \quad (14)$$

The resulting dimensionless numbers can be used to differentiate the streams when considering the properties individually. They can also be combined to give an index that reflects the severity of a process stream in case of a leakage leading to a fire and/or explosion. This combined index (PSI) is expressed in equation 15.

$$\mathbf{PSI} = \mathbf{A_0} \times (\mathbf{I_e} \times \mathbf{I_p} \times \mathbf{I_r} \times \mathbf{I_{FL}}) \quad (15)$$

The empirical constant $\mathbf{A_0}$ used is to increase or decrease the magnitude of the resulting numbers for the calculation of PSI. For this work, $\mathbf{A_0}$ is chosen as 10 and the units of heating value, pressure, density, and ΔFL are (kcal/kg), (kPa), (kg/m^3), and volume %, respectively. Table 15**Error! Reference source not found.** and Table 16 show the PSI value calculations for the streams in Base Case and Integrated Case with Intensification respectively.

Table 15: PSI Values for streams in the Base Case

Stream No.	I_e	I_p	I_r	I_{fl}	PSI
119	0.86	1.71	5.41	0.70	**55.49**
114	0.91	2.53	2.30	0.95	**50.56**
113	0.91	2.58	1.76	1.07	**44.37**
122	2.23	1.43	0.10	2.39	**7.72**
105	0.89	0.88	0.98	0.64	**4.86**
118	0.89	0.82	1.08	0.56	**4.42**
112	0.91	0.74	0.49	0.81	**2.67**
106	0.89	0.70	0.26	1.09	**1.76**
107	0.90	0.55	0.19	1.11	**1.03**
108	0.90	0.40	0.13	1.12	**0.52**
109	0.90	0.25	0.08	1.10	**0.19**
110	0.91	0.23	0.07	1.09	**0.16**
111	0.91	0.18	0.15	0.43	**0.11**

Table 16: PSI values for streams in Integrated Case with Intensification

Stream No.	I_e	I_p	I_r	I_{fl}	PSI
135	0.9	2.3	3.0	0.9	**55.7**
132	0.9	2.0	2.7	0.9	**43.1**
134	0.9	2.0	2.7	0.9	**43.1**
119	0.9	1.5	3.4	0.8	**34.6**
129	1.0	2.2	1.2	1.1	**29.1**
128	1.0	2.2	1.1	1.2	**27.7**
130	0.9	1.3	1.8	0.8	**15.2**
131	0.9	1.2	1.7	0.7	**14.3**
114	1.0	0.6	1.5	0.9	**7.9**
122	2.3	1.2	0.1	2.6	**4.8**
105	0.9	0.7	0.6	0.7	**3.0**
118	0.9	0.7	0.7	0.6	**2.8**
123	0.9	0.7	0.2	1.2	**1.7**
126	1.0	0.6	0.3	0.9	**1.6**
127	1.0	0.6	0.3	0.8	**1.5**
106	0.9	0.6	0.2	1.2	**1.1**
107	0.9	0.5	0.1	1.2	**0.6**
108	0.9	0.3	0.1	1.2	**0.3**
109	1.0	0.2	0.0	1.2	**0.1**
110	1.0	0.2	0.0	1.2	**0.1**
124	1.0	0.2	0.1	0.6	**0.1**
125	1.0	0.2	0.1	0.4	**0.1**

Figure 11 shows the Integrated case with Intensification flowsheet with the high-risk streams highlighted in red based on their relative PSI values. As can be seen from the figure, the heat pump compressor system in the PP Splitter section has effectively introduced the highest risk streams within the process. This makes logical sense as these streams have very high flow rates (due to high reflux ratios required in the PP Splitter) and are at high pressures (due to the heat pump compressor). In addition, the Hydrogen streams are also classified as high risk due to the large range of flammability limits. Some of the vapor streams in the Reactor Effluent Compressor sections (second stage discharge) also have to be paid attention. It is to be noted that the PSI numbers represent the Inherent Safety values of each of the streams highlighted. However, additional PSM mitigation techniques such as LOPA and HAZOP analysis can lead to identifying advanced control measures to minimize the risk associated with these streams. Some observations made based on the PSI method are:

- PSI does account for the high pressure streams, but fails to account for streams with pressure lower than atmospheric (vacuum) which could lead to air ingress and cause explosion
- In the current case study, Reactor Effluent is very low pressure (potentially vacuum) stream at very high temperature which can be hazardous
- Temperature accounted for only indirectly through the UFL and LFL corrections and note direct measurements. Small ranges of UFL/LFL values can potentially offset the risk of high temperature streams

Finally, it should be noted that PSI is only a measurement of relative safety between several process streams. There may be a scenario that we are comparing streams within an extremely hazardous process flow-scheme which should not be implemented. Therefore, it should be used in conjunction with other safety indices which provide more insight into the inherent safety of the overall process, and not independently.

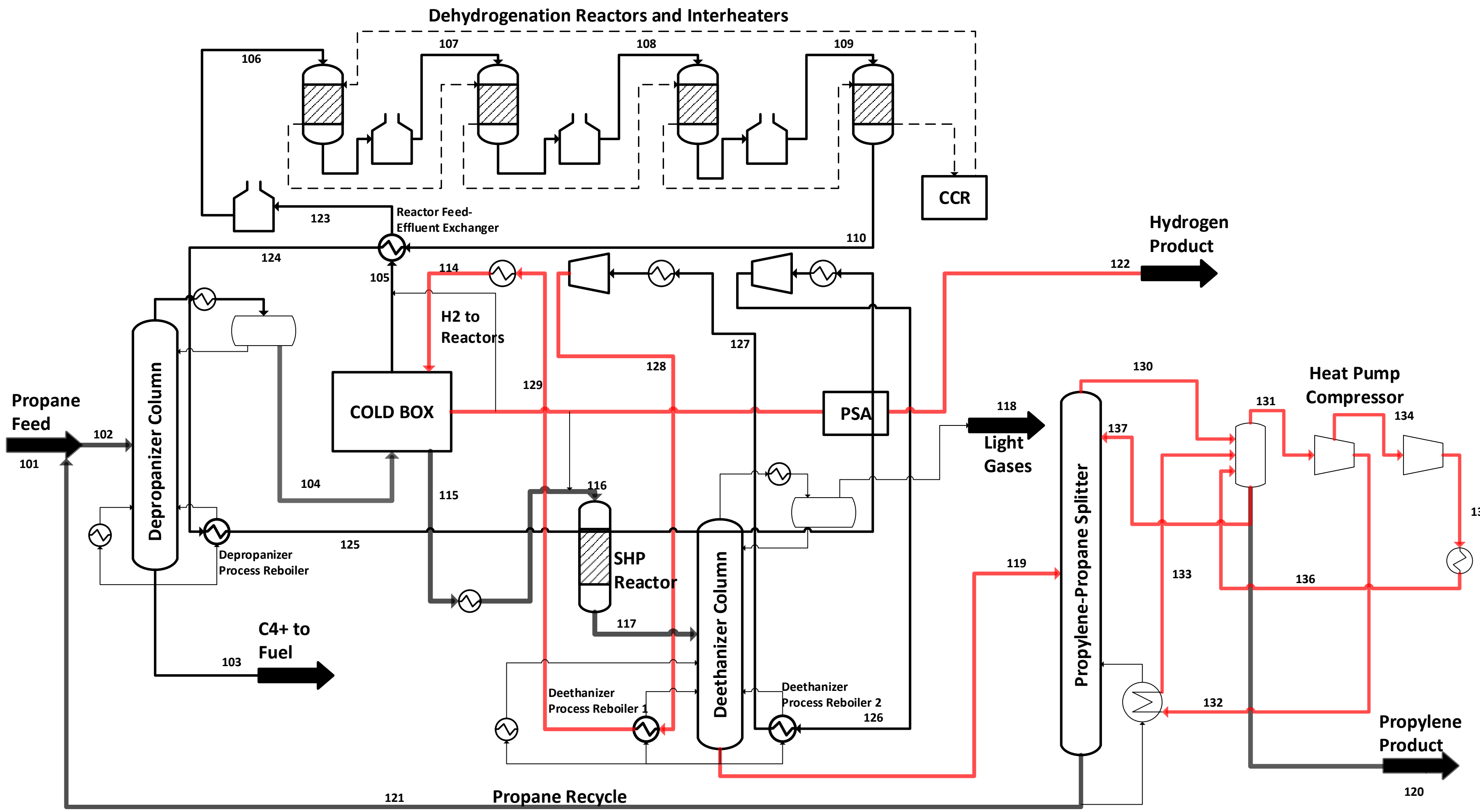

Figure 11: Simplified PFD of the Integrated Case with Intensification highlighting the High Risk streams in Red

5. CONCLUSIONS

This paper provided a systematic way of developing a sustainable process design with illustration of on-purpose propylene production. Starting with two gross economic metrics, a quick economic profitability calculation provided information to select a competitive process option for on-purpose propylene production. Then, a base case design provides the economic, energy, and emissions profile for the selected PDH process. Following this, a thorough process analysis provided the energy hotspots. An initial thermal pinch analysis identified the potential heat exchanges, and where they should be implemented. The entire process flowsheet was changed from the base case to the integrated case to include four heat exchangers and associated changes for reduced external utility consumption. After this, the process still demonstrated significant energy consumption for the propane-propylene splitter since the boiling points are very close for the two components. A process intensification scheme using a heat pump compression system was utilized and subsequent changes in splitter configuration (number of trays, operating pressure etc.) were implemented for an integrated and intensified case. It was noticed at this stage that significant reduction in both capital and operating costs were achieved through implementing these design changes. The water consumption in the process was significantly reduced, leading to a lower water footprint.

The next step was the emissions analysis whereby each source of emission was analyzed. Emission factors for electricity generation, boilers, and furnaces were considered from EPA AP 42 standards and other published sources to estimate the total emission for all the design cases. It was observed that a significant amount of heat was being wasted in the fired heaters, which could be further utilized to generate steam, thereby reducing the steam consumption in the process. Another source of energy through the offgas recovery system was also identified through the emissions analysis. These were included in the process analysis. It was observed that through the utilization of the waste heat and off gas recovery addition, the overall utility consumption in the process was reduced, thereby saving in purchased utility costs and resulting emissions. An economic study revealed the most profitable options. The impact of all these case studies on the sustainability metrics was determined by calculating the SWROI for all individual cases to select the most desirable flowsheet configuration.

Finally, inherent safety metrics (PRI and PSI) were evaluated for all the process flowsheets and the high-risk areas in the process were identified. Suggestions to improve inherent safety of the process were derived.

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APPENDIX

A.1. MISR and GVM Background Calculations

A.1.1. Propane Dehydrogenation

Propane Dehydrogenation							
			$C3H8 \rightarrow C3H6 + H2$				
			Selectivity	**100%**			
	Stoich. Coeff.	**Mol Weight**	**Flow Rates**		**Unit Prices**	**MISR**	**GVM Calc**
		kg/kgmole	KMTA	kmol*10^3/yr	$/lb		$/KMTA Propylene
Reactants						2.07	0.535
Propane	-1	44	-628.57	-14.286	0.217		
Products							
Propylene	1	42	600	14.286	0.431		
Hydrogen	1	2	28.57	14.286	0.817		

A.1.2. Methanol to Olefins

MTO							
			$2CH3OH \rightarrow C2H4 + 2H2O$				
			$CH3OH + C2H4 \rightarrow C3H8 + H2O$				
		Selectivity to olefin production		**100%**	**P/E Ratio**	**1.8**	
	Stoich. Coeff.	**Mol Weight**	**Flow Rates**		**Unit Prices**	**MISR**	**GVM Calc**
		kg/kgmole	KMTA	kmol*10^3/yr	$/lb		$/KMTA Propylene
Reactants						1.29	0.268
Methanol	-7.25	32	-1841.27	-57.540	0.136		
Products							
Propylene	1.8	42	600	14.286	0.431		
Ethylene	1	28	222.22	7.937	0.293		
Water	7.25	18	1035.71	57.540	0.000		

A.1.3. Olefin Metathesis

Olefin Metathesis							
			$C2H4 + C4H8 \rightarrow 2C3H6$				
			Selectivity	**100%**			
	Stoich. Coeff.	**Mol Weight**	**Flow Rates**		**Unit Prices**	**MISR**	**GVM Calc**
		kg/kgmole	KMTA	kmol*10^3/yr	$/lb		$/KMTA Propylene
Reactants						0.95	-0.045
Ethylene	-1	28	-200.00	-7.143	0.293		
Butylene	-1	56	-400.00	-7.143	0.531		
Products							
Propylene	2	42	600	14.286	0.431		

A.2. Capital Costs Estimation (Equipment Wise)

A.2.1. Columns, Vessels and Reactors

List of Equipments	Tag No.	Equipment Name	Hand Calculations for Cost														
			Size Parameter	S Value			a	b	n	Prchased Equipment Cost (2016)			Fm	Hand Factor	Installed Cost (2016)		
				Base Case	Integrated Case	Integration + HPC				Base Case	Integrated Case	Integration + HPC			Base Case	Integrated Case	Integration + Intensification
Columns	1301	Depropanizer Column	Shell Mass, kg	398163	398163	398163	11600	34	0.85	2,018,931	2,018,931	2,018,931	1	4	8,075,723	8,075,723	8,075,723
		DeC3 Trays	Diameter, m	3.66	3.66	3.66	130	440	1.8	575,258	575,258	575,258	1	1	575,258	575,258	575,258
	1360	Deethanizer Column	Shell Mass, kg	1274121	1274121	1274121	11600	34	0.85	5,406,158	5,406,158	5,406,158	1	4	21,624,633	21,624,633	21,624,633
		DeC2 Trays	Diameter, m	6.71	6.71	6.71	130	440	1.8	1,499,000	1,499,000	1,499,000	1	1	1,499,000	1,499,000	1,499,000
	1370	PP Splitter	Shell Mass, kg	3243217	3243217	1900322	11600	34	0.85	11,947,173	11,947,173	7,589,051	1	4	47,788,691	47,788,691	30,356,202
		PP Splitter Trays	Diameter, m	12.2	12.2	11.4	130	440	1.8	10,208,739	10,208,739	9,092,746	1	1	10,208,739	10,208,739	9,092,746
															89,772,044	**89,772,044**	**71,223,562**
Vessels	1302	Depropanizer Receiver	Shell Mass, kg	27297	27297	27297	10200	31	0.85	198,000	198,000	198,000	1	4	792,000	792,000	792,000
	1320	Reactor Effluent	Shell Mass, kg	18406	18406	18406	11600	34	0.85	159,034	159,034	159,034	1	4	636,135	636,135	636,135
	1321	REC Interstage Drum	Shell Mass, kg	22170	22170	22170	11600	34	0.85	184,248	184,248	184,248	1	4	736,992	736,992	736,992
	1322	REC Discharge Drum	Shell Mass, kg	37261	37261	37261	11600	34	0.85	279,855	279,855	279,855	1.07	4	1,197,778	1,197,778	1,197,778
	1330	High pressure Separator	Shell Mass, kg	67902	67902	67902	11600	34	0.85	458,175	458,175	458,175	1.07	4	1,960,988	1,960,988	1,960,988
	1331	Intermediate Pressure	Shell Mass, kg	9782	9782	9782	11600	34	0.85	97,873	97,873	97,873	1.07	4	418,895	418,895	418,895
	1332	LP Separator (Cold Box)	Shell Mass, kg	8333	8333	8333	11600	34	0.85	86,916	86,916	86,916	1.07	4	372,001	372,001	372,001
	1333	Flash Drum (Cold Box)	Shell Mass, kg	2291	2291	2291	11600	34	0.85	36,936	36,936	36,936	1.07	4	158,087	158,087	158,087
	1361	Deethanizer Receiver	Shell Mass, kg	83139	83139	83139	11600	34	0.85	541,973	541,973	541,973	1	4	2,167,893	2,167,893	2,167,893
	1371	Heat Pump Compressor Suction Drum	Shell Mass, kg	241436	241436	241436	11600	34	0.85	1,323,749	1,323,749	1,323,749	1	4	5,294,997	5,294,997	5,294,997
															13,735,767	**13,735,767**	**13,735,767**
Reactors	1310	Reactor 1	Volume, m3	241.3245464	241.3245464	241.3245464	61500	32500	0.8	2,748,354	2,748,354	2,748,354	1	4	10,993,417	10,993,417	10,993,417
	1311	Reactor 2	Volume, m3	241.3245464	241.3245464	241.3245464	61500	32500	0.8	2,748,354	2,748,354	2,748,354	1	4	10,993,417	10,993,417	10,993,417
	1312	Reactor 3	Volume, m3	241.3245464	241.3245464	241.3245464	61500	32500	0.8	2,748,354	2,748,354	2,748,354	1	4	10,993,417	10,993,417	10,993,417
	1313	Reactor 4	Volume, m3	241.3245464	241.3245464	241.3245464	61500	32500	0.8	2,748,354	2,748,354	2,748,354	1	4	10,993,417	10,993,417	10,993,417
	1399	SHP Reactor	Volume, m3	28.35920724	28.35920724	28.35920724	61500	32500	0.8	547,323	547,323	547,323	1	4	2,189,293	2,189,293	2,189,293
															46,162,960	**46,162,960**	**46,162,960**

A.2.2. Exchangers

List of Equipments	Tag No.	Equipment Name	Hand Calculations for Cost														
			Size Parameter	S Value			a	b	n	Prchased Equipment Cost (2016)			Fm	Hand Factor	Installed Cost (2016)		
				Base Case	Integrated Case	Integration + HPC				Base Case	Integrated Case	Integration + HPC			Base Case	Integrated Case	Integration + Intensification
	1401	Depropanizer Condenser	Area, m2	4759.47	4759.47	4759.47	32000	70	1.2	1,891,452	1,891,452	1,891,452	1	3.5	6,620,081	6,620,081	6,620,081
	1420	Reactor Effluent Cooler	Area, m2	2005.84	620.39	620.39	32000	70	1.2	691,812	194,006	194,006	1	3.5	2,421,342	679,021	679,021
	1421	REC Interstage Cooler	Area, m2	1093.92	868.19	868.19	32000	70	1.2	351,174	274,069	274,069	1	3.5	1,229,109	959,240	959,240
	1422	REC Discharge Cooler	Area, m2	1088.93	893.67	893.67	32000	70	1.2	349,432	282,590	282,590	1	3.5	1,223,011	989,066	989,066
	1476	Propylene Trim Condenser (Integrated	Area, m2	0.00	0.00	1917.02	32000	70	1.2	0	0	656,950	1	3.5	0	0	2,299,326
	1481	PP Splitter Condenser (Base case)	Area, m2	33323.86	33323.86	0.00	32000	70	1.2	19,238,444	19,238,444	0	1	3.5	67,334,553	67,334,553	0
	1402	Depropanizer Reboiler	Area, m2	377.46	209.56	209.56	30400	122	1.1	116,678	75,934	75,934	1	3.5	408,373	265,769	265,769
Exchangers	1402A	Depropanizer Process Reboiler	Area, m2	0.00	1047.21	1047.21	30400	122	1.1	0	293,858	293,858	1	3.5	0	1,028,504	1,028,504
	1440	SHP Feed Heater	Area, m2	85.80	85.80	85.80	28000	54	1.2	40,298	40,298	40,298	1	3.5	141,042	141,042	141,042
	1461	Deethanizer Steam Reboiler	Area, m2	527.92	211.97	211.97	30400	122	1.1	154,836	76,501	76,501	1	3.5	541,926	267,755	267,755
	1461A	Deethanizer Process Reboiler-REC Interstage	Area, m2	0.00	1416.32	1416.32	30400	122	1.1	0	397,333	397,333	1	3.5	0	1,390,665	1,390,665
	1461B	Deethanizer Process Reboiler-REC Discharge	Area, m2	0.00	1403.12	1403.12	30400	122	1.1	0	393,580	393,580	1	3.5	0	1,377,530	1,377,530
	1480	PP Splitter Reboiler	Area, m2	2997.16	2997.16	0.00	30400	122	1.1	866,331	866,331	0	1	3.5	3,032,157	3,032,157	0
	1415	Hot Combined Feed Exchanger	Area, m2	0.00	5433.13	5433.13	32000	70	1.2	0	2,211,445	2,211,445	1	3.5	0	7,740,056	7,740,056
	1430	Cold Combined Feed Exchanger (Cold Box)	Area, m2	26090.51	26090.51	26090.51	1600	210	0.95	3,381,524	3,381,524	3,381,524	1.07	3.5	12,663,806	12,663,806	12,663,806
	1432	Feed Chiller (Cold Box)	Area, m2	4130.68	4130.68	4130.68	1600	210	0.95	588,406	588,406	588,406	1.07	3.5	2,203,580	2,203,580	2,203,580
	1475	PP Splitter Reboiler Condenser	Area, m2	0.00	0.00	11730.33	30400	122	1.1	0	0	3,777,675	1	3.5	0	0	13,221,861
	1460	Deethanizer Condenser	Area, m2	1876.40	1876.40	1876.40	32000	70	1.2	641,113	641,113	641,113	1	3.5	2,243,897	2,243,897	2,243,897
															100,062,877	**108,936,722**	**54,091,199**

A.2.3. Fired Heaters, Pumps, Compressors, Packages and Totals

List of Equipments	Tag No.	Equipment Name	Hand Calculations for Cost														
			Size Parameter	S Value			a	b	n	Prchased Equipment Cost (2016)			Fm	Hand Factor	Installed Cost (2016)		
				Base Case	Integrated Case	Integration + HPC				Base Case	Integrated Case	Integration + HPC			Base Case	Integrated Case	Integration + Intensification
Fired Heaters	1201	Charge Heater	Duty, MW	127.52	23.07	23.07	43000	111000	0.8	5,549,805	1,446,252	1,446,252	1	2	11,099,609	2,892,503	2,892,503
	1202	Interheater 1	Duty, MW	21.32	21.32	21.32	43000	111000	0.8	1,360,604	1,360,604	1,360,604	1	2	2,721,207	2,721,207	2,721,207
	1203	Interheater 2	Duty, MW	21.36	21.36	21.36	43000	111000	0.8	1,362,688	1,362,688	1,362,688	1	2	2,725,376	2,725,376	2,725,376
	1204	Interheater 3	Duty, MW	21.01	21.01	21.01	43000	111000	0.8	1,345,121	1,345,121	1,345,121	1	2	2,690,242	2,690,242	2,690,242
															19,236,434	**11,029,328**	**11,029,328**
Pumps	1501	Depropanizer Overhead	Flow, litres/sec	183.37	183.37	183.37	8000	240	0.9	35,011	35,011	35,011	1	4	140,044	140,044	140,044
	1540	Flash Drum Pumps	Flow, litres/sec	107.28	107.28	107.28	8000	240	0.9	24,752	24,752	24,752	1	4	99,007	99,007	99,007
	1560	Deethanizer Reflux	Flow, litres/sec	186.77	186.77	186.77	8000	240	0.9	35,459	35,459	35,459	1	4	141,835	141,835	141,835
	1580	Propylene Product Pumps	Flow, litres/sec	1577.26	1577.26	75.20	8000	240	0.9	194,135	194,135	20,224	1	4	776,538	776,538	80,897
	1578	Propane Recycle Pumps	Flow, litres/sec	45.83	45.83	45.83	8000	240	0.9	15,902	15,902	15,902	1	4	63,609	63,609	63,609
															1,221,034	**1,221,034**	**525,392**
Compressors	1531	HP Expander (Cold Box)	Flow, m3/hr	7054.292925	7054.292925	7054.292925	4450	57	0.8	74,655	74,655	74,655	1	2.5	186,638	186,638	186,638
	1532	LP Expander (Cold Box)	Flow, m3/hr	6164.011255	6164.011255	6164.011255	4450	57	0.8	67,485	67,485	67,485	1	2.5	168,711	168,711	168,711
	1520A	Reactor Effluent	Power, kW	13621.32	13621.32	13621.32	580000	20000	0.6	6,797,678	6,797,678	6,797,678	1	2.5	16,994,196	16,994,196	16,994,196
	1520B	Reactor Effluent	Power, kW	12012.44	12012.44	12012.44	580000	20000	0.6	6,347,092	6,347,092	6,347,092	1	2.5	15,867,731	15,867,731	15,867,731
	1540	SHP Hydrogen	Power, kW	36.96	36.96	36.96	260000	2700	0.75	308,194	308,194	308,194	1	2.5	770,484	770,484	770,484
	1575A	Heat Pump Compressor	Power, kW	0.00	0.00	14407.43	580000	20000	0.6	0	0	7,010,047	1	2.5	0	0	17,525,117
	s	Heat Pump Compressor	Power, kW	0.00	0.00	128.20	580000	20000	0.6	0	0	972,298	1	2.5	0	0	2,430,745
	15xx	Turbine for REC Stage 1															
	15xx	Turbine for REC Stage 2															
	15xx	Turbine for HPC															
															33,987,760	**33,987,760**	**53,943,623**
Packages	01	PSA															
	02	RED's and Feed Pretreatment															
	03	Propyelene Refrigerant (DeC2 Condenser)													**17,148,895**	**17,148,895**	**17,148,895**
		Refrigerant Compressor	Power, kW	8862.00	8862.00	8862.00	580000	20000	0.6	5,387,530	5,387,530	5,387,530	1	2.5	13,468,826	13,468,826	13,468,826
		Condenser (CW)	Area, m2	2883.44	2883.44	2883.44	32000	70	1.2	1,051,448	1,051,448	1,051,448	1	3.5	3,680,070	3,680,070	3,680,070

Total Costs of Equipment (Installed, ($2016))		321,327,772	321,994,511	267,860,726
	OSBL%	30%		
	DEC%	30%		
	Contingency	10%		
Total Fixed Capital Costs (MM$, 2016)		**584.8**	**586.0**	**487.5**

A.3. Utility Costs

A.3.1. Cooling Water and LP Steam

Cooling Water							
		CW Flow			CW Price		
		Base Case	Integrated Case	Integration +HPC	Base Case	Integrated Case	Integration +HPC
		lb/hr			$/yr		
1401	Depropanizer Condenser	3,193,104	3,121,637	3,121,637	271,823	265,739	265,739
1420	Reactor Effluent Cooler	48,833,905	1,181,946	1,181,946	4,157,143	100,617	100,617
1421	REC Interstage Cooler	6,771,749	3,149,893	3,149,893	576,467	268,145	268,145
1422	REC Discharge Cooler	6,290,712	3,242,343	3,242,343	535,517	276,015	276,015
1476	Propylene Trim Condenser	0	0	2,862,219	0	0	243,656
1481	PP Splitter Condenser	32,869,591	31,042,550	0	2,798,129	2,642,597	0
				Total Cooling Water Costs	8,339,079	3,553,112	1,154,171
					0.8341		

LP Steam							
		LPS_Flow			LPS_Cost		
		Base Case	Integrated Case	Integration +HPC	Base Case	Integrated Case	Integration +HPC
		lb/hr			$/yr		
1402	Depropanizer Reboiler	86,340	49,605	49,605	3,461,277	1,988,595	1,988,615
1440	SHP Feed Heater	15,637	15,622	15,622	626,856	626,254	626,270
1461	Deethanizer Reboiler	85,499	34,527	34,527	3,427,570	1,384,161	1,384,153
1480	PP Splitter Reboiler	697,095	696,675	0	27,945,859	27,928,992	0
1531	Reactor Effluent Compressor Stage 1	0	0	0	0	0	0
1532	Reactor Effluent Compressor Stage 2	0	0	0	0	0	0
1575A	Heat Pump Compressor Stage 1	0	0	0	0	0	0
1575B	Heat Pump Compressor Stage 2	0	0	0	0	0	0
				Total LP steam Costs	35,461,561	31,928,002	3,999,038

A.3.2. Natural Gas and Power Costs

Natural Gas

			NG_Flow	NG_Cost		
			Base Case	Base Case	Integrated Case	Integration +HPC
			SCFH	$/yr		
1201	Charge Heater		411,765	10,480,420	1,896,072	1,896,072
1202	Interheater 1		68,851	1,752,421	1,752,421	1,752,421
1203	Interheater 2		68,987	1,755,889	1,755,889	1,755,889
1204	Interheater 3		67,840	1,726,697	1,726,697	1,726,697
		Total Natural Gas Firing Costs		15,715,427	7,131,079	7,131,079

Power

		Shaft Power			Cost		
		Base Case	Integrated Case	Integration +HPC	Base Case	Integrated Case	Integration +HPC
		hP			$/yr		
1501	Depropanizer Overhead Pumps	77	77	77	30,842	30,842	30,842
1540	Flash Drum Pumps (Cold Box)	728	728	728	293,045	293,045	293,045
1560	Deethanizer Reflux Pumps	116	116	116	46,695	46,695	46,695
1578	Propane Recycle Pumps	121	121	121	48,656	48,656	48,656
1580	Propylene Product Pumps	78	78	78	31,256	31,256	31,256
					450,495	450,495	450,495
		Shaft Power			Cost		
		Base Case	Integrated Case	Integration +HPC	Base Case	Integrated Case	Integration +HPC
		hP			$/yr		
1520A	Reactor Effluent Compressor Stage 1	18,399	18,399	18,399	7,401,987	7,401,987	7,401,987
1520B	Reactor Effluent Compressor Stage 2	16,325	16,325	16,325	6,567,559	6,567,559	6,567,559
1540	SHP Hydrogen Compressor	49	49	49	19,880	19,880	19,880
1575A	Heat Pump Compressor Stage 1	0	0	19,321	0	0	7,772,809
1575B	Heat Pump Compressor Stage 2	0	0	172	0	0	69,156
		35,893	35,893	55,386	13,989,426	13,989,426	21,831,391
		Total Electricity Costs ($/yr)			14,439,921	14,439,921	22,281,886

A.3.3. Refrigeration Equipment and Totals

Refrigerant Section							
		Shaft Power/CW Flow			Cost		
		Base Case	Integrated Case	Integration +HPC	Base Case	Integrated Case	Integration +HPC
		hP/lb/hr			$/yr		
1460	Refrigerant Compressor	11,884	11,884	11,884	4,781,013	4,781,013	4,781,013
	Refrogerant Condenser (CW)	505,448	505,448	505,448	43,028	43,028	43,028
		47,777					

	Base Case	Integrated Case	Integration + HPC
Total Utility Costs ($/yr)	78,780,029	61,876,155	39,390,215
Total Cooling Water Costs	8,382,107	3,596,140	1,197,199
Total LP steam Costs	35,461,561	31,928,002	3,999,038
Total Natural Gas Firing Costs	15,715,427	7,131,079	7,131,079
Total Electricity Costs ($/yr)	19,220,934	19,220,934	27,062,899

A.4. Pinch Analysis Data

A.4.1. Streams extracted for Base Case

Stream Name	Supply Temperature	Target Temperature	Heat Duty	Heat Flow	Stream Type	Supply Shift	Target Shift
	°F	°F	kW	kW		°C	°C
DeC3_Cond_S1	113.1	111.8	93.000	93.0	HOT	38.1	37.4
DeC3_Cond_S2	111.8	110.2	16340.000	16340.0	HOT	37.4	36.5
DeC3_Cond_S3	110.2	108.6	5043.000	5043.0	HOT	36.5	35.6
REC_Cooler_S1	1054	92	99964.000	99964.0	HOT	560.8	26.4
REC_Int_Cooler_S1	267.39	92	13862.000	13862.0	HOT	123.8	26.4
REC_Dis_Cooler_S1	252.1	92	12878.000	12878.0	HOT	115.3	26.4
PP_Cond_S1	106.7	106	122705.000	122705.0	HOT	34.6	34.2
PP_Cond_S2	106	105.4	41017.000	41017.0	HOT	34.2	33.8
PP_Cond_S3	105.4	104.4	18915.000	18915.0	HOT	33.8	33.3
DeC2_Cond_S1	35.6	26.6	11057.000	11057.0	HOT	-4.9	-9.9
DeC2_Cond_S2	26.6	11	7264.000	7264.0	HOT	-9.9	-18.6
DeC3_Reb_S1	123.8	124.5	23173.000	23173.0	COLD	57.9	58.3
SHP_Htr_S1	98.3	140	4195.000	4195.0	COLD	43.8	66.9
DeC2_Reb_S1	176.7	176.8	23081.000	23081.0	COLD	87.3	87.4
PP_Reb_S1	127.4	127.5	143874.000	143874.0	COLD	59.9	60.0
PP_Reb_S2	127.5	127.7	43228.000	43228.0	COLD	60.0	60.1
CH_S1	84.3	1112	106261.000	106261.0	COLD	36.0	606.9
IH1_S1	994.3	1130	17768.000	17768.0	COLD	541.6	616.9
IH2_S1	1012.9	1148	17805.000	17805.0	COLD	551.9	626.9
IH3_S1	1034	1166	17509.000	17509.0	COLD	563.6	636.9

A.4.2. Streams Extracted for Integrated Case with Intensification

Stream Name	Supply Temperature	Target Temperature	Heat Duty	Heat Flow	Stream Type	Supply Shift	Target Shift
	°F	°F	kW	kW		°C	°C
DeC3_Cond_S1	113.1	111.8	92.724	92.724	HOT	38.1	37.4
DeC3_Cond_S2	111.8	110.2	16339.681	16339.6808	HOT	37.4	36.5
DeC3_Cond_S3	110.2	108.6	5042.764	5042.7642	HOT	36.5	35.6
REC_Cooler_S1	125	92	2415.650	2415.6502	HOT	44.7	26.4
REC_Int_Cooler_S1	176.8	92	6423.729	6423.729	HOT	73.5	26.4
REC_Dis_Cooler_S1	176.8000001	92	6612.265	6612.2654	HOT	73.5	26.4
DeC2_Cond_S1	35.59617729	26.56208644	11057.428	11057.4283	HOT	-4.9	-10.0
DeC2_Cond_S2	26.56208644	10.95774771	7264.376	7264.3756	HOT	-10.0	-18.6
DeC3_Reb_S1	123.7956395	124.5819285	13329.568	13329.5685	COLD	57.9	58.4
SHP_Htr_S1	98.30367719	140	4195.415	4195.4146	COLD	43.8	66.9
DeC2_Reb_S1	176.7200928	177	9272.322	9272.3218	COLD	87.3	87.5
CH_S1	963.7653556	1112	19224.239	19224.239	COLD	524.6	606.9
IH1_S1	994.2503082	1130	17768.012	17768.0124	COLD	541.5	616.9
IH2_S1	1012.8704	1148	17804.911	17804.9109	COLD	551.9	626.9
IH3_S1	1034.014554	1166	17508.994	17508.9938	COLD	563.6	636.9

A.5. Emissions Calculations

A.5.1. Base Case

Emission Calculations - Base Case				
		Base Case	Base Case + WHR	Base Case + WHR + OGR
	Metric for Estimation	Metric Value	Metric Value	Metric Value
Natural Gas Combustion	Natural Gas consumption, MMSCFH	**1.581**	**1.357**	**1.357**
Steam Boiler (Offsites)		0.998	0.774	0.774
Fired Heater (Reactor Section)		0.583	0.583	0.583
Electricity Consumption	Power, MW	**26.77**	**26.77**	**26.77**
Product Stream Flaring (100% Combustion)	CO2 Flow Rate, lbhr	**48689**	**48689**	**5309**
Deethanizer Off Gas		43380	43380	0
Flash Gas from Cold Box		3498	3498	3498
DeC3 Bottoms		1811	1811	1811
	Pollutant	**Base Case**	**Base Case + WHR**	**Base Case + WHR + OGR**
		lb/yr	lb/hr	lb/hr
	CO2	2,232,770,283	2,009,267,883	1,649,213,883
	Methane	48355	44071	44071
	SO2	7874	6756	6756
	TOC	144354	123867	123867
	VOC	72177	61933	61933
Assume Low Nox Burners in Heaters	**N2O**	10976	9784	9784

A.5.2. Integrated Case

Emission Calculations - Integrated Case				
		Integrated Case	**Integrated Case with WHR**	**Integrated case +WHR+OGR**
	Metric for Estimation	Metric Value	Metric Value	Metric Value
Natural Gas Combustion	Natural Gas consumption, MMSCFH	**1.156**	**1.057**	**1.057**
Steam Boiler (Offsites)		0.891	0.792	0.792
Fired Heater (Reactor Section)		0.265	0.265	0.265
Electricity Consumption	Power, MW	**26.77**	**26.77**	**26.77**
Product Stream Flaring (100% Combustion)	CO2 Flow Rate, lbhr	**48689**	**48689**	**5309**
Deethanizer Off Gas		43380	43380	0
Flash Gas from Cold Box		3498	3498	3498
DeC3 Bottoms		1811	1811	1811
	Pollutant	**Integrated Case**	**Integrated Case with WHR**	**Integrated case +WHR+OGR**
		lb/yr	lb/hr	lb/hr
	CO2	1,808,872,683	1,710,467,883	1,350,413,883
	Methane	40231	38344	38344
	SO2	5754	5262	5262
	TOC	105497	96477	96477
	VOC	52749	48238	48238
Assume Low Nox Burners in Heaters	**N2O**	8715	8190	8190

A.5.3. Integrated Case with Intensification

Emission Calculations - Integrated and Intensified Case				
		Integrated +HPC Case	**Integrated + HPC Case with WHR**	**Integrated +HPC case +WHR+OGR**
	Metric for Estimation	Metric Value	Metric Value	Metric Value
Natural Gas Combustion	Natural Gas consumption, MMSCFH	**0.377**	**0.265**	**0.265**
Steam Boiler (Offsites)		0.113	0.000	0.000
Fired Heater (Reactor Section)		0.265	0.265	0.265
Electricity Consumption	Power, MW	**41.30**	**41.30**	**41.30**
Product Stream Flaring (100% Combustion)	CO2 Flow Rate, lbhr	**48689**	**48689**	**5309**
Deethanizer Off Gas		43380	43380	0
Flash Gas from Cold Box		3498	3498	3498
DeC3 Bottoms		1811	1811	1811
	Pollutant	**Integrated +HPC Case**	**Integrated + HPC Case with WHR**	**Integrated +HPC case +WHR+OGR**
		lb/yr	lb/hr	lb/hr
	CO2	1,171,659,267	1,059,410,067	699,356,067
	Methane	35244	33092	33092
	SO2	1879	1318	1318
	TOC	34447	24158	24158
	VOC	17224	12079	12079
Assume Low Nox Burners in Heaters	**N2O**	5981	5382	5382

A.6. Economic Calculations

A.6.1. DCFROR - Base Case

Owner's Name		Capital Cost Basis Year	2006
Plant Location		Units	○ English ○ Metric
Case Description		On Stream	8,300 hr/yr 345.83 day/yr

REVENUES AND PRODUCTION COSTS

	$MM/yr
Main product revenue	554.4
Byproduct revenue	47.1
Raw materials cost	322.1
Utilities cost	78.8
Consumables cost	10.0
VC	363.8
Salary and overheads	15.0
Maintenance	20.0
Interest	0.0
Royalties	0.0
FC	35.0

CAPITAL COSTS

	$MM
ISBL Capital Cost	321.0
OSBL Capital Cost	96.3
Engineering Costs	125.2
Contingency	41.7
Total Fixed Capital Cost	584.2
Working Capital	58.4

CONSTRUCTION SCHEDULE

Year	% FC	% WC	% FC	%VC
1	25.00%			
2	75.00%	100.00%		
3			100.00%	50.00%
4			100.00%	100.00%
5			100.00%	100.00%
6			100.00%	100.00%
7+			100.00%	100.00%

ECONOMIC ASSUMPTIONS

Cost of equity		Debt ratio		Tax rate	0.4
Cost of debt				Depreciation method	MACRS
Cost of capital	0.07			Depreciation period	7 years

CASH FLOW ANALYSIS

All figures in $MM unless indicated

Project year	Cap Ex	Revenue	Total Costs	Gr. Profit	Deprcn	Taxbl Inc	Tax Paid	Cash Flow	PV of CF	NPV
1	146.1	0.0	0.0	0.0	0.0	0.0	0.0	-146.1	-136.5	-136.5
2	496.6	0.0	0.0	0.0	0.0	0.0	0.0	-496.6	-433.7	-570.2
3	0.0	277.2	216.9	60.3	83.5	-23.2	0.0	60.3	49.2	-521.0
4	0.0	554.4	398.8	155.6	143.1	12.5	-9.3	164.8	125.8	-395.3
5	0.0	554.4	398.8	155.6	73.0	82.6	5.0	150.6	107.3	-287.9
6	0.0	554.4	398.8	155.6	52.2	103.4	33.0	122.5	81.6	-206.3
7	0.0	554.4	398.8	155.6	52.1	103.4	41.4	114.2	71.1	-135.2
8	0.0	554.4	398.8	155.6	52.2	103.4	41.4	114.2	66.5	-68.7
9	0.0	554.4	398.8	155.6	26.1	129.5	41.4	114.2	62.1	-6.6
10	0.0	554.4	398.8	155.6	0.0	155.6	51.8	103.8	52.7	46.1
11	0.0	554.4	398.8	155.6	0.0	155.6	62.2	93.3	44.3	90.5
12	0.0	554.4	398.8	155.6	0.0	155.6	62.2	93.3	41.4	131.9
13	0.0	554.4	398.8	155.6	0.0	155.6	62.2	93.3	38.7	170.7
14	0.0	554.4	398.8	155.6	0.0	155.6	62.2	93.3	36.2	206.8
15	0.0	554.4	398.8	155.6	0.0	155.6	62.2	93.3	33.8	240.7
16	0.0	554.4	398.8	155.6	0.0	155.6	62.2	93.3	31.6	272.3
17	0.0	554.4	398.8	155.6	0.0	155.6	62.2	93.3	29.5	301.8
18	0.0	554.4	398.8	155.6	0.0	155.6	62.2	93.3	27.6	329.5
19	0.0	554.4	398.8	155.6	0.0	155.6	62.2	93.3	25.8	355.3
20	-58.4	554.4	398.8	155.6	0.0	155.6	62.2	151.8	39.2	394.5

ECONOMIC ANALYSIS

Average cash flow	110.4 $MM/yr	NPV	10 years	46.1 $MM	IRR	10 years	8.9%
Simple pay-back period	5.823516017 yrs		15 years	240.7 $MM		15 years	13.9%
Return on investment (10 yrs)	10.38%		20 years	394.5 $MM		20 years	15.6%
Return on investment (15 yrs)	14.99%	NPV to yr	1	-136.5 $MM			

A.6.2. DCFROR - Integrated Case

Owner's Name		Capital Cost Basis Year	2006		
Plant Location		Units	English	Metric	
Case Description		On Stream	8,300 hr/yr	345.83 day/yr	

REVENUES AND PRODUCTION COSTS

	$MM/yr
Main product revenue	554.4
Byproduct revenue	47.1
Raw materials cost	322.1
Utilities cost	61.9
Consumables cost	10.0
VC	346.9
Salary and overheads	15.0
Maintenance	20.0
Interest	0.0
Royalties	0.0
FC	35.0

CAPITAL COSTS

	$MM
ISBL Capital Cost	322.0
OSBL Capital Cost	96.6
Engineering Costs	125.6
Contingency	41.9
Total Fixed Capital Cost	586.0
Working Capital	58.6

CONSTRUCTION SCHEDULE

Year	% FC	% WC	% FC	%VC
1	25.00%			
2	75.00%	100.00%		
3			100.00%	50.00%
4			100.00%	100.00%
5			100.00%	100.00%
6			100.00%	100.00%
7+			100.00%	100.00%

ECONOMIC ASSUMPTIONS

Cost of equity		Debt ratio	Tax rate	0.4	
Cost of debt			Depreciation method	MACRS	
Cost of capital	0.07		Depreciation period	7	years

CASH FLOW ANALYSIS

All figures in $MM unless indicated

Project year	Cap Ex	Revenue	Total Costs	Gr. Profit	Deprcn	Taxbl Inc	Tax Paid	Cash Flow	PV of CF	NPV
1	146.5	0.0	0.0	0.0	0.0	0.0	0.0	-146.5	-136.9	-136.9
2	498.1	0.0	0.0	0.0	0.0	0.0	0.0	-498.1	-435.1	-572.0
3	0.0	277.2	208.4	68.7	83.7	-15.0	0.0	68.7	56.1	-515.9
4	0.0	554.4	381.9	172.5	143.5	29.0	-6.0	178.5	136.2	-379.7
5	0.0	554.4	381.9	172.5	73.2	99.3	11.6	160.9	114.7	-265.0
6	0.0	554.4	381.9	172.5	52.3	120.1	39.7	132.8	88.5	-176.5
7	0.0	554.4	381.9	172.5	52.3	120.2	48.1	124.4	77.5	-99.1
8	0.0	554.4	381.9	172.5	52.3	120.1	48.1	124.4	72.4	-26.7
9	0.0	554.4	381.9	172.5	26.1	146.3	48.1	124.4	67.7	41.0
10	0.0	554.4	381.9	172.5	0.0	172.5	58.5	113.9	57.9	98.9
11	0.0	554.4	381.9	172.5	0.0	172.5	69.0	103.5	49.2	148.1
12	0.0	554.4	381.9	172.5	0.0	172.5	69.0	103.5	45.9	194.0
13	0.0	554.4	381.9	172.5	0.0	172.5	69.0	103.5	42.9	237.0
14	0.0	554.4	381.9	172.5	0.0	172.5	69.0	103.5	40.1	277.1
15	0.0	554.4	381.9	172.5	0.0	172.5	69.0	103.5	37.5	314.6
16	0.0	554.4	381.9	172.5	0.0	172.5	69.0	103.5	35.1	349.7
17	0.0	554.4	381.9	172.5	0.0	172.5	69.0	103.5	32.8	382.4
18	0.0	554.4	381.9	172.5	0.0	172.5	69.0	103.5	30.6	413.1
19	0.0	554.4	381.9	172.5	0.0	172.5	69.0	103.5	28.6	441.7
20	-58.6	554.4	381.9	172.5	0.0	172.5	69.0	162.1	41.9	483.6

ECONOMIC ANALYSIS

Average cash flow	120.8	$MM/yr	NPV	10 years	98.9	$MM	IRR	10 years	11.0%
Simple pay-back period	5.338470379	yrs		15 years	314.6	$MM		15 years	15.8%
Return on investment (10 yrs)	12.29%			20 years	483.6	$MM		20 years	17.3%
Return on investment (15 yrs)	17.12%		NPV to yr	1	-136.9	$MM			

A.6.3. DCGROR - Integrated Case with Intensification

Owner's Name				Capital Cost Basis Year	2006				
Plant Location				Units		English		Metric	
Case Description				On Stream	8,300	hr/yr		345.83 day/yr	

REVENUES AND PRODUCTION COSTS

	$MM/yr
Main product revenue	554.4
Byproduct revenue	47.1
Raw materials cost	322.1
Utilities cost	39.4
Consumables cost	10.0
VC	324.4
Salary and overheads	15.0
Maintenance	20.0
Interest	0.0
Royalties	0.0
FC	35.0

CAPITAL COSTS

	$MM
ISBL Capital Cost	267.8
OSBL Capital Cost	80.3
Engineering Costs	104.4
Contingency	34.8
Total Fixed Capital Cost	487.4
Working Capital	48.7

CONSTRUCTION SCHEDULE

Year	% FC	% WC	% FC	%VC
1	25.00%			
2	75.00%	100.00%		
3			100.00%	50.00%
4			100.00%	100.00%
5			100.00%	100.00%
6			100.00%	100.00%
7+			100.00%	100.00%

ECONOMIC ASSUMPTIONS

Cost of equity		Debt ratio	Tax rate	0.4	
Cost of debt			Depreciation method	MACRS	
Cost of capital	0.07		Depreciation period	7	years

CASH FLOW ANALYSIS

All figures in $MM unless indicated

Project year	Cap Ex	Revenue	Total Costs	Gr. Profit	Deprcn	Taxbl Inc	Tax Paid	Cash Flow	PV of CF	NPV
1	121.8	0.0	0.0	0.0	0.0	0.0	0.0	-121.8	-113.9	-113.9
2	414.3	0.0	0.0	0.0	0.0	0.0	0.0	-414.3	-361.8	-475.7
3	0.0	277.2	197.2	80.0	69.6	10.3	0.0	80.0	65.3	-410.4
4	0.0	554.4	359.4	195.0	119.4	75.6	4.1	190.8	145.6	-264.8
5	0.0	554.4	359.4	195.0	60.9	134.1	30.2	164.7	117.4	-147.4
6	0.0	554.4	359.4	195.0	43.5	151.4	53.6	141.3	94.2	-53.2
7	0.0	554.4	359.4	195.0	43.5	151.5	60.6	134.4	83.7	30.5
8	0.0	554.4	359.4	195.0	43.5	151.4	60.6	134.4	78.2	108.7
9	0.0	554.4	359.4	195.0	21.7	173.2	60.6	134.4	73.1	181.8
10	0.0	554.4	359.4	195.0	0.0	195.0	69.3	125.7	63.9	245.7
11	0.0	554.4	359.4	195.0	0.0	195.0	78.0	117.0	55.6	301.2
12	0.0	554.4	359.4	195.0	0.0	195.0	78.0	117.0	51.9	353.2
13	0.0	554.4	359.4	195.0	0.0	195.0	78.0	117.0	48.5	401.7
14	0.0	554.4	359.4	195.0	0.0	195.0	78.0	117.0	45.4	447.1
15	0.0	554.4	359.4	195.0	0.0	195.0	78.0	117.0	42.4	489.5
16	0.0	554.4	359.4	195.0	0.0	195.0	78.0	117.0	39.6	529.1
17	0.0	554.4	359.4	195.0	0.0	195.0	78.0	117.0	37.0	566.1
18	0.0	554.4	359.4	195.0	0.0	195.0	78.0	117.0	34.6	600.8
19	0.0	554.4	359.4	195.0	0.0	195.0	78.0	117.0	32.3	633.1
20	-48.7	554.4	359.4	195.0	0.0	195.0	78.0	165.7	42.8	675.9

ECONOMIC ANALYSIS

Average cash flow	132.0	$MM/yr	NPV	10 years	245.7 $MM	IRR	10 years	18.2%
Simple pay-back period	4.060950323	yrs		15 years	489.5 $MM		15 years	22.1%
Return on investment (10 yrs)	19.45%			20 years	675.9 $MM		20 years	23.2%
Return on investment (15 yrs)	25.09%		NPV to yr	1	-113.9 $MM			