SOCIAL, SAFETY, AND SUSTAINABLE PROCESS SELECTION APPROACH FOR ON-PURPOSE PROPYLENE PRODUCTION

A Thesis

by

JOSEPH ALEXANDER HERNANDEZ

Submitted to the Office of Graduate and Professional Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

Chair of Committee,	Mahmoud M. El-Halwagi
Co-Chair of Committee,	Chad V. Mashuga
Committee Member,	M. Sam Mannan
Head of Department,	M. Nazmul Karim

May 2018

Major Subject: Chemical Engineering

ABSTRACT

A systematic method for process selection is proposed by using accurate and reliable metrics that consider environmental, safety, and social impacts. This method provides measures in the form of three stages. The high-level process surveying and screening stage focuses on accumulating and preliminarily evaluating numerous process routes for the desired project. The targeted process selection stage ranks the designs by using metrics and reducing the number of designs considered for detailed analysis. Lastly, the Safety and Sustainability Weighted Return on Investment Metric (SASWROIM) integrates the information for decision-making before proceeding to the detailed analysis. To illustrate the approach, case studies on social indicators for process selection and on-purpose propylene production are considered.

DEDICATION

To my magnificent mother without whom this thesis would not have been written—may this paper be a testament to the power behind a mother's love and words of encouragement.

ACKNOWLEDGEMENTS

I would like to thank my committee chair, Dr. Mahmoud M. El-Halwagi, my co-chair, Dr. Chad V. Mashuga, and my committee member, Dr. M. Sam Mannan, for their guidance and support. Thanks also go to Dr. James Harris and Dr. Debalina Sengupta for inspiring me to pursue a graduate degree. Thanks go to the department faculty and staff for teaching and providing me the tools to succeed. Thanks to my friends and fellow colleagues for a great experience at Texas A&M University. Finally, thanks to my mother, father, and siblings for their encouragement.

CONTRIBUTORS AND FUNDING SOURCES

This work was supported by a thesis committee consisting of my advisor Professor Mahmoud M. El-Halwagi, and committee members, Professor M. Sam Mannan, Professor Chad V. Mashuga, and Professor M. Nazmul Karim of the Artie McFerrin Department of Chemical Engineering. The data analyzed for the propylene case study was provided by Ashwin Agarwal, Professor Debalina Sengupta of the Gas and Fuels Research Center for Texas A&M Engineering Experiment Station (TEES), and Professor Mahmoud M. El-Halwagi. All other work conducted for the thesis was completed independently by the student. No financial contributions were received or made for this thesis.

NOMENCLATURE

2TISI	Two-Tier Inherent Safety Index
3TISQ	Three-Tier Inherent Safety Quantification
A	Area (ft^3)
A_0	User Specified Constant
A_{tot}	Total Impact Area (ft^3)
A_{E}	Process Energy Area (ft^3)
A_{I}	Installation Area (ft^3)
A_{P}	Products & Byproducts Area (ft^3)
A_{R}	Raw Material & Feedstock Area (ft^3)
A_{S}	Staff Area (ft^3)
AEP	Annual Economic Profit ($)
ASP	Annual Sustainability Profit ($)
ASSP	Annual Safety and Sustainability Profit ($)
a	Cost Adjustment Addition Factor
a_{in}	Specific Inhabitant Capacity Area (ft^3-yr/capacity)
a_{tot}	Specific Sustainable Service Area (ft^3-yr/service)
b	Cost Adjustment Multiplication Factor
C_{eq}	Purchased Equipment Cost ($)
C4+	Hydrocarbons with molecular weights equal to or greater than butane
C5+	Hydrocarbons with molecular weights equal to or greater than pentane
CEPCI	Chemical Engineering Process Cost Index

CER	CO_2 Emission Reduction (10^3 tons/yr)
CM	Control Measure
CML	Control Measure Level
CTD	Cumulative Trauma Disease
CWB	Comprehensive Well-Being
DI	Damage Index
DMDS	Dimethyl-disulfide
DME	Dimethyl-ether
E	Energy (BTU)
ΔE_{fuel}	Net Energy Used as Primary Fuel Equivalent (BTU or BTU/yr)
ECC	Engineering and Construction Cost ($)
ED	Exposure Duration (min)
EE	Enclosed and Local Exhaust Ventilation Engineering Controls
EEe	Effective Engineering Control Measures
EEn	No Engineering Control Measures
EEp	Partially Effective Engineering Control Measures
EES	Electrical Energy Savings (MW)
EGP	Economic Gross Product ($/yr)
EHI	Exposure Hazard Index
EHI_{cor}	Exposure Hazard Index: Corrected
EHI_{ES}	Exposure Hazard Index: Expert System
EI	Exposure Index
EI_{ES}	Exposure Index: Expert System

EIM	Energy Intensity Metric (BTU/Ω or BTU/yr-Ω)
EIA	U.S. Energy Information Administration
FCC	Fluid Catalytic Cracking
FCI	Fixed Capital Investment ($)
FSM	Fuel Savings Metric (MW)
GC	Gasoline Column
GDP	Gross Domestic Product ($MM/person)
GGRM	Greenhouse Gas Release Metric (lbm/Ω or lbm/yr-Ω)
Δh_c	Heat of Combustion (kcal/mol)
HAP	Hazardous Air Pollutants
HDI	Human Development Index
HDO	Hydrodeoxygenation Process
HI	Hazard Index
I_{FL}	Stream Flammability Limit Indicator
I_e	Stream Heating Value Indicator
I_P	Stream Pressure Indicator
I_ρ	Stream Density Indicator
I2SI	Integrated Inherent Safety Index
IChemE	Institute of Chemical Engineers
IRA	Inherent Risk Assessment
ISL	Inherent Safety Level
ISBL	Inside Battery Limits
ISCI	Inherent Safety Cost Index

ISIM	Inherent Safety Index Model
ISPI	Inherent Safety Potential Index
i	Summation Counter Variable
k	Cost Adjustment Exponential Factor
LFL	Lower Flammability Limit (vol%)
LFL_{25}	Lower Flammability Limit at 25 °C (vol%)
$\mathrm{LFL}_{\mathrm{m}}$	Lower Flammability Limit of Mixture (vol%)
$\mathrm{LFL}_{\mathrm{T}}$	Lower Flammability Limit at Temperature T^{C} (vol%)
LGC	Light Gas Column
LHV	Lower Heat Value (kJ/hr)
M	Total Mass (lbm)
M_{Base}	Base Mass Flowrate (lbm/yr)
M_{gg}	Total Mass of Carbon Dioxide Equivalents Emitted (lbm or lbm/yr)
M_p	Project Mass Flowrate (lbm/yr)
M_{poll}	Total Mass of Pollutant Equivalents Emitted (lbm or lbm/yr)
M_{prod}	Total Mass of Products (lbm or lbm/yr)
M_{raw}	Total Mass of Raw Materials (lbm or lbm/yr)
M_{toxic}	Total Mass of Toxic Release (lbm or lbm/yr)
$M_{\mathrm{waste,s}}$	Total Mass of Solid Wastes (lbm or lbm/yr)
MeOH	Methanol
MI	Management Index
$\mathrm{MI}_{\mathrm{ES}}$	Management Index: Expert System
MIM	Material Intensity Metric (lbm/Ω or lbm/yr-Ω)

MISR	Metric for Inspecting Sales and Reactants
MSDS	Material Safety Data Sheet
MTO	Methanol-to-Olefins Process
MTP	Methanol-to-Propylene Process
MW	Molecular Weight (kg/kmol)
m	Mass Flowrate (lbm/yr)
N	Number of Management Measures
$N_{\text{chemicals}}$	Total Number of Chemicals
$N_{\text{Indicators}}$	Total Number of Indicators
N_{streams}	Total Number of Streams
n	Surveyed Count
O	Occasion
OEL-TWA	Occupational Exposure Level Time Weighted Average (ppm)
OMT	Olefin Metathesis Process
OSBL	Outside Battery Limits
OSHA	Occupational Safety and Health Administration
OWB	Objective Well-Being
P	Pressure (kPa)
PDH	Propane Dehydrogenation Process
PDI	Protection Deficiency Index
PEL	Permissible Exposure Limit
PFD	Process Flow Diagram
PHCI	Process and Hazard Control Index

PI	Protection Index
PPE	Personal Protective Equipment
PPEe	Effective Personal Protective Equipment
PPEn	No Personal Protective Equipment
PRM	Pollutant Release Metric (lbm/Ω or lbm/yr-Ω)
PRI	Process Route Index
PSA	Pressure Swing Adsorption
PSI	Process Stream Index
$\wp$	Power (MW)
p	Project
R^2	Coefficient of Determination
RSM	Refrigerant Savings Metric (10^6 kg/hr)
ROI	Return on Investment ($/$)
S	Size Parameter
S_{lower}	Lower Boundary of Size
S_R	Size Parameter of Reactor
S_{upper}	Upper Boundary of Size
S_{tot}	Annual Services (service/yr)
SASWROIM	Safety and Sustainability Weighted Return on Investment Metric ($/$)
SDS	Safety Data Sheet
SIA	Social Impact Assessment
SOP	Standard Operating Procedure
SPI	Sustainable Process Index

SWB	Subjective Well-Being
SWM	Solid Wastes Metric (lbm/Ω or lbm/yr-Ω)
SWROIM	Sustainability Weighted Return on Investment Metric ($/$)
T	Temperature (K)
T^{C}	Temperature (°C)
TCI	Total Capital Investment ($)
TI	Toxicity Index
$\mathrm{TI_{ES}}$	Toxicity Index: Expert System
TID	Temperature Interval Diagram
TPI	Total Project Investment ($MM)
TRM	Toxic Release Metric (lbm/Ω or lbm/yr-Ω)
TST	Twu-Sim-Tassone
TWA	Time Weighted Average (ppm)
t	Time (yr)
UFL	Upper Flammability Limit (vol%)
$\mathrm{UFL_{25}}$	Upper Flammability Limit at 25 °C (vol%)
$\mathrm{UFL_m}$	Upper Flammability Limit of Mixture (vol%)
$\mathrm{UFL_T}$	Upper Flammability Limit at Temperature T^{C} (vol%)
V_{water}	Volume of Fresh Water Used (gal or gal/yr)
VOC	Volatile Organic Compounds
VRM	VOC Reduction Metric (tons/yr)
WHR	Waste Heat Reduction
WIM	Water Intensity Metric (gal/Ω or gal/yr-Ω)

WRM	Water Reduction Metric (10^6 kg/hr)
w_i	Weight Factor of Indicator *i*
x	Dependent Variable from Plot
x_{A}	Batch Plant Capacity (kg/day)
x_{B}	Average Plant Capacity (kg/day)
x_{C}	Continuous Plant Capacity (kg/day)
y	Independent Variable from Plot
y_{A}	Batch Plant Operating Labor (hr/day-step)
y_{B}	Average Plant Operating Labor (hr/day-step)
y_{C}	Continuous Plant Operating Labor (hr/day-step)
y_i	Mole Fraction (mol/mol)
y_{tot}	Service Yield (service/ft^3-yr)
μ_{FL}	Stream Flammability Limit Mean (vol%)
μ_e	Stream Heating Value Mean (kJ/hr)
μ_P	Stream Pressure Mean (kPa)
μ_ρ	Stream Density Mean (kg/m^3)
ρ	Density (kg/m^3)
Ω	Output Value, which could either be Mass of Product (lbm or lbm/yr), Revenue ($), or Value-Added ($)

TABLE OF CONTENTS

Page

LIST OF FIGURES

Page

LIST OF TABLES

Page

LIST OF EQUATIONS

Page

1. INTRODUCTION

1.1 Need for Tracking Environmental, Safety, and Social Impacts

In current engineering practice, the criteria for design decision-making relies mainly on technological and economic considerations. Other consequences, such as environmental, safety, and social impacts of the designs, are usually neglected. Currently, companies are pushing to become more sustainable and safer than in the past. Future engineering practices must try to meet this trend and better align with the core values of a company. The method developed in this paper addresses that need.

1.2 Importance of Societal Equity

How a project impacts society is very important. Projects can either benefit or detriment individuals in the short term or the long term. Companies hope each project they complete can not only profit economically or help the environment but also improve the lives of those impacted, e.g. increase the number of jobs available in society.

Societal equity is also one of the principles of sustainability, but it is the least quantified and potentially least understood by most engineers. “While environmental sustainability examines living within the limits of the natural world, social sustainability emphasizes living in ways that can be sustained because they are healthy and satisfying for people and communities” [1]. There are many indicators that quantify the economic, environmental, and safety impacts of a project in the preliminary design stages. For ages, projects’ economic risks can be assessed using a Return on Investment (ROI) metric. It has become common to track a project’s carbon footprint as a means for measuring environmental impacts. Safety has relative risk charts based on the number of hazards present to determine safety impacts. As of now, there are very few indicators of societal equity.

As it stands now, societal equity is understood very subjectively. Society's opinions of and tendencies towards certain views of what is important change with time. As a result, it is difficult to determine a basis. Indicators, or metrics, require an objective standard of measure in which to compare other measurements. Therefore, subjective societal equity cannot be used for indicators. Instead, objective societal equity first needs to be better understood in order for appropriate indicators to be created and utilized. This paper provides some clear objective social metrics.

1.3 Propylene and the Shale Gas Boom

With the shale gas boom, two events are predicted to occur for propylene. First, propylene production via light naphtha cracking will decrease. Before the shale gas boom, light naphtha cracking was a common process route to separate petroleum. Propylene came out as a byproduct in large enough quantities to not upset the market. Now with shale gas in the market, chemical companies are seeking new process routes with shale gas as their feedstock. Consequently, the supply of propylene will decrease and drive its cost up. Thus, propylene becomes a more profitable product than before the shale gas boom. Second, chemical companies will seek on-purpose propylene routes with shale gas as their feedstock. Research towards these routes should benefit both academia and industry. This paper provides a case study for selecting the optimal propylene process route using a systematic method.

1.4 Problem Statement

In current engineering practice, the criteria for process decision-making rely heavily on techno-economic considerations, which neglects the environmental and social impacts of the process. Other important objectives such as safety and sustainability impact are typically

addressed after the initial design has been generated. The main goal of this work is to include these critical metrics early enough during conceptual process design, integration, and selection.

1.5 Objectives

The objective is to find and verify objective safety, environmental, and social metrics for process selection and to demonstrate a systematic method for process selection of propylene by using various accurate and reliable metrics that consider safety, economic, environmental, and social impacts.

2. LITERATURE REVIEW

A literature review was conducted to gather data and information. The data used is open-access, so that any individual may be able to access the same information and form similar conclusions. Additionally, the technique implemented in this paper can be applied without proprietary information.

2.1 Economic Indicators & Metrics

Companies must determine whether or not a project route or project is economically viable and assess the level of associated risk before decision-making. There are multiple indicators and metrics that assess the economic implications before detailed analysis. Listed below are some of those metrics.

2.1.1 Metric Inspecting Sales and Reactants (MISR)

The Metric Inspecting Sales and Reactants (MISR) compares the annual cost of product generation to the annual cost of reactants consumed, shown by Equation 1.

Equation 1 Metric Inspecting Sales and Reactants (MISR) reprinted from [2]

$$\text{MISR} = \frac{\sum_{p=1}^{N_{products}} \text{Annual production rate of product p} * \text{Selling price of product p}}{\sum_{r=1}^{N_{reactants}} \text{Annual feed rate of reactant r} * \text{Purchased price of reactant r}}$$

If the MISR is greater than 1, then the process route requires more analysis to check the economic viability. The greater the value of MISR, the more likely the process route will be economically viable. If the MISR is less than or equal to 1, then the process route is not economically viable. With MISR, some process routes may be eliminated before higher level of analysis.

2.1.2 Economic Gross Potential (EGP)

The Economic Gross Potential (EGP) is the difference between the annual cost of product generation to the annual cost of reactants consumed, shown in Equation 2.

Equation 2 Economic Gross Potential (EGP) reprinted from [2]

$$\text{EGP} = \sum_{p=1}^{N_{products}} \text{Annual production rate of product p} * \text{Selling price of product p} - \sum_{r=1}^{N_{reactants}} \text{Annual feed rate of reactant r} * \text{Purchased price of reactant r}$$

If the EGP is greater than 0, then the process route requires more analysis to check the economic viability. The greater the value of EGP, the more likely the process route will be economically viable. If the EGP is less than or equal to 0, then the process route is not economically viable. With EGP, some process routes may be eliminated before higher level of analysis.

2.1.3 Fixed Capital Investment (FCI)

The Fixed Capital Investment (FCI) contains four major components, shown in Table 1:

Table 1 FCI Components reprinted from [3]

1. Inside Battery Limits (ISBL) Investment
2. Outside Battery Limits (OSBL) Investment
3. Engineering and Construction Cost (ECC)
4. Contingency Charges

ISBL is the cost of the plant itself, which includes equipment, piping, labor, installation, and more. OSBL is the cost of modifications and additions to the existing plant. ECC is the cost of designing the plant. Contingency charges are funds set aside in case there are any mishaps or errors in design or construction.

2.1.4 Return On Investment (ROI)

Another metric is the conventional Return on Investment (ROI), shown in Equation 3.

Equation 3 Return on Investment (ROI)

$$\mathrm{ROI}_p = \frac{\mathrm{AEP}_p}{\mathrm{TCI}_p}$$

The Return on Investment of project p, ROI_p is the Annual Net Economic Profit of project p, AEP_p over the Total Capital Investment of project p, TCI_p.

Companies can decide if a project is economically viable by setting a threshold. They can determine the level of risk associated with the project by comparing the project's ROI to the ROI threshold. A project with a higher ROI than another project's ROI is deemed a safer investment, and vice versa.

2.1.5 IChemE Economic Metrics

Table 2 contains economic metrics by the Institute of Chemical Engineers (IChemE):

Table 2 IChemE Economic Metrics reprinted from [4]

Profit, Value, and Tax
• Value added[a] ($/yr) • Value added per unit value of sales ($/$) • Value added per direct employee ($/yr) • Gross margin[b] per direct employee ($/yr) • Return on average capital employed (%/yr) • Taxes paid as percent of net income before tax (%)
Direct Investments
• Percentage increase (decrease) in capital employed (%/yr) • R&D expenditure as % sales (%) • Employees with post-school qualification[c] (%) • New appointments/number of direct employees (%/yr) • Training expense as percentage of payroll expense (%)
Indirect Investments
• Ratio of indirect jobs[d]/number of direct employees • Investment in education[e]/employee training expense ($/$) • Charitable gifts as percentage of net income before tax[f] (%)

[a] Value added equals the value of sales minus the cost of goods, raw materials, required energy, and services purchased.
[b] Gross margin equals the value of sales minus all variable costs.
[c] Technicians, graduates, and others who have had at least two years of education or training after leaving secondary school.
[d] Number of indirect jobs includes contractors and service workers.
[e] Education does not include specifically for benefit of employees.
[f] This metric is a measure of the investment in the community.

The method, in which to calculate these metrics, can be found through its source article in the REFERENCE section.

2.1.6 Cost Curves for Purchased Equipment Costs

Cost curves are used to estimate equipment costs. Most equipment is sized by one key parameter. Similarly, cost is typically directly proportional to the same key factor. Thus, the cost of the equipment can be estimated from the key parameter. One set of correlations are provided by Towler and Sinnott through Equation 4:

Equation 4 Purchased Equipment Cost Correlation reprinted from [5]

$$C_{\mathrm{eq}} = a + bS^k$$

The purchased equipment cost, C_{eq} is the sum of the cost adjustment addition factor, a and the cost adjustment multiplication factor, b by the size parameter, S taken to the cost adjustment exponential factor, k. Towler and Sinnott provided a table of parameters for purchased equipment costs, shown in Table 3:

Table 3 Cost Curves for Purchased Equipment Costs reprinted from [5]

Equipment	**Units for *S***	S_{lower}	S_{upper}	***a***	***b***	***k***
Compressor: Centrifugal	driver power, kW	75	30,000	580,000	20,000	0.6
Dryers: Direct contact rotary	m^2	11	180	15,000	10,500	0.9
Exchangers: U-tube shell and tube	area, m^2	10	1,000	28,000	54	1.2
Pressure Vessels: Vertical, cs	shell mass, kg	160	250,000	11,600	34	0.85
Pressure Vessels: Horizontal, cs	shell mass, kg	160	50,000	10,200	31	0.85
Pumps and Drivers: Single stage centrifugal	flow, L/s	0.2	126	8,000	240	0.9
Trays: Sieve trays (based on stack of 30)	diameter, m	0.5	5	130	440	1.8

All costs are U.S. Gulf Coast basis, Jan. 2010 (CEPCI index = 532.9, NF refinery inflation index = 2281.6) [5]. The correlations in the table are only valid for the lower and upper boundaries of S indicated. It is assumed the equipment are based on carbon steel unless otherwise specified.

2.1.7 MTP Plant Cost

Estimates and correlations are practical if no real data of plant cost are found. Actual plant cost is necessary to validate if the estimate is reasonable (within 5-10% accuracy).

Fortunately, Meyers provides an investment cost of a 520 tonne per year MTP plant in January 2002, shown in Table 4:

Table 4 MTP 2002 Plant Cost reprinted from [6]

Description	Value	Units
Capacity	520,000	t/a
Jan. 2002 CEPCI	395.6	----
Investment Cost	215	$MM

This datum will be used for comparison in the RESULTS & DISCUSSION section.

2.1.8 MTP Reactor Estimation

Correlations are great estimates of most purchased equipment. Correlations are not good estimates of reactors. Reactors strongly dependent on the reaction occurring rather than simply a size or rated quantity. Therefore, actual data of MTP reactors were sought for.

The reaction process for Fluid Catalytic Cracking (FCC) are quite similar to the reaction process used for MTP. Thus, the reactor cost of FCC projects is shown in Table 5:

Table 5 FCC Project Costs reprinted from [7]

Total FCC Projects Costs	Large Scale Plant	Small Scale Plant
Gas Oil Feed Rate (BPSD)	62,000	2,500
Reactor/Regen TPI ($MM)	102.6	11
Total Project Investment ($MM)	191.6	20.5
Total Investment/BBL Feed ($)	~3,000	~8,200
Sizing Exponential	0.7	

This datum will be used for comparison in the RESULTS & DISCUSSION section.

2.2 Environmental Indicators & Metrics

Companies would like to predict and assess the environmental impact of process routes or projects before decision-making. There are multiple indicators and metrics that assess the environmental implications before detailed analysis. Listed below are some of those metrics.

2.2.1 Sustainable Process Index (SPI)

Sustainable Process Index (SPI) focuses on tracking the ecological impact of factors on the landscape and any life [8]. This indicator works well, since processes need more land area to produce more products and vice versa. It does by calculating the mass and energy usage of systems across areas and then comparing the value to the specific inhabitant capacity area. The SPI can be calculated by determining the total impact area, the annual services, the specific sustainable service area, and the specific inhabitant capacity area, as shown in Equation 5.

Equation 5 Total Impact Area (A_{tot}) reprinted from [8]

$$A_{\mathrm{tot}} = A_{\mathrm{R}} + A_{\mathrm{E}} + A_{\mathrm{I}} + A_{\mathrm{S}} + A_{\mathrm{P}}$$

The total impact area, A_{tot} is the sum of all the impacted areas: raw material and feedstock (A_{R}), process energy area (A_{E}), installation area (A_{I}), staff area (A_{S}), and products and byproducts area (A_{P}). Other impacted areas can be included as well.

Equation 6 Specific Sustainable Service Area (a_{tot}) reprinted from [8]

$$a_{\mathrm{tot}} = \frac{1}{y_{\mathrm{tot}}} = \frac{A_{\mathrm{tot}}}{S_{\mathrm{tot}}}$$

In Equation 6, the specific sustainable service area, a_{tot} is the inverse of the service yield, y_{tot} or the total impact area, A_{tot} over the annual services, S_{tot}. The annual services are the number of unit services, or product units, completed in a given year. For example, a unit service could be 580 MMlbm of product in one year for a 600 MMlbm/yr capacity plant.

Equation 7 Sustainable Process Index (SPI) reprinted from [8]

$$\mathrm{SPI} = \frac{a_{\mathrm{tot}}}{a_{\mathrm{in}}}$$

In Equation 7, the Sustainable Process Index, SPI is the specific sustainable service area, a_{tot} over the specific inhabitant capacity area, a_{in}. "Low SPI values indicate processes that are competitive under sustainable conditions and that are environmentally compatible in the long-term view" [8].

2.2.2 BRIDGES Sustainability Metrics

Listed below are BRIDGES' Sustainability Metrics based on basic resource usage, as shown by Table 6:

Table 6 BRIDGES' Sustainability Metrics reprinted from [9]

Basic Resource Usage
• Material Intensity, MI (lbm/Ω or lbm/yr-Ω) • Water Intensity, WI (gal/Ω or gal/yr-Ω) • Energy Intensity, EI (BTU/Ω or BTU/yr-Ω) • Toxic Release, TR (lbm/Ω or lbm/yr-Ω) • Solid Wastes, SW (lbm/Ω or lbm/yr-Ω) • Pollution Release, PR (lbm/Ω or lbm/yr-Ω) • Greenhouse Gas Release, GGR (lbm/Ω or lbm/yr-Ω)

Equation 8 Material Intensity Metric (MIM) reprinted from [9]

$$\mathrm{MIM} = \frac{M_{\mathrm{raw}} - M_{\mathrm{prod}}}{\Omega}$$

In Equation 8, the Material Intensity Metric, MIM is the difference between the mass of raw material, M_{raw} and the mass of products, M_{prod} over the output value, Ω. The output value can be one of three types: mass of product, dollars of revenue, or dollars of value added [9]. The unit of the output value is consistent for the following equations in this section.

Equation 9 Water Intensity Metric (WIM) reprinted from [9]

$$\text{WIM} = \frac{V_{\text{water}}}{\Omega}$$

In Equation 9, the Water Intensity Metric, WIM is the volume of fresh water used, V_{water} over the output value, Ω. The amount should exclude rainwater, since the amount of rainfall is site-specific. "This metric includes evaporation and misting losses from cooling water (7% of cooling water usage is the default if no data are available), water vapor vented to the atmosphere, water lost through waste treatment or disposal, and water lost through deep-well injection" [9].

Equation 10 Energy Intensity Metric (EIM) reprinted from [9]

$$\text{EIM} = \frac{\Delta E_{\text{fuel}}}{\Omega}$$

In Equation 10, the Energy Intensity Metric, EIM is the net energy used as primary fuel equivalent, ΔE_{fuel} over the output value, Ω. The primary fuel equivalent is a measure of the heat and power usage, i.e. utility usage, of the project.

Equation 11 Toxic Release Metric (TRM) reprinted from [9]

$$\text{TRM} = \frac{M_{\text{toxic}}}{\Omega}$$

In Equation 11, the Toxic Release Metric, TRM is the total mass of recognized toxics released, M_{toxic} over the output value, Ω. The US EPA provides a list of toxic chemicals that must be reported on the Toxic Chemical Release Inventory Form (Form R) under Section 313 of the Emergency Planning and Community Right-to-Know Act.

Equation 12 Solid Wastes Metric (SWM) reprinted from [9]

$$\text{SWM} = \frac{M_{\text{waste,s}}}{\Omega}$$

In Equation 12, the Solid Wastes Metric, SWM is the total mass of solid wastes, $M_{\text{waste,s}}$ over the output value, Ω. Solid wastes are any solid material that cannot be used or sold by the company as a result of the process route and must be disposed.

Equation 13 Pollution Release Metric (PRM) reprinted from [9]

$$\text{PRM} = \frac{M_{\text{poll}}}{\Omega}$$

In Equation 13, the Pollution Release Metric, PRM is the total mass of pollutant equivalents, M_{poll} over the output value, Ω. Pollutant equivalents are any substances that negatively affects the atmosphere, water, or land, e.g. volatile organic compounds (VOCs).

Equation 14 Greenhouse Gas Release Metric (GGRM) reprinted from [9]

$$\text{GGRM} = \frac{M_{\text{gg}}}{\Omega}$$

In Equation 14, the Greenhouse Gas Release Metric, GGRM is the total mass of carbon dioxide equivalents emitted, M_{gg} over the output value, Ω. Carbon dioxide equivalent is a measure than translates greenhouse gases and their global warming potential into carbon dioxide's global warming potential. This metric always for the total global warming potential to be summed under one gas for measure and understanding—CO_2.

2.2.3 IChemE Environmental Metrics

Table 7 contains environmental metrics by IChemE:

Table 7 IChemE Environmental Metrics reprinted from [4]

Energy of Resource Usage
• Total net primary energy usage rate = imports - exports (MMBTU/yr) • Percentage total net primary energy sourced from renewables (%) • Total net primary energy usage per mass of product (BTU/lbm) • Total net primary energy usage per unit value added (BTU/$)
Materials of Resource Usage (Excluding Fuel and Water)
• Total raw materials used per mass of product (lbm/lbm) • Total raw materials used per unit of value added (lbm/$) • Fraction of raw materials recycled within company (lbm/lbm) • Fraction of raw materials recycled from consumers (lbm/lbm) • Hazardous raw material per mass of product (lbm/lbm)
Water of Resource Usage
• Net water consumed per unit mass of product (lbm/lbm) • Net water consumed per unit value added (lbm/$)
Land Resource Usage
• Total land occupied + affected for value added[a] (ft^2-yr/$) • Rate of land restoration[b] (ft^2/ft^2-yr)
Atmospheric Impacts of Emissions, Effluents, and Waste
• Atmospheric acidification burden per unit value added (lbm/$) • Global warming burden per unit value added (lbm/$) • Human health burden per unit value added (lbm/$) • Ozone depletion burden per unit value added (lbm/$) • Photochemical ozone burden per unit value added (lbm/$)
Aquatic Impacts of Emissions, Effluents, and Waste
• Aquatic acidification per unit value added (lbm/$) • Aquatic oxygen demand per unit value added (lbm/$) • Metallic ecotoxicity to aquatic life per unit value added (lbm/$) • Other ecotoxicity to aquatic life per unit value added (lbm/$) • Eutrophication per unit value added (lbm/$)
Impacts to Land of Emissions, Effluents, and Waste
• Hazardous solid waste per unit value added (lbm/$) • Non-hazardous solid waste per unit value added (lbm/$)

[a] Land affected might be, e.g. land used in mining raw material or in dumping waste product.
[b] The areas of land occupied and affected are those at the start of the reporting period, and the land restored is that area restored during the reporting period.

The methods, in which to calculate these metrics, can be found through its source article in the REFERENCE section.

2.2.4 Environmental Indicators Across Projects

Agarwal *et al.* used various mass and energy indicators to compare the environmental impact of plants or projects against one another. They compare water reduction using the following equation:

Equation 15 Water Reduction Metric (WRM)

$$\text{WRM} = \frac{M_{\text{Base},i} - M_{p,i}}{M_{\text{Base},i}}$$

In Equation 15, the Water Reduction Metric, WRM is the base mass flowrate of water difference between the base case, M_{Base} and assessed project, M_p over the base case. Next, Agarwal *et al.* compare electrical energy savings using the following equation:

Equation 16 Electrical Energy Savings (EES) adapted from [10]

$$\text{EES} = \frac{\wp_{\text{Base},i} - \wp_{p,i}}{\wp_{\text{Base},i}}$$

In Equation 16, the Electrical Energy Savings, EES is the base energy flowrate of electricity consumed difference between the base case, $\wp_{\text{Base}}$ and assessed project, $\wp_p$ over the base case. Then, Agarwal *et al.* compare fuel savings using the following equation:

Equation 17 Fuel Savings Metric (FSM) adapted from [10]

$$\text{FSM} = \frac{\wp_{\text{Base},i} - \wp_{p,i}}{\wp_{\text{Base},i}}$$

In Equation 17, the Fuel Savings Metric, FSM is the base energy flowrate of fuel consumed difference between the base case, $\wp_{\text{Base}}$ and assessed project, $\wp_p$ over the base case. Agarwal *et al*. compare CO_2 emission reduction using the following equation:

Equation 18 CO_2 Emission Reduction (CER) adapted from [10]

$$\text{CER} = \frac{M_{\text{Base},i} - M_{p,i}}{M_{\text{Base},i}}$$

In Equation 18, the CO_2 Emission Reduction, CER is the base mass flowrate of CO_2 difference between the base case, M_{Base} and assessed project, M_p over the base case. Similarly, Agarwal *et al.* compare VOC reduction using the following equation:

Equation 19 VOC Reduction Metric (VRM) adapted from [10]

$$\text{VRM} = \frac{M_{\text{Base},i} - M_{p,i}}{M_{\text{Base},i}}$$

In Equation 19, the VOC Reduction Metric, VRM is the base mass flowrate of VOC difference between the base case, M_{Base} and assessed project, M_p over the base case. Lastly, refrigerant savings can also be compared on a mass basis.

Equation 20 Refrigerant Savings Metric (RSM) adapted from [10]

$$\text{RSM} = \frac{M_{\text{Base},i} - M_{p,i}}{M_{\text{Base},i}}$$

In Equation 20, the Refrigerant Savings Metric, RSM is the base mass flowrate of refrigerant difference between the base case, M_{Base} and assessed project, M_p over the base case. These metrics will be implemented in the RESULTS & DISCUSSION section.

2.3 Safety Indicators & Metrics

Companies would like to assess the safety of process routes or projects before decision-making. There are multiple indicators and metrics that assess the level of safety before detailed analysis. Listed below are some of those metrics.

2.3.1 Integrated Inherent Safety Index (I2SI)

The Integrated Inherent Safety Index (I2SI) compares the applicability of inherent safety principles (or guidewords) against the damage potential of a process [11].

Equation 21 Hazard Index (HI) reprinted from [11]

$$\mathrm{HI} = \frac{\mathrm{DI}}{\mathrm{PHCI}}$$

In Equation 21, the Hazard Index, HI is the Damage Index, DI over the Process and Hazard Control Index, PHCI. HI is an index tracking the damage potential. The hazard index can come from a variety of indices: the Dow Fire and Explosion Index, Dow Chemical Exposure Index, Safety Weighted Hazard Index, Environmental Risk Management Screening Tool, Transportation Risk Screening Model, Hazardous Waste Index, Mond Index, Toxicity Hazard Index, and many more. The HI is only calculated for the base process design and remains the same as alterations have been made to formulate the integrated design. Thus, factors that affect safety in the integrated design can be quantified after each change.

Equation 22 Integrated Inherent Safety Index (I2SI) reprinted from [11]

$$\mathrm{I2SI} = \frac{\mathrm{ISPI}}{\mathrm{HI}}$$

In Equation 22, the Integrated Inherent Safety Index, I2SI is the Inherent Safety Potential Index, ISPI over the Hazard Index, HI. ISPI is an index tracking the applicability of inherent safety principles. The integrated design with the highest I2SI value is the inherently safer option. This fact, however, does not necessarily mean the design is safe—just safer.

The method, in which to calculate these metrics, can be found through its source article in the REFERENCE section. In particular for this method, focus on the flowcharts presented the figures.

2.3.2 Inherent Safety Index Model (ISIM)

The Inherent Safety Index Model (ISIM) builds off I2SI. ISIM focuses on gathering process information from a process design simulator and applying I2SI to track the Inherent Safety Level (ISL) [12]. Through a series of steps and calculation, a base design can be

optimized to an acceptable level during preliminary design stages. The model is presented and demonstrated in its source article, which can be found in the REFERNCE section.

2.3.3 Two-Tier Inherent Safety Index (2TISI)

The Two-Tier Inherent Safety Index (2TISI) is a framework that checks a process route through two levels of safety indices [13]. The approach is a matter of taking the common Inherent Risk Assessment (IRA) and applying an additional index—the Process Route Index (PRI). PRI "ranks all process routes using an overall index to determine the inherently safer option for further evaluation" [13]. The PRI is a function of the mass, energy, and combustibility of each process stream, as shown by Equation 23:

Equation 23 Process Route Index (PRI) reprinted from [13]

$$\text{PRI} = A_0 \mu_P \mu_\rho \mu_e \mu_{\text{FL}}$$

The Process Route Index, PRI is the product of the stream pressure mean, μ_P, stream density mean, μ_ρ, stream heating value mean, μ_e, stream flammability limit mean, μ_{FL}, and a user specified constant, A_0. A_0 is typically 10^{-8} for PRI.

One method to track flammability limit is by calculating the Lower Flammability Limit (LFL) and Higher Flammability Limit (UFL) at various temperatures.

Equation 24 Lower Flammability Limit at Temperature T^{C} (LFL_{T}) reprinted from [3]

$$\text{LFL}_{\text{T}} = \text{LFL}_{25}\left[1 - \frac{0.75(T^{\text{C}} - 25)}{\Delta h_{\text{c}}}\right]$$

In Equation 24, the Lower Flammability Limit at temperature T in Celsius, LFL_{T} is a function of the Lower Flammability Limit at 25 °C, LFL_{25} multiplied by a temperature factor based on the heat of combustion in kcal/mol, Δh_{c} and the measured temperature T^{C}.

Equation 25 Upper Flammability Limit at Temperature T^{C} ($\mathrm{UFL_T}$) reprinted from [3]

$$\mathrm{UFL_T} = \mathrm{UFL_{25}}\left[1 + \frac{0.75(T^{\mathrm{C}} - 25)}{\Delta h_{\mathrm{c}}}\right]$$

In Equation 25, the Upper Flammability Limit at temperature T in Celsius, $\mathrm{UFL_T}$ is a function of the Upper Flammability Limit at 25 °C, $\mathrm{UFL_{25}}$ multiplied by a temperature factor based on the heat of combustion in kcal/mol, Δh_{c} and the measured temperature T^{C}.

PRI can also be a function of density, pressure, energy, and combustibility of individual components in a stream based on the combustibility of the mixture.

Equation 26 Lower Flammability Limit of Mixture ($\mathrm{LFL_m}$) reprinted from [3]

$$\mathrm{LFL_m} = \frac{1}{\sum_i^{N_{\mathrm{chemicals}}} \frac{y_i}{\mathrm{LFL}_i}}$$

In Equation 26, the Lower Flammability Limit of a mixture, $\mathrm{LFL_m}$ is the inverse sum of the component molar fraction, y_i over the component LFL.

Equation 27 Upper Flammability Limit of Mixture ($\mathrm{UFL_m}$) reprinted from [3]

$$\mathrm{UFL_m} = \frac{1}{\sum_i^{N_{\mathrm{chemicals}}} \frac{y_i}{\mathrm{UFL}_i}}$$

In Equation 27, the Upper Flammability Limit of a mixture, $\mathrm{UFL_m}$ is the inverse sum of the component molar fraction, y_i over the component UFL.

The method, in which to calculate these metrics in more detail, can be found through its source article in the REFERENCE section. In particular for this method, focus on the flowcharts presented the figures.

If toxicity is a factor that needed to be tracked more heavily than combustibility, another safety index, called the Three-Tier Inherent Safety Quantification (3TISQ), for toxic release can be applied instead [14].

2.3.4 Process Stream Index (PSI)

Shariff *et al.* sought an indicator that captures the stream's mass, energy, and combustibility. The Process Stream Index (PSI) is a function of the stream density, pressure, energy, and combustibility, as shown by Equation 28:

Equation 28 Process Stream Index (PSI) reprinted from [15]

$$\mathrm{PSI} = A_0 I_P I_\rho I_e I_{\mathrm{FL}}$$

The Process Stream Index, PSI is the product of the stream pressure indicator, I_P, stream density indicator, I_ρ, stream heating value indicator, I_e, stream flammability limit indicator, I_{FL}, and a user specified constant, A_0. A_0 is typically 10 for PSI.

Equation 29 Stream Pressure Indicator (I_P) reprinted from [15]

$$I_P = \frac{P}{\mu_P}$$

In Equation 29, the stream pressure indicator, I_P is the ratio of the stream pressure, P over the stream pressure mean, μ_P.

Equation 30 Stream Density Indicator (I_ρ) reprinted from [15]

$$I_\rho = \frac{\rho}{\mu_\rho}$$

In Equation 30, the stream density indicator, I_ρ is the ratio of the stream density, ρ over the stream density mean, μ_ρ.

Equation 31 Stream Heating Value Indicator (I_e) reprinted from [15]

$$I_e = \frac{\mathrm{LHV}}{\mu_e}$$

In Equation 31, the stream heating value indicator, I_e is the ratio of the stream Lower Heating Value, LHV over the stream heating value mean, μ_e.

Equation 32 Stream Flammability Limit Indicator (I_{FL}) reprinted from [15]

$$I_{\mathrm{FL}} = \frac{\mathrm{UFL_m} - \mathrm{LFL_m}}{\mu_{\mathrm{FL}}}$$

In Equation 32, the stream density indicator, I_{FL} is the ratio of the difference between the UFL of the stream mixture, $\mathrm{UFL_m}$ and the LFL of the stream mixture, $\mathrm{LFL_m}$ over the stream density mean, μ_{FL}.

To get an estimate of the PSI for the entire project, the average of all streams can be taken as shown below:

Equation 33 PSI of Project (PSI_p)

$$\mathrm{PSI}_p = \frac{1}{N_{\mathrm{streams}}} \sum_{i}^{N_{\mathrm{streams}}} \mathrm{PSI}_i$$

In Equation 33, the Process Stream Index of the project, PSI_p is the average of all the stream PSI.

2.4 Social Indicators & Metrics

Companies would like to predict and assess the social impact of process routes or projects before decision-making. There are multiple indicators and metrics that assess the social implications before detailed analysis. Listed below are some of those metrics.

2.4.1 Social Impact Assessment (SIA)

Social Impact Assessment (SIA) is defined as "the process of identifying the future consequences of a current or proposed action which are related to individuals, organizations, and social macro-systems" [16]. It attempts to measure the consequences of current or future actions by introducing steps into the initial and main phase of project development. The steps for the SIA Project are shown in the Table 8:

Table 8 Social Impact Assessment (SIA) Project reprinted from [16]

Initial Phase
1. Problem analysis and communication strategy 2. System analysis 3. Baseline analysis 4. Trend analysis and monitoring design 5. Project design
Main Phase
1. Scenario design 2. Design of strategies 3. Assessment of impacts 4. Ranking of strategies 5. Mitigation of negative impacts 6. Reporting 7. Stimulation of implementation 8. Auditing and ex-post evaluation

Each step requires targets, or baselines, to be employed. Data for these targets can be determined from historical accounts or trends in the social system. The method, in which to calculate these metrics, can be found through its source article in the REFERENCE section.

2.4.2 IChemE Social Metrics

Table 9 contains social metrics by IChemE:

Table 9 IChemE Social Metrics reprinted from [4]

Employment Workplace
• Benefits as percentage of payroll expense (%) • Employee turnover (%) • Promotion rate (%) • Working hours lost as percent of total hours worked (%) • Income + benefit ratio (top 10%/bottom 10%)
Health and Safety Workplace
• Lost-time accident frequency (number per million hours worked) • Expenditure on illness and accident prevention relative to payroll expense
Society
• Number of stakeholder meetings per unit value-added (1/$) • Indirect community benefit per unit value-added ($/$) • Number of complaints per unit value-added (1/$) • Number of legal actions per unit value-added (1/$)

The method, in which to calculate these metrics, can be found through its source article in the REFERENCE section.

2.4.3 Community Resilience Dimensions

Community resilience is the existence, development, and engagement of community resources by community members to thrive in an environment characterized by change, uncertainty, unpredictability, and surprise [17]. Table 10 contains the community resilience dimensions:

Table 10 Community Resilience Dimensions and Examples adapted from [17]

Community Resources
The extent to which community members • Understand opportunities in environment • Understand limitations in environment • Network (by community leaders) to external resources (e.g. government, businesses) • Believe change is inevitable • Believe in community adaptability
Development of Community Resources
The extent to which community members • Form new businesses and employment opportunities over the last ten years • Prepare youth with work habits (e.g. quality work, timeliness, reliability) • Prepare youth to become involved citizens (e.g. vote) • Keep the status quo
Engagement of Community Resources
The extent to which • Community government effectively handles problems • Community organizations contribute leadership and volunteers • Communities generate ideas to address change
Active Agents
The extent to which community members • Believe to affect community's well-being • Involve various groups and generate events • Address major issues in self-reliance
Collective Action
The extent to which community members • Facilitate collaboration between groups • Engage diverse perspectives in decision-making • Reflect cultural difference in decision-making • Share supports, resources, knowledge, and expertise from diverse groups
Strategic Action
The extent to which community members • Use resource in planning endeavors • Generate community-wide commitment to a common future • Seek outside resources
Equity
The extent to which community members • Provide access to natural resources for various groups • Involve various groups in planning and leadership • Welcome and include various groups

Table 10 Continued

Impact
The extent to which • Changes in participation and collaboration occur over time • Changes in community's capacity to respond to change occur over time • Change in community's resources occur over time

Each of these dimensions could be considered for social metrics. They focus more so on the community aspects of a project's impact than from the project itself.

2.4.4 Human Well-Being Dimensions

Human well-being is a multidimensional and content-specific concept that addresses both objective (e.g. material wealth and physical health) and subjective components (e.g. quality of social relationships or feelings of happiness) [1]. Some of these components include material living standards, health, education, work, leisure, agency, political voice, social relationships, stable ecosystems, physical security, economic security, and more. All these components are interrelated and can be tracked through measures. Table 11 contains some measures of human well-being:

Table 11 Human Well-Being Measures adapted from [1]

Objective Well-Being (OWB)
• Gross Domestic Product (GDP) per capita • Human Development Index (HDI) • Personal security
Subjective Well-Being (SWB)
• Happiness index • Equality in social relations
Comprehensive Well-Being (CWB)
• Physical well-being (e.g. basic human needs of survival) • Emotional and social well-being (e.g. basic needs of social beings)

Because of the multidimensional aspect of well-being, any measure of it has both objective and subjective components. Table 12 contains human needs form CWB:

Table 12 Human Needs for Comprehensive Well-Being reprinted from [1]

Physical Well-Being
• Nutritious food • Clean water • Adequate shelter • Health (protection from disease, provision of elements needed for good health, etc.) • Security (protection from inflicted physical harm, crime, conflict, and disasters) • Material goods needed for decent life • Energy source (solar, wind, water, animal, fuel) • Work or means of earning a living • Exercise, relaxation, and rest
Emotional and Social Well-Being
• Strong families • Strong community and social interactions • Social equality with others (non-discrimination) • Ability to trust others • Identify, autonomy, and self-determination • Freedom to move about and choose job, home, and social relationships • Political voice and empowerment • Education, knowledge • Fulfillment and creative outlet • Time and space for recreation • Connection with nature and beauty • Belief system and sense of meaning • Hope for the future

These elements are fundamental to current society, even if society does not provide access to all the elements listed above. “Social sciences research does make clear the need to replace the consumer culture with something more supportive of human social and emotional needs, diminish inequalities within and between societies, and develop economic and political policies and institutions that serve human well-being in all its dimensions” [1]. A huge shift in thinking and lifestyle would have to occur.

Nevertheless, one thing remains consistent across cultures: basic human needs. It could be the basis of social indicators. Metrics could be developed to track how well a project meets those needs. The target would be specified by the consumer as to what the project is desired to achieve.

2.4.5 Jobs and Plant Capacity

Another method in which projects impact society is through the number of jobs created. From a flowsheet and drawings, the labor can be estimated based on process equipment and work required to be performed for each unit. Peters *et al.* compare a plant's capacity to the operating labor based on daily employee-hours per processing step in the Figure 1.

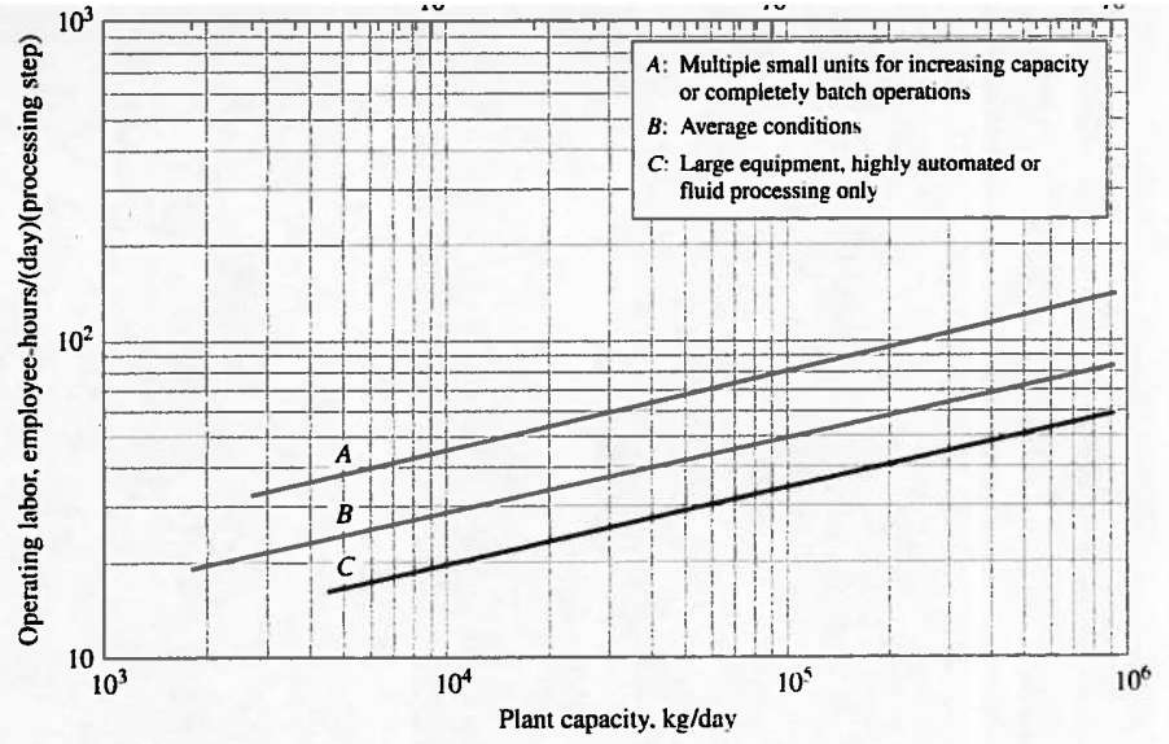


Figure 1 Operating labor requirements in the chemical process industry reprinted from [18].

There's a logarithmic relationship between plant capacity and labor per process step. "A process step is defined as any unit operation, unit process, or combination thereof that takes place in one or more units of distillation, evaporation, drying, filtration, etc." [18]. The more automated the process, the less operating labor hours are required. The vice versa is true as well.

As a reminder, this figure is only an estimation. Due to new technology and automation controls, the expected operating labor could vary dramatically. "For chemical processes, operating labor usually amounts to about 10 to 20 percent of the total product cost" [18]. Consequently, Peters *et al.* propose a rule of thumb for plant labor requirements in Table 13:

Table 13 Rule of Thumb for Plant Labor Requirements reprinted from [18]

Type of Processing Plant	Employee-Hours per 1000 kg	Example
Fluids	0.33-to-2	Ethylene Oxide Plant
Solid-Fluids	2-to-4	Shale-Oil Plant
Solids	4-to-8	Coal Briquetting Plant

2.4.6 Health Hazards

Another method to track the social impacts of a project is how the project affects people's health or the health hazards associated. "A health hazard can be defined as any process, material, or energy at the place of employment which has the potential by itself and by interaction with other variables (including human agency) of causing disease or significant health impairment upon repeated exposure at a level or intensity which is beyond a certain threshold limit." [19] The health hazards of chemicals can be studied in three different ways, based on industrial toxicology: entry, contamination, and effects.

There are five routes of entry: inhalation, skin penetration or absorption, ingestion, eye penetration or absorption, or injection. Considering these pathways with each chemical used in a

project can help predict the hazard intensity or severity of exposure. Process steps should be carefully analyzed under different scenarios as to how chemicals can enter a person. This analysis could start in the early stages of plant design and be refined over time.

There are eleven forms of contamination: solid, liquid, gas, vapor, fume, mist, fog, aerosol, smoke, dust, and solution. Contamination is harder to predict since it is heavily dependent on process conditions. The pressure, temperature, and system environment will drastically affect how the chemical will behave. Only once the project has reached detailed design can these forms be considered with reason.

There are thirteen types of toxic effects: irritation, asphyxiation, anesthesia, hepatoxic (liver) effects, nephrotoxic (kidney) effects, neurotoxic (brain and nervous system) effects, pneumoconiosis (lung scarring), chemical carcinogenesis, chemical mutagenesis, chemical teratogenesis (e.g. birth defects), radiation disease, hearing loss, and cumulative trauma disease (CTD). The potential side effects of exposure to a chemical should also be listed on its Safety Data Sheet (SDS). Information on a SDS is easily and readily available. Thus, health hazard analysis can be completed in the early stages of project creation.

Despite knowing these various forms of better understanding health hazards, it is all still very qualitative—more subjective in understanding than objective. A quantitative understanding of these health hazards is necessary to objectively measure occupational risk.

Wang *et al.* developed a semi-quantitative model for chemical exposures to predict occupational risk. They proposed a model, surveyed manufacturing industries, and corrected their model using an expert system. The Exposure Hazard Index (EHI) considered toxicity and two factors that reflect exposure potential:

Equation 34 Exposure Hazard Index (EHI) reprinted from [20]

$$\mathrm{EHI} = (\mathrm{TI})(\mathrm{EI})(\mathrm{PDI})$$

In Equation 34, the Exposure Hazard Index, EHI is the product of the Toxicity Index, TI, Exposure Index, EI, and Protection Deficiency Index, PDI. TI is an index correlating a chemical's toxicity to a dimensionless semi-quantitative value.

Equation 35 Toxicity Index: Expert System ($\mathrm{TI_{ES}}$) reprinted from [20]

$$\mathrm{TI_{ES}} = 2^{[4.16-\mathrm{lo}\ (\mathrm{OELTWA})]}$$

In Equation 35, the Toxicity Index: Expert System, $\mathrm{TI_{ES}}$ is a logarithmic relationship of the difference between a theoretical maximum Time Weighted Average, TWA and a chemical's Occupational Exposure Limit Time Weighted Average, OEL-TWA in units of parts per million. The expert system accuracy is for OEL-TWA between 0.01 and 1000 ppm at $R^2 = 0.97$ and $n = 7$. After comparing Wang's OEL-TWA for surveyed compounds to Occupational Safety and Health Administration (OSHA)'s list of PEL for chemical contaminants, the values are the same (i.e. Wang's OEL-TWA is equivalent to OSHA's PEL).

Equation 36 Exposure Index: Expert System ($\mathrm{EI_{ES}}$) reprinted from [20]

$$\mathrm{EI_{ES}} = 0.0023 \cdot \mathrm{ED} - 0.0037$$

In Equation 36, the Exposure Index: Expert System, $\mathrm{EI_{ES}}$ is a linear relationship of the Exposure Duration, ED in units of minutes. ED is total exposed time for a worker to a chemical. The expert system accuracy is for ED between 0 and 300 minutes at $R^2 = 0.97$ and $n = 7$.

Equation 37 Protection Deficiency Index (PDI) reprinted from [20]

$$\mathrm{PDI} = 1 - (\mathrm{MI})(\mathrm{PI})$$

In Equation 37, the Protection Deficiency Index, PDI is the lack of effect due to the Management Index, MI and the Protection Index, PI. PI is determined from two controls set in place for a

chemical: enclosed and local exhaust ventilation engineering controls, EE and Personal Protective Equipment, PPE administrative controls. Table 14 summarizes these controls.

Table 14 Engineering Controls for Determining PI: Expert System (PI_{ES}) adapted from [20]

Combination	PI_{ES}
EEn + PPEn	0.00 ± 0.00
EEn + PPEe	0.18 ± 0.06
EEp + PPEn	0.42 ± 0.03
EEp + PPEe	0.61 ± 0.12
EEe + PPEn	0.74 ± 0.04
EEe + PPEe	1.00 ± 0.00

EEn represents no engineering control measures. EEp represents partially effective engineering control measures. EEe represents effective engineering control measures. PPEn represents no personal protective equipment. PPEe represents effective personal protective equipment.

Equation 38 Management Index: Expert System (MI_{ES}) reprinted from [20]

$$\mathrm{MI_{ES}} = 0.21 \cdot \mathrm{N} + 0.18$$

In Equation 38, the Management Index: Expert System, MI_{ES} is a linear relationship of the number of implemented management measures, N. N can be determined from "the availability of safety and health personnel, the material safety data sheet (MSDS), standard operating procedures (SOP), and training programs for handling hazardous materials" [20]. The expert system accuracy is for N between 1 and 4 measures at $R^2 = 0.99$ and $n = 7$.

Equation 39 Exposure Hazard Index: Expert System (EHI_{ES}) reprinted from [20]

$$\mathrm{EHI_{ES}} = 1.05 \cdot \mathrm{EHI_{cor}} - 0.27$$

In Equation 39, the Exposure Hazard Index: Expert System, EHI_{ES} is a linear relationship of the Corrected Exposure Hazard Index, EHI_{cor}. EHI_{cor} comes from the seven surveyed manufacturing

industries, while EHI_{ES} correlates the EHI_{cor} data. The expert system accuracy is for EHI_{cor} between 0 and 40 at $R^2 = 0.94$ and $n = 7$. In the end, Wang *et al.* adopted EHI_{cor} for their model.

Lastly, the health of both people in the workplace and people in the surrounding community should be considered. Chemical exposure does not just affect those directly working with the chemicals but also those in the surrounding areas indirectly. For example, VOC emissions will contaminate the air of the local area, which community dwellers will breathe.

2.5 Integrating Indicators & Metrics

Annual Sustainability Profit (ASP) is a sustainability factor adjustment to the Annual Economic Profit (AEP) based on indicators and their respective targets, shown by Equation 40.

Equation 40 Annual Sustainability Profit (ASP) reprinted from [21]

$$\mathrm{ASP}_p = \mathrm{AEP}_p \left[1 + \sum_{i=1}^{N_{\mathrm{Indicators}}} w_i \left(\frac{\mathrm{Indicator}_{p,i}}{\mathrm{Indicator}_i^{\mathrm{Target}}} \right) \right]$$

For project p, the sustainability factor adjustment consists of the following components: i is an index for the different sustainability indicators and the weighing factor and w_i is a ratio representing the relative importance of the i^{th} sustainability indicator compared to the AEP for the total number of indicators, $N_{\mathrm{Indicators}}$.

The Sustainability Weighted Return on Investment Metric (SWROIM) extends "the conventional ROI concept by incorporating process integration targeting, or benchmarking, and relevant sustainability metrics" [21].

Equation 41 Sustainability Weighted Return on Investment Metric (SWROIM) reprinted from [21]

$$\mathrm{SWROIM}_p = \frac{\mathrm{ASP}_p}{\mathrm{TCI}_p}$$

In Equation 41, SWROIM is the ASP over the Total Capital Investment, TCI for project p.

Annual Safety and Sustainability Profit (ASSP) is a safety and sustainability factor adjustment to the AEP based on indicators and their respective targets, shown by Equation 42.

Equation 42 Annual Safety and Sustainability Profit (ASSP) reprinted from [22]

$$\mathrm{ASSP}_p = \mathrm{AEP}_p \left[1 + \sum_{i=1}^{N_{\mathrm{Indicators}}} w_i \left(\frac{\mathrm{Indicator}_{\mathrm{Base},i} - \mathrm{Indicator}_{p,i}}{\mathrm{Indicator}_{\mathrm{Base},i} - \mathrm{Indicator}_{\mathrm{Target},i}} \right) \right]$$

For project p, the safety and sustainability factor adjustment consists of w_i times a ratio representing the relative importance of the i^{th} safety or sustainability indicator compared to the AEP. The ratio of indicator differences represents "the fractional contribution of the p^{th} design option toward meeting the target performance associated with the i^{th} safety or sustainability metric" [22].

Safety and Sustainability Weighted Return on Investment (SASWROIM) "provides an economic basis for the real cost/value of a project based on the directly tangible financial performance as well as the indirectly tangible impact on the environment and safety using ROI as a unifying basis of multiple objectives" [22].

Equation 43 Safety and Sustainability Weighted Return on Investment (SASWROIM) reprinted from [22]

$$\mathrm{SASWROIM}_p = \frac{\mathrm{ASSP}_p}{\mathrm{TCI}_p}$$

In Equation 43, SASWROIM is ASSP over the TCI for project p.

Weights are determined by core values of the company conducting the design evaluation.

2.6 Other Decision Criteria

The indicators and metrics listed above is only a finite amount of the possible ways to evaluate a process route or project. "Many other factors have to be considered when evaluating projects, such as those listed below" in Table 15 [5]:

Table 15 Other Potential Project Criteria reprinted from [5]

1.	Safety
2.	Environmental problems (waste disposal)
3.	Political considerations (government policies and incentives)
4.	Location of customers and suppliers (supply chain)
5.	Availability of labor and supporting services
6.	Corporate growth strategies
7.	Company experience in the particular technology

More data and information is needed to properly use and assess some of these criteria.

2.7 Propylene Data

Data to accurately calculate the cost of propylene was collected.

2.7.1 Identifying On-Purpose Propylene Routes

There are an infinite number of process routes to generate propylene. However, not all routes are economical. Theoretically, it is possible to go from octane to propylene, but it may take four-to-five reactions. As the number of reactions required to get from substance A to propylene increases, the less economical the route becomes. Each reaction has a set of mass and energy requirements that increase capital cost. Each new reaction adds its own capital cost, like an economic burden. Therefore, it is reasonable to seek for process routes that only require one or two reactions to generate propylene and, consequently, minimize the economic burden.

There are only a finite number of process routes to generate propylene via one reaction. Table 16 contains the four on-purpose propylene process routes and their respective reactions.

Table 16 On-Purpose Propylene Process Routes & Reactions

Process Route	Abbrev.	Reaction
Propane Dehydrogenation	PDH	$C_3H_8 \rightarrow C_3H_6 + H_2$
Methanol-to-Propylene	MTP	$3\ CH_3OH \rightarrow C_3H_6 + 3\ H_2O$
Hydrodeoxygenation	HDO	$C_3H_8O_3 + 2\ H_2 \rightarrow C_3H_6 + 3\ H_2O$
Olefin Metathesis	OMT	$C_2H_4 + C_4H_8 \rightarrow 2\ C_3H_6$

These reactions identify the key feedstock consumed and byproducts produced from each process route.

2.7.2 Seeking Data for Chemical Prices

Chemical pricing is required to perform any economic analysis. Prices were sought via creditable sources, such as the U.S. Energy Information Administration (EIA) and the Independent Chemical Information Service (ICIS). Table 17 contains the historical prices of key components for on-purpose propylene routes.

Table 17 Prices for Chemicals

Chemicals	**Historical Prices**	**Time & Sources**
2-butene	1.18 $/kg	2017 Platts [23]
ethylene	0.65 $/kg	2017 ICIS [24]
hydrogen	1.50-2.00 $/kg	2013-2015 Noureldin [25] [26]
gasoline	1.778-2.125 $/gal	2017 EIA [27]
glycerol	0.82-1.05 $/lbm	2008 ICIS Prices [28]
methanol	330 $/MT	2017 Methanex (Europe) [29]
natural gas	3.89-6.93 $/1000SCFT	2010 EIA Price [30]
propane	0.48 $/kg	2017 US EIA [31]
propylene	0.95 $/kg	2015 PGPI [32]
water	0.50-1.50 $/m^3	2012 El-Halwagi [2]

Although these values are not current prices for each chemical, historical data for natural gas and propane have not changed significantly or beyond the range listed above for an extended period of time. Therefore, the values can be used for current pricing.

2.7.3 Propane Dehydrogenation (PDH) Process Design

Agarwal *et al.* provides a detailed account of on-purpose propylene production and intensification via Propane Dehydrogenation (PDH). Figure 2 shows the process flow diagram of PDH:

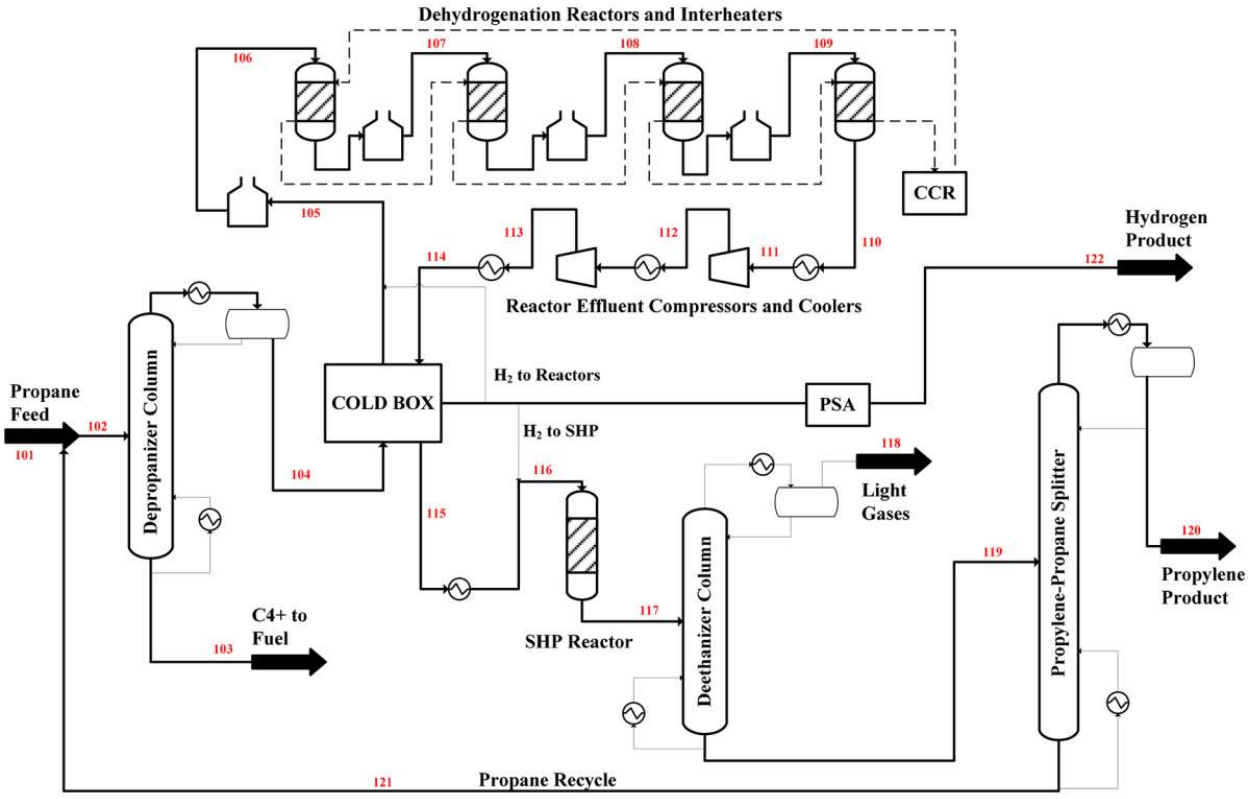


Figure 2 Propane Dehydrogenation Process Flow Diagram reprinted from [10].

Data for the base case design of an Oleflex PDH plant are shown below in Table 18:

Table 18 Conditions & Composition of Base Case PDH Inlets & Outlets adapted from [10]

Stream	Inlet	Outlet	Outlet	Outlet	Outlet
Conditions	**Propane Feed**	**C4+ to Fuel**	**Hydrogen Product**	**Light Gases**	**Propylene Product**
Vapor Fraction	0	0	1	1	0
Temperature, K	313.1	328.4	308.4	220.0	284.3
Pressure, kPa	6894.8	1647.8	777	446.1	894.2
Molar Flow, kmol/hr	1950	6	1564	265	1730
Mass Flow, kg/hr	85,049	274	3152	6663	72,828
Components (Mole Fraction)					
Hydrogen	0.0000	0.0000	1.0000	0.0546	0.0000
Methane	0.0027	0.0000	0.0000	0.2079	0.0000
Ethylene	0.0001	0.0000	0.0000	0.2669	0.0000
Ethane	0.0290	0.0000	0.0000	0.4689	0.0001
Propene	0.0000	0.0000	0.0000	0.0015	0.9947
Propane	0.9675	0.9069	0.0000	0.0003	0.0052
Propadiene	0.0000	0.0000	0.0000	0.0000	0.0000
m-Acetylene	0.0000	0.0000	0.0000	0.0000	0.0000
i-Butane	0.0006	0.0856	0.0000	0.0000	0.0000
n-Butane	0.0000	0.0047	0.0000	0.0000	0.0000
Benzene	0.0000	0.0024	0.0000	0.0000	0.0000
Toluene	0.0000	0.0003	0.0000	0.0000	0.0000

The selectivity toward propylene is 90 mol% and the once-through conversion is 40 mol% [33]. Furthermore, the base case utility costs from propane dehydrogenation are provided in Table 19:

Table 19 Base Case Utility Costs adapted from [10]

Utility Type	Unit Cost
Cooling Water	$\$0.023/m^3$
LP Steam	\$10.7/kg
Natural Gas	\$10.1/MW-hr
Electricity	\$0.065/kW-hr

Agarwal's data and analysis using SWROIM can be further improved upon by applying SASWROIM. Lastly, after reviewing key units of the PDH design, the following chemicals could be assumed to be those listed in Table 20:

Table 20 Chemicals in PDH Plant

Unit	Chemicals
Inlets & Outlets	See Base Case Composition Table
Reactor/CCR Section	DEH-16/DEH-14 Catalyst, DMDS, Coke
Feed Treatment	Sulfur, Mercury, and Arsine Removal, GB-236/GB-238
SHP	Zeolite Catalyst
Dehydration	UI-94

The Depropanizer, Cold Box, Reactor Effluent Compressors and Coolers, Deethanizer, Pressure Swing Adsorption (PSA), and PP-Splitter sections were assumed to not have any additional chemicals that are not already listed above.

2.7.4 Methanol-to-Propylene (MTP) Process Design

Jasper *et al*. provide a detailed account of on-purpose propylene production via Methanol-to-Olefins (MTO) or Methanol-to-Propylene (MTP). Figure 3 shows the process flow diagram of MTP:

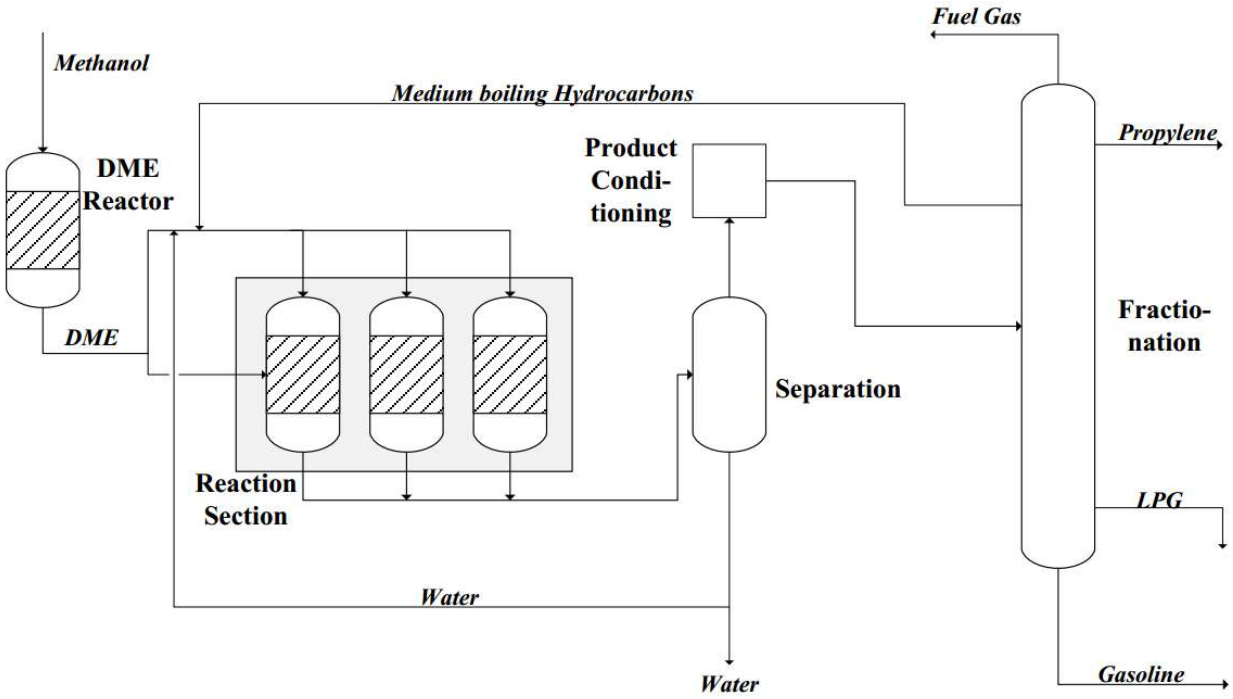


Figure 3 Methanol-to-Propylene Process Flow Diagram reprinted from [34].

Data for the base case design of a Lurgi MTP plant are shown below in Table 21:

Table 21 Flowrates of Base Case MTP Inlets & Outlets adapted from [34]

Chemical Stream	Type	Flowrate (ktonne/yr)
Methanol	Inlet	1825
Propylene	Outlet	568
Gasoline	Outlet	157

Jasper's data and analysis can be further improved upon by applying SASWROIM. Lastly, after reviewing key units of the MTP design, the following chemicals could be assumed to be those listed in Table 22:

Table 22 Chemicals in MTP Plant

Unit	Chemicals
Inlets & Outlets	See Base Case Composition Table
Reactor Section	ZSM-5 Catalyst, DME, Coke
Feed Treatment	Sulfur, Mercury, and Arsine Removal, GB-236/GB-238
Dehydration	UI-94

The Separation, Product Conditioning, and Fractionation sections were assumed to not have any additional chemicals that are not already listed above.

Furthermore, Ehlinger *et al.* provides a detailed account of shale gas to methanol technologies. Multiple cases and shale gas stream are listed. The composition of her shale gas to methanol process is shown below in Table 23:

Table 23 Methanol Process Stream from Shale Gas adapted from [35]

Conditions	**Value**
Temperature, °F	113
Pressure, psia	1096
Total Flow, lbmol/hr	13,021.8
Total Flow, lbm/h	415,835
Components	**Molar Flowrate (lbmol/hr)**
Hydrogen	0.0
Water	2.7
Methane	30.8
Nitrogen	2.1
Ethane	0.0
Propane	0.0
Carbon Monoxide	403.7
Methanol	12,524.5
Butanol	1.8
Dimethyl-ether	0.4
Acetone	0.7
Oxygen	0.0
Carbon Dioxide	55.1

Over a H-ZSM-5 catalyst, the MTP reactor will have a production distribution shown below provided by Onel *et al* in Table 24:

Table 24 MTP Product Distribution adapted from [36]

Species	**MTP (mol%)**
CH4	0.56
C2H4	0
C2H6	0.69
C3H6	71.37
C3H8	2.31
C4H8	0
C4H10	5.22
C5+	19.85

2.7.5 Green Propylene Routes

There are various process routes to produce propylene from bio-based materials. Some of these routes are listed in Figure 4:

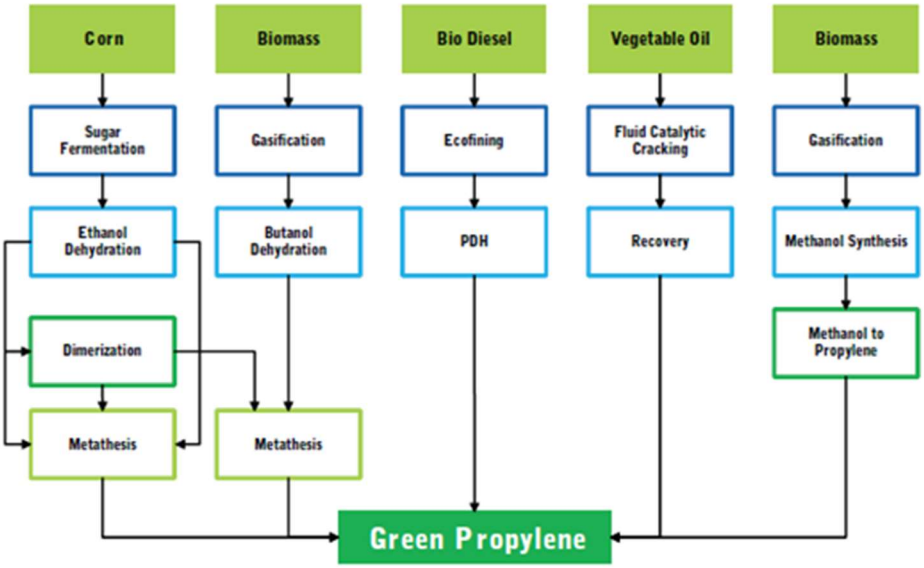


Figure 4 Routes to Green Propylene reprinted from [37].

These process routes produce propylene through various reactions, as shown in Table 25:

Table 25 Reactions of Routes to Green Propylene

Process Box	Reaction	Sources
Sugar Fermentation	$2(C_6H_{10}O_5)_n + nH_2O \rightarrow n\ C_{12}H_{22}O_{11}$ $C_{12}H_{22}O_{11} + H_2O \rightarrow 2\ C_6H_{12}O_6$ $C_6H_{12}O_6 \rightarrow 2\ C_2H_5OH + 2\ CO_2$	[38]
Gasification	$\text{biomass} + H_2O \rightarrow CO + H_2$ $\text{biomass} + 2H_2O \rightarrow CO_2 + H_2$ $\text{biomass} + CO_2 \rightarrow 2\ CO$ etc.	[39]
Ecofining	$\text{triglyceride} + 3\ CH_3OH \overset{NaOH}{\rightarrow} C_3H_8O_3 + 3\ R_xCOOCH_3$	[40]
Fluid Catalytic Cracking	$C_{7+} \rightarrow C_3H_6 + \text{others}$	[41]
Ethanol Dehydration	$C_2H_5OH \overset{H_2SO_4}{\rightarrow} C_2H_4 + H_2O$	----
Butanol Dehydration	$C_4H_9OH \overset{H_2SO_4}{\rightarrow} C_4H_8 + H_2O$	----
Propane Dehydrogenation (PDH)	$C_3H_8 \rightarrow C_3H_6 + H_2$	[41]
Methanol Synthesis	$CO + 2\ H_2 \rightarrow CH_3OH$	[42]
Dimerization	$\text{methyl propene} \rightarrow \text{propene}$	[43]
Methanol-to-Propylene (MTP)	$3\ CH_3OH \rightarrow C_3H_6 + 3\ H_2O$	[41]
Metathesis (Olefin Metathesis)	$C_2H_4 + C_4H_8 \rightarrow 2\ C_3H_6$	[44]
Hydrodeoxygenation	$C_3H_8O_3 + 2\ H_2 \rightarrow C_3H_6 + 3\ H_2O$	[45]

Knowing which reactions occur for each process route, we can determine which components are necessary to produce propylene.

2.8 Shale Gas and Biofuels Data

Unfortunately, components do not exist naturally in pure states. They exist in mixtures with other components. Therefore, feedstock compositions must be sought after in order to accurately represent where propylene comes from.

2.8.1 Shale Gas Composition

The average shale gas composition from the Marcellus well is shown below in Table 26:

Table 26 Average Shale Gas Composition from Marcellus Well adapted from [35]

Component	**wt%**
Methane	85.2
Ethane	11.3
Propane	2.9
CO2	0.4
N2	0.3
Total	100.1

Other compositions of shale gas from the Barnett, Fayetteville, New Albany, Antrim, or Haynesville wells could have been used. The Marcellus well composition was recorded and used in this paper, since it had the highest total hydrocarbon composition that could be converted to propylene.

2.8.2 Corn Composition

Corn is an easy crop to mass produce and collect for various purposes—grain, food, silage, etc. A generic composition of corn is shown below in Table 27:

Table 27 Generic Corn Composition reprinted from [46]

Component	**wt%**
Starch	62
Cellulose	4
Sugars	2
Hemicellulose	6
Protein	6
Oil	4
Ash	1
Water	15
Total	100

This composition is completely theoretical for El-Halwagi's stoichiometric targeting but still reasonably represents what corn will be consist of.

2.8.3 Biodiesel Production

Another bio-based fuel that can be easily be converted into propylene is biodiesel. "Biodiesel fuel can be produced by transesterification of virtually any triglyceride feedstock" [47]. The composition of biodiesel derived from corn is shown below in Table 28:

Table 28 Biodiesel (Corn) Composition adapted from [48]

Component	**wt%**
Palmitic (16:0)	11.5
Palmitoleic (16:1)	0.2
Heptadecenoic (17:1)	0.1
Stearic (18:0)	1.9
Oleic (18:1)	26.6
Linoleic (18:2)	58.7
Linolenic (18:3)	0.6
Arachidic (20:0)	0.3
Gondoic (20:1)	0.1
Behenic (22:0)	0.1
Erucic (22:1)	0.1
Lignoceric (24:0)	0.1
Other/Unknown	0.3
Total	100.6

The composition of biodiesel derived from canola oil is shown below in Table 29:

Table 29 Biodiesel (Canola) Composition adapted from [48]

Component	wt%
Capric (10:0)	0.1
Palmitic (16:0)	4.2
Palmitoleic (16:1)	0.3
Heptadecanoic (17:0)	0.1
Heptadecenoic (17:1)	0.1
Stearic (18:0)	2
Oleic (18:1)	60.4
Linoleic (18:2)	21.2
Linolenic (18:3)	9.6
Arachidic (20:0)	0.7
Gondoic (20:1)	1.5
Eicosadiensic (20:2)	0.1
Behenic (22:0)	0.3
Erucic (22:1)	0.5
Lignoceric (24:0)	0.2
Nervonic (24:1)	0.2
Other/Unknown	2.2
Total	103.7

Many more compositions of biodiesel were listed in the journal article; however, only two were selected. The corn biodiesel composition was selected to be compared against the generic corn composition, while the canola biodiesel composition was selected to be compared as an alternative to the corn biodiesel.

2.8.4 Farmers and Farmland

Research into the number of farmers and amount of farmland in use was sought after in order to estimate the number of jobs produced. In the 2012 U.S. Census, 3,180,074 farmers were employed covering 914,527,657 acres of farmland [49].

3. METHODOLOGY

The objective is to determine an on-purpose propylene route using economic, environmental, safety, and social indicators with minimal data. Economic indicators eliminate non-viable process routes and provide a comparable measure across various projects. Environmental, safety, and social indicators help identify which of the remaining process routes has the least detrimental impact.

3.1 Approach & Procedure for Social Indicator Case Study

Of the various social indicators founded in the literature review, a few were selected in a case study to verify that the metrics could be used with reasonable results.

The operating labor chart data was extracted via a web plot digitizer for Figure 5:

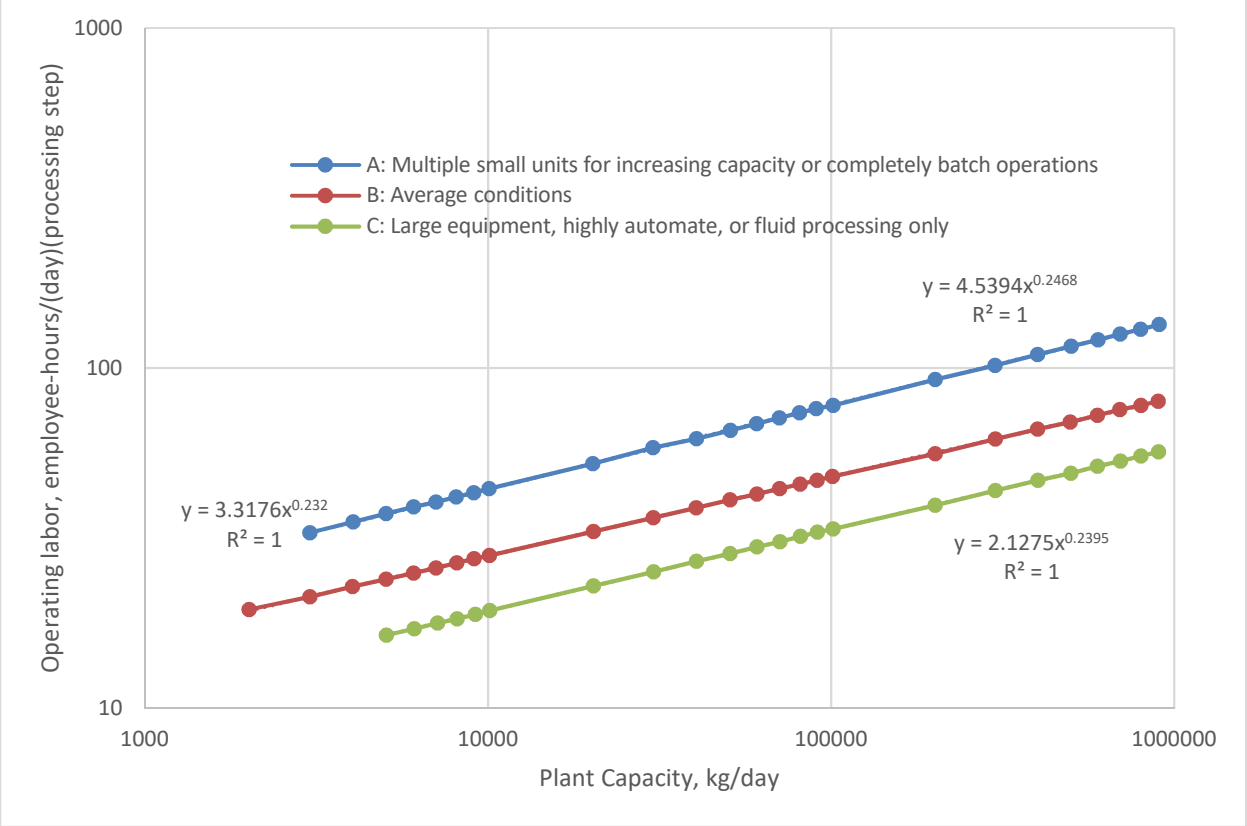


Figure 5 Operating Labor Requirements in Chemical Industry adapted from [18].

After digitizing and recording the data points in excel, Equations 44, 45, and 46 were modeled:

Equation 44 Batch Plant Operating Labor (y_A) adapted from [18]

$$y_A = 4.5394 x_A^{0.2468}$$

Equation 45 Average Plant Operating Labor (y_B) adapted from [18]

$$y_B = 3.3176 x_B^{0.232}$$

Equation 46 Continuous Plant Operating Labor (y_C) adapted from [18]

$$y_C = 2.1275 x_C^{0.2395}$$

The operating labor, y is in units of hours per day per process step and the plant capacity, x is in units of kilograms per day.

The number of jobs was estimated based on the operating labor requirement, number of process steps, number of jobs per person, and the daily man hours expected of a worker, shown by Equation 47.

Equation 47 Number of Jobs

$$(\text{no. jobs}, \text{job}) = \frac{\left(\text{op. labor}, \frac{\text{hr}}{\text{day} \cdot \text{step}}\right)(\text{no. of process steps}, \text{step})\left(\text{jobs per person}, \frac{\text{job}}{\text{person}}\right)}{\left(\text{daily manhours}, \frac{\text{hr}}{\text{day} \cdot \text{person}}\right)}$$

ED was estimated based on the number of interactions per year, the duration period in which the workers handle or may be exposed to the chemical in hours, and the total working hours per year of the individual. The number of time in an 8-hour work schedule is 480 minutes. Equation 48 shows this relationship.

Equation 48 Exposure Duration Estimate (ED)

$$\text{ED} = \frac{(\text{no. interaction per year})(\text{duration period in hours})}{(\text{total working hours per year})} * 480 \text{ minutes}$$

For the semi-quantitative occupational risk prediction model, the EHI is determined from individual chemicals. For a project, multiple chemicals must be considered. Fortunately, in the EHI model study, they "assume the toxic effects of all involved chemicals are additive (i.e., assuming no synergistic or antagonistic effects for a co-exposure). Therefore, the summation of EHI for each of all chemicals used in the enterprise [project] was considered to be representative of the EHI of the enterprise [project]" [20]. Therefore, the EHI model equations can be adjusted for projects by summing the EHI of individual chemicals in Table 30.

Table 30 EHI Equations for Projects (EHI_p) adapted from [20]

Indices	**Wang *et al.*, 2013** [20]	**Social Indicator Case Study**
Exposure Hazard Index	$\mathrm{EHI} = (\mathrm{TI})(\mathrm{EI})(\mathrm{PDI})$	$\mathrm{EHI}_p = \sum_{i}^{N_{\mathrm{chemicals}}} (\mathrm{TI}_i)(\mathrm{EI}_i)(\mathrm{PDI}_i)$
Toxicity Index	$\mathrm{TI}_{\mathrm{ES}} = 2^{[4.16-\log(\mathrm{OELTWA})]}$	$\mathrm{TI}_i = 2^{[4.16-\log(\mathrm{OELTWA})_i]}$
Exposure Index	$\mathrm{EI}_{\mathrm{ES}} = 0.0023 \cdot \mathrm{ED} - 0.0037$	$\mathrm{EI}_i = 0.0023 \cdot \mathrm{ED}_i - 0.0037$
Protection Deficiency Index	$\mathrm{PDI} = 1 - (\mathrm{MI})(\mathrm{PI})$	$\mathrm{PDI}_i = 1 - (\mathrm{MI}_i)(\mathrm{PI}_i)$
Management Index	$\mathrm{MI}_{\mathrm{ES}} = 0.21 \cdot \mathrm{N} + 0.18$	$\mathrm{MI}_i = 0.21 \cdot \mathrm{N}_i + 0.18$

EHI_{cor} was adopted for Wang *et al.* study. Therefore, this social indicator case study will do so also and not EHI_{ES}.

For simplicity, the combination of engineering controls and PPE administrative controls were categorized into five different levels. The PI for each control measure level is directly associated with the PI of the expert system, as shown in Table 31.

Table 31 Control Measure Level (CML) adapted from [20]

Combination	CML	PI_{ES}
EEn + PPEn	CM0	0.00
EEn + PPEe	CM1	0.18
EEp + PPEn	CM2	0.42
EEp + PPEe	CM3	0.61
EEe + PPEn	CM4	0.74
EEe + PPEe	CM5	1.00

The approach to address the social indicator case study is shown in Figure 6:

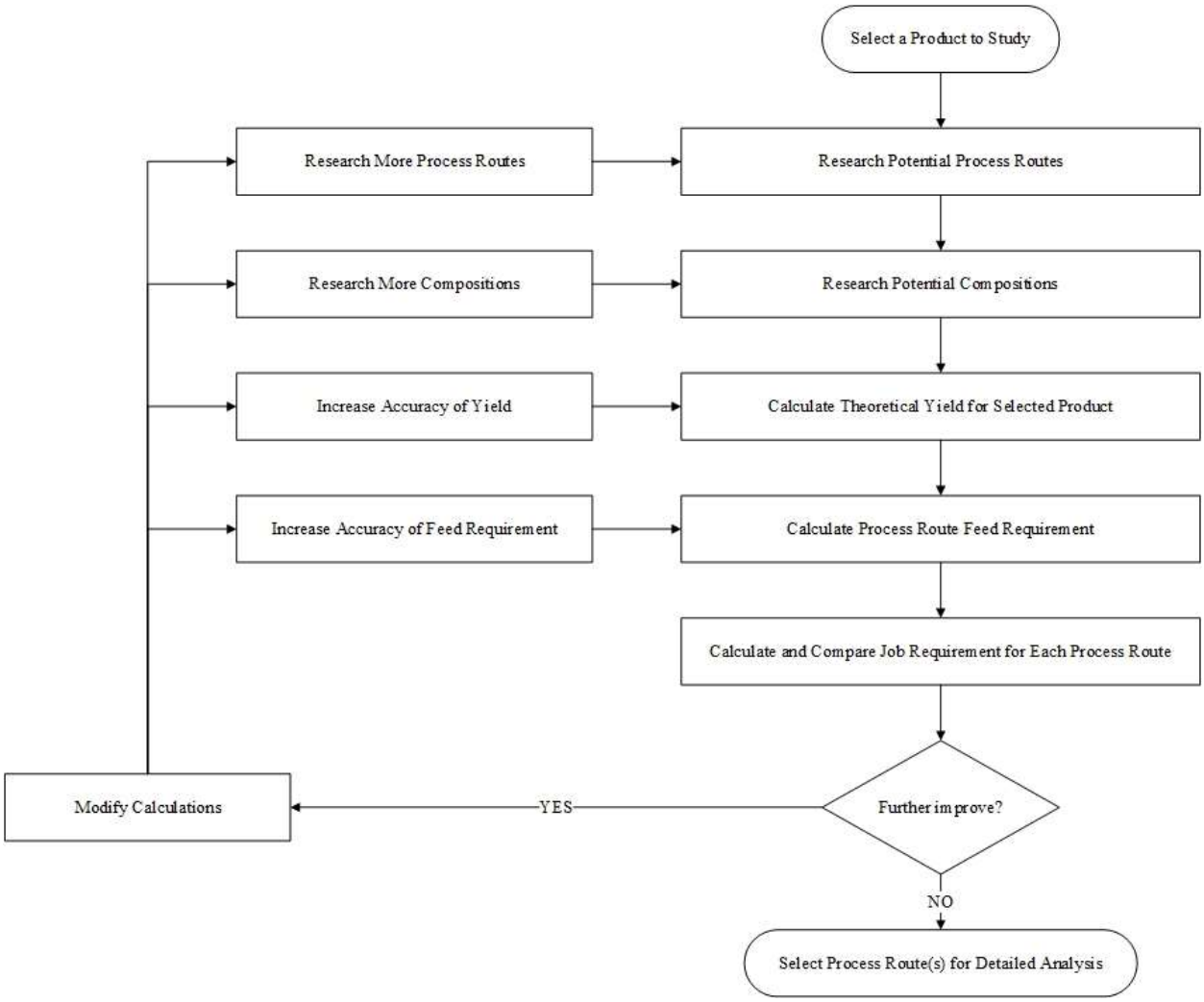


Figure 6 Social Indicator Approach Flowchart.

First, a product was selected to study, along with a basis of production. Various potential process routes were found with their associated reactions and feedstock. Then, potential compositions of those feedstock were found to use as a starting point for the calculations. Next, the theoretical yield from the feedstock components to the selected product was calculated for each process route. Initially, 100% mass yield conversion is assumed. The process route feed requirement was then back-calculated from the basis of product production. Lastly, the job requirement was calculated from the feed requirement. The job requirement for each process route can be compared. If the approach could have been further improved, then it was modified by either further research or increasing the accuracy of the calculations with data. If the approach did not need further improvement, then one or multiple process routes were taken into detailed analysis.

3.2 Approach & Procedure for On-Purpose Propylene Case Study

Various on-purpose propylene production routes are analyzed along with the application of an integrated metric, called the Safety and Sustainability Weighted Return on Investment Metric (SASWROIM). It is implemented in the final selection of the approach. It provides an economic basis for the project as well as tangible impacts from safety, social, and environmental factors. The SASWROIM approach to address the objective is shown in Figure 7:

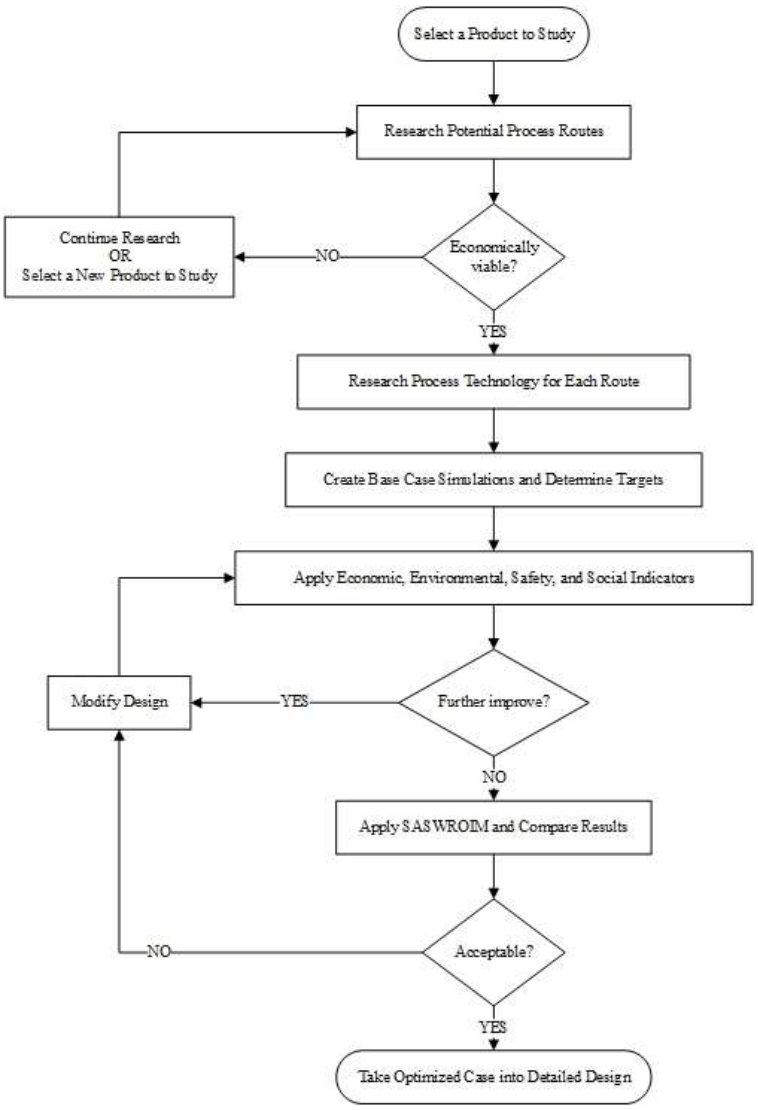


Figure 7 SASWROIM Approach Flowchart.

First, a product was selected to study. Various potential process routes were found and researched. Each process route was tested for economic viability via MISR and/or EGP. If the process route was not viable, then either more research was conducted or a new product to study was selected. If it was viable, then research into process technology routes was conducted. A base case simulation was modeled in Aspen HYSYS V10 based on the data found. Targets for indicators were determined from each of the base case designs. Then, economic, safety, environmental, and social indicators were applied to each design. If the design could have been

further improved, then it was modified and indicators were reapplied. If the design did not need further improvement, then the integrated indicator SASWROIM was applied. If a decision was not reached, then the designs were further modified. Otherwise, the selected optimized case design was taken into detailed design.

4. RESULTS AND DISCUSSION: SOCIAL INDICATORS CASE STUDY

For this case study, social indicators found in the literature review were applied comparing various propylene production process routes from shale gas and bio-based fuels.

4.1 Chemical Data

Chemical data was determined first for the case study to stay within a reasonable realm of accuracy. The chemical data includes molecular weights and theoretical yields for various components.

4.1.1 Molecular Weights

Table 32 lists molecular weights for various components used for this case study:

Table 32 Component Molecular Weights (MW)

Component	Symbol	C	H	O	Component MW
Methane	CH4	1	4	0	16.0423
Ethane	C2H6	2	6	0	30.0688
Propane	C3H8	3	8	0	44.0953
Butane	C4H10	4	10	0	58.1218
Pentane	C5H12	5	12	0	72.1483
Hexane	C6H14	6	14	0	86.1748
Ethylene	C2H4	2	4	0	28.053
Propylene	C3H6	3	6	0	42.0795
Butylene	C4H8	4	8	0	56.106
Pentylene	C5H10	5	10	0	70.1325
Hexylene	C6H12	6	12	0	84.159
Water	H2O	0	2	1	18.0152
Carbon Dioxide	CO2	1	0	2	44.0095
Hemicellulose	C5H10O5	5	10	5	150.1295
Starch/Cellulose	C6H10O5	6	10	5	162.1402
Glucose	C6H12O6	6	12	6	180.1554
Lauric Acid	C12H24O2	12	24	2	200.3168
Myristic Acid	C14H28O2	14	28	2	228.3698
Myristoleic Acid	C14H26O2	14	26	2	226.354
Palmitic Acid	C16H32O2	16	32	2	256.4228
Palmitoleic Acid	C16H30O2	16	30	2	254.407

Table 32 Continued

Component	Symbol	C	H	O	Component MW
Stearic Acid	C18H36O2	18	36	2	284.4758
Oleic Acid	C18H34O2	18	34	2	282.46
Linoleic Acid	C18H32O2	18	32	2	280.4442
Linolenic Acid	C18H30O2	18	30	2	278.4284
Arachidic Acid	C20H40O2	20	40	2	312.5288
Gondoic Acid	C20H38O2	20	38	2	310.513
Behenic Acid	C22H44O2	22	44	2	340.5818
Erucic Acid	C22H42O2	22	42	2	338.566

The atomic molecular weights used for carbon, hydrogen, and oxygen were 12.0107 amu, 1.0079 amu, and 15.9994 amu respectively [50].

4.1.2 Theoretical Yield

The theoretical 100% yield was calculated strictly from an atomic level. The component would react with or produce either water, carbon dioxide, or both to produce the selected product (i.e. propylene). The stoichiometric mass yield could be determined from an atomic balance of a compound to propylene. An example of starch ($C_6H_{10}O_5$) to propylene (C_3H_6) is shown below:

$$C_6H_{10}O_5 \rightarrow \frac{4}{3}C_3H_6 + 1\ H_2O + 2\ CO_2$$

$$1\frac{\text{kg } C_6H_{10}O_5}{\text{kg } C_6H_{10}O_5} \cdot \left(\frac{\text{kmol } C_6H_{10}O_5}{162.14\text{ kg}}\right) \cdot \left(\frac{4/3\text{ kmol } C_3H_6}{1\text{ kmol } C_6H_{10}O_5}\right) \cdot \left(\frac{42.0795\text{ kg}}{\text{kmol } C_3H_6}\right) = 0.346\frac{\text{kg } C_3H_6}{\text{kg } C_6H_{10}O_5}$$

Table 33 summarizing the theoretical 100% yields is shown below:

Table 33 Theoretical 100% Yield

Component	Molar Yield (mol/mol)	Mass Yield (kg/kg)
CH4	0.444	1.166
C2H6	0.778	1.088
C3H8	1.111	1.060
C4H10	1.444	1.046
C5H12	1.778	1.037
C6H14	2.111	1.031
C2H4	0.667	1.000
C3H6	1.000	1.000
C4H8	1.333	1.000
C5H10	1.667	1.000
C6H12	2.000	1.000
H2O	0.000	0.000
CO2	0.000	0.000
C5H10O5	1.111	0.311
C6H10O5	1.333	0.346
C6H12O6	1.333	0.311
C12H24O2	3.778	0.794
C14H28O2	4.444	0.819
C14H26O2	4.333	0.806
C16H32O2	5.111	0.839
C16H30O2	5.000	0.827
C18H36O2	5.778	0.855
C18H34O2	5.667	0.844
C18H32O2	5.556	0.834
C18H30O2	5.444	0.823
C20H40O2	6.444	0.868
C20H38O2	6.333	0.858
C22H44O2	7.111	0.879
C22H42O2	7.000	0.870

The actual yield of propylene from these chemicals cannot be greater than the value listed above.

4.2 Basis, Constraints, and Assumptions

The basis for propylene production was set to 200 MMlbm/yr. Table 34 lists all constraints and assumptions for this calculation:

Table 34 Social Indicator Case Study Basis

Basis	**Value**	**Units**
Propylene Production	200	MMlbm/yr
Plant On-Stream Efficiency	92	%
Farm On-Stream Efficiency	85	%
Employee Hours	3	hr/1000 kg
Work Hours Per Year	2040	hr/yr
Baseline Number of Jobs	6	jobs
Target Number of Jobs	20	jobs
Kilogram-to-Bushel	25.4	kg/bushel
Bushel Production	150	bushel/acre-yr
Acres per Farmer	287.58	acre/job
Acres per Farmer per Year	287.58	acre/job-yr
Density of Water	3.7854	kg/gal
Specific Gravity of Biodiesel (Corn)	0.883	----
Specific Gravity of Biodiesel (Canola)	0.003	----
Biodiesel Yield from Corn	19	gal/acre
Biodiesel Yield from Canola	127.5	gal/acre

The employee hours were determined from Peters *et al.* rule of thumb table for solid-fluid plants [18]. The baseline number of jobs was determined from the expected number of jobs created from a shale gas process route. The target number of jobs was selected arbitrarily for this case study; however, this value would be determined by decision-makers as the number of jobs they wish to create via any process route. The kilogram-to-bushel and bushel production conversions were determined from El-Halwagi's textbook example [46]. The acres per farmer and acres per farmer per year were determined by dividing the total acres of US farmland by the total number of U.S. farmers pulled from the 2012 Census. The specific gravity of corn and canola biodiesel and the biodiesel yields were determined from Hoekman *et al.* study on biodiesel [48].

4.3 Process Routes

Five separate routes were analyzed for this case study, as shown in Table 35:

Table 35 Social Indicators Case Study Routes

#	**Feed Composition**	**Mass Yield Method**
1	Shale Gas	Stoichiometric
2	Generic Corn	Stoichiometric
3	Generic Corn	Processes
4	Biodiesel (Corn)	Stoichiometric
5	Biodiesel (Canola Oil)	Stoichiometric

The feed compositions are listed in the literature review. The mass yield was calculated based on either stoichiometry or processes. The stoichiometric mass yield has been shown in a previous section. The processes mass yield is determined by taking into account process units and their respective reactions. An example of starch ($C_6H_{10}O_5$) to propylene (C_3H_6) is in Table 36:

Table 36 Corn to Propylene via Process Units

Process Units	**Reactions**
Sugar Fermentation	$C_6H_{10}O_5 + \frac{1}{2}H_2O \rightarrow \frac{1}{2}C_{12}H_{22}O_{11}$ $\frac{1}{2}C_{12}H_{22}O_{11} + \frac{1}{2}H_2O \rightarrow C_6H_{12}O_6$ $C_6H_{12}O_6 \rightarrow 2\ C_2H_5OH + 2\ CO_2$
Ethanol Dehydration	$2\ C_2H_5OH \xrightarrow{H_2SO_4} 2\ C_2H_4 + 2\ H_2O$
Metathesis	$2\ C_2H_4 + 2\ C_4H_8 \rightarrow 4\ C_3H_6$
Overall	$C_6H_{10}O_5 + 2\ C_2H_4 \xrightarrow{H_2SO_4} 4\ C_3H_6 + H_2O + 2\ CO_2$

$$1\frac{\text{kg } C_6H_{10}O_5}{\text{kg } C_6H_{10}O_5} \cdot \left(\frac{\text{kmol } C_6H_{10}O_5}{162.14\text{ kg}}\right) \cdot \left(\frac{4\text{ kmol } C_3H_6}{1\text{ kmol } C_6H_{10}O_5}\right) \cdot \left(\frac{42.0795\text{ kg}}{\text{kmol } C_3H_6}\right) = 1.04\frac{\text{kg } C_3H_6}{\text{kg } C_6H_{10}O_5}$$

Since this method was applied to the generic corn composition, the mass yields for sugar and hemicellulose are 0.934 kg C_3H_6/kg $C_6H_{12}O_6$ and 0.934 kg C_3H_6/kg $C_5H_{10}O_5$ respectively.

4.4 Comparison

Following the social indicators case study methodology and the information listed above, the finals are presented below in Table 37:

Table 37 Social Indicators Case Study Results

Route		**1**	**2**	**3**	**4**	**5**
100% Mass Yield	kg C_3H_6/kg feed	1.146	0.2533	0.7600	0.8334	0.8161
Feed Requirement	kg/day	9824	44,440	14,810	13,510	13,790
Employee Hours	hr/day	29.47	----	----	----	----
Land Area	acres	----	86,850	28,950	212.7	9526
Jobs	jobs	6	303	101	1	34
Ratio to Shale Gas		1.00	50.5	16.8	0.17	5.67

Notably, most of the biofuel based feed for propylene requires more labor, and consequently, provides more jobs than shale gas feed.

5. RESULTS AND DISCUSSION: ON-PURPOSE PROPYLENE CASE STUDY

Propylene was selected as the case study product. Propane dehydration and methanol-to-propylene technologies were simulated and analyzed.

5.1 Product Economic Viability Analysis

A preliminary economic analysis verifies if there are currently known process routes that are economically viable for high-level analysis.

5.1.1 Standardize Chemical Prices

The prices of chemicals were converted into prices with identical units and averaged for comparable measurements, as shown below in Table 38:

Table 38 Adjusted Prices for Chemicals

Chemicals	Average Prices ($/kg)
2-butene	1.180
ethylene	0.650
hydrogen	1.750
gasoline	0.813
glycerol	2.061
methanol	0.330
natural gas	0.267
propane	0.480
propylene	0.950
water	0.001

Volumetric prices, e.g. $/1000SCFT, were multiplied by their respective component densities into prices per unit mass. The Engineering Toolbox provided gas densities [51]. The ranges were averaged to provide a singular reference price for each component.

5.1.2 Stoichiometric Analysis

Stoichiometric indicators are easy, low-level analysis tools to identify benchmarks of a process route. By taking a basis of propylene product, the feedstock consumed and byproducts generated can easily be determined from each process route's reactions, as shown in Table 39:

Table 39 Stoichiometric Mass Balance of Reactions

Routes	C_3H_8	CH_3OH	$C_3H_8O_3$	C_2H_4	C_4H_8	C_3H_6	H_2	H_2O
MW	44.10	32.04	92.10	28.05	56.11	42.08	2.016	18.02
PDH	-104.8	----	----	----	----	+100.0	+4.791	----
MTP	----	-228.4	----	----	----	+100.0	----	+128.5
HDO	----	----	-218.9	----	----	+100.0	-9.582	+128.5
OMT	----	----	----	-33.33	-66.67	+100.0	----	----

Basis: 100 kg/yr of propylene (C_3H_6) & 100% yield

5.1.3 Application of MISR & EGP

With the production and consumption rates known for each process route, the MISR and EGP can be applied to determine if any routes are not economically viable options.

Table 40 MISR & EGP of On-Purpose Propylene Routes

Process Route	**MISR**	**EGP**	**Result**
Propane Dehydrogenation (PDH)	2.055	53.08	more analysis required
Methanol-to-Propylene (MTP)	1.262	19.76	more analysis required
Hydrodeoxygenation (HDO)	0.203	-372.9	not economically viable
Olefin Metathesis (OMT)	0.947	-5.335	not economically viable

5.1.4 Preliminary Economic Analysis Conclusion

From Table 40, there are at least two process routes that are economically viable—PDH and MTP. In the literature review, the Oleflex technology was found for PDH, whereas Lurgi was found for MTP.

5.2 MTP Base Case Design

The basis for both designs is 600,000 MTA polymer-grade propylene. Agarwal *et al*. provides a detailed account of the PDH process at this basis. MTP was simulated in Aspen HYSYS V10 with Twu-Sim-Tassone (TST) Fluids Thermodynamic Package. TST accounts for hydrocarbon and non-ideal systems. TST is most typically used with glycol.

5.2.1 Feed Composition

Feed composition for MTP was created based on the Ehlinger *et al.* composition from shale gas to methanol and summarized in Table 41:

Table 41 MTP Base Case Feed Composition

Components	**Molar Fraction**
Acetone	0.00005
n-Butane	0.00000
1-Butanol	0.00014
1-Butene	0.00000
CO	0.03100
CO2	0.00423
DME	0.00004
Ethane	0.00000
H2	0.00000
Methane	0.00236
Methanol	0.96180
N2	0.00016
1-Pentene	0.00000
Propane	0.00000
Propene	0.00000
H2O	0.00021
Total	1.00000

The pressure (1096 psia or 7557 kPa) and temperature (113 °F or 318.15 K) also matched their conditions. The feed flowrate was adjusted to produce 600,000 MTA of propylene, which ended up being approximately 288,200 kg/hr.

5.2.2 Assumptions

The on-stream efficiency of the plant is ~92% (8060 hr/yr). Polymer-grade propylene is assumed to be a minimum of 99.5 mol% propylene in product stream. No side reactions, such as propane cracking to light gases, occur in either simulation. Compressors operated at 78% polytrophic efficiency. The discharge temperature of compressors was also determined to be below 225 °F (380 K) [53]. A 5 psi (34.47 kPa) pressure drop was selected across heater, coolers, and heat exchangers.

5.2.3 Reactions

The MTP design had the following reactions based on the product distribution in the literature review, shown in Table 42:

Table 42 MTP Reactions

#	**Reaction adapted from [53]**	**CH_3OH Conversion (%)**	**CH_3OCH_3 Conversion (%)**
1	$CH_3OH \rightarrow CO + 2\ H_2$	0.95	
2	$2\ CH_3OH \rightarrow CH_3OCH_3 + H_2O$	18.43	
3	$CH_3OCH_3 + 2\ H_2 \rightarrow 2\ CH_4 + H_2O$		0.89
4	$CH_3OCH_3 + H_2 \rightarrow C_2H_6 + H_2O$		18.91
5	$3\ CH_3OH \rightarrow C_3H_6 + 3\ H_2O$	80.62	
6	$2\ C_2H_6 + CH_3OCH_3 \rightarrow 2\ C_3H_8 + H_2O$		8.35
7	$2\ C_3H_6 + CH_3OCH_3 \rightarrow 2\ C_4H_8 + H_2O$		31.75
8	$2\ C_3H_8 + CH_3OCH_3 \rightarrow 2\ C_4H_{10} + H_2O$		8.35
9	$2\ C_4H_8 + CH_3OCH_3 \rightarrow 2\ C_5H_{10} + H_2O$		31.75
--	**Total**	100	100

C_5H_{10} represents gasoline (C_{5+}). Based on the reaction listed above, the MTP reactors follow the reaction scheme below in Figure 8.

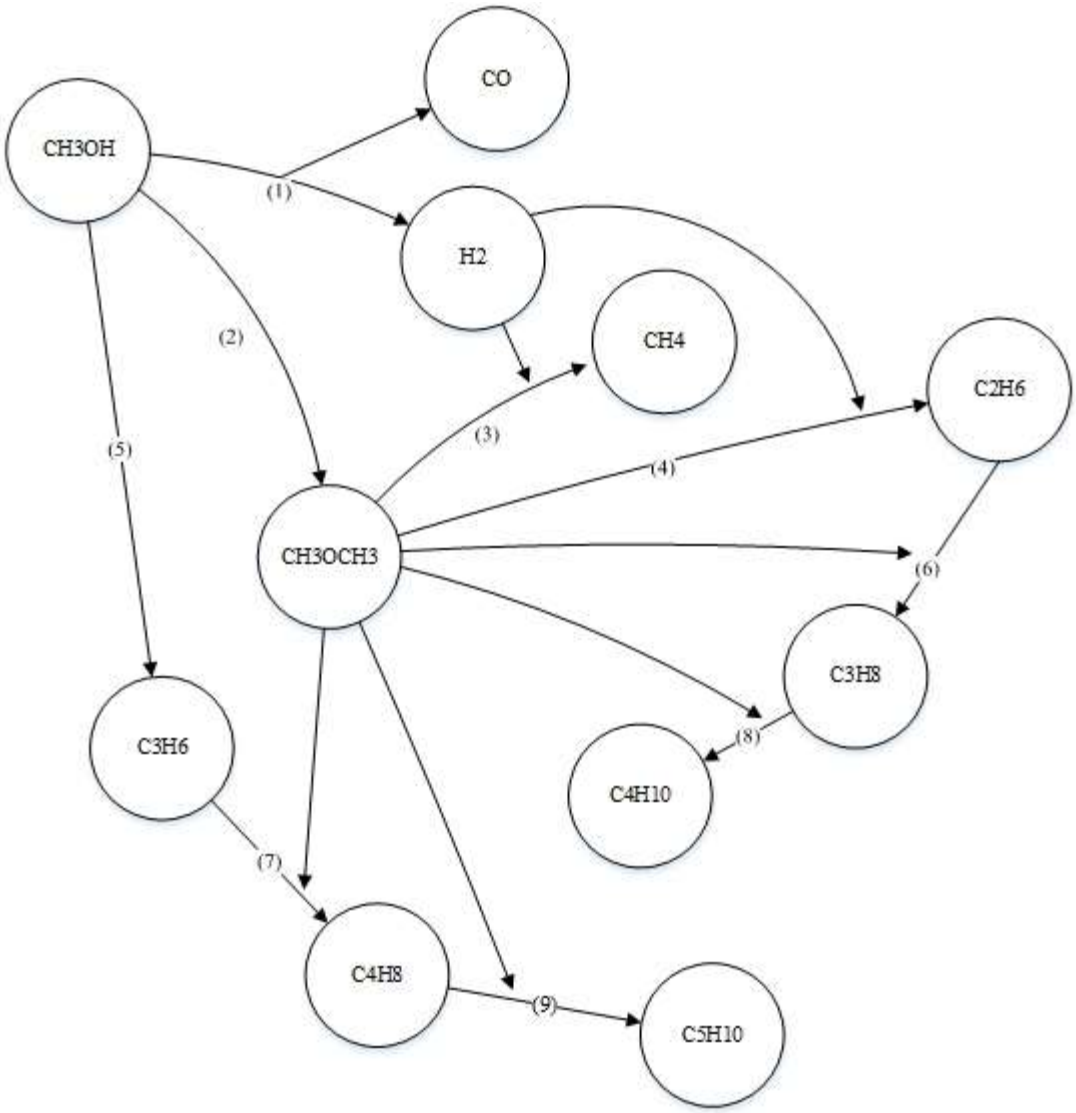


Figure 8 MTP Reaction Pathway.

Water is not shown on the MTP Reaction Pathway figure.

5.2.4 Base Case Process Flow Diagram

The MTP base case was simulated. A Process Flow Diagram (PFD) representing the MTP process is shown below in Figure 9:

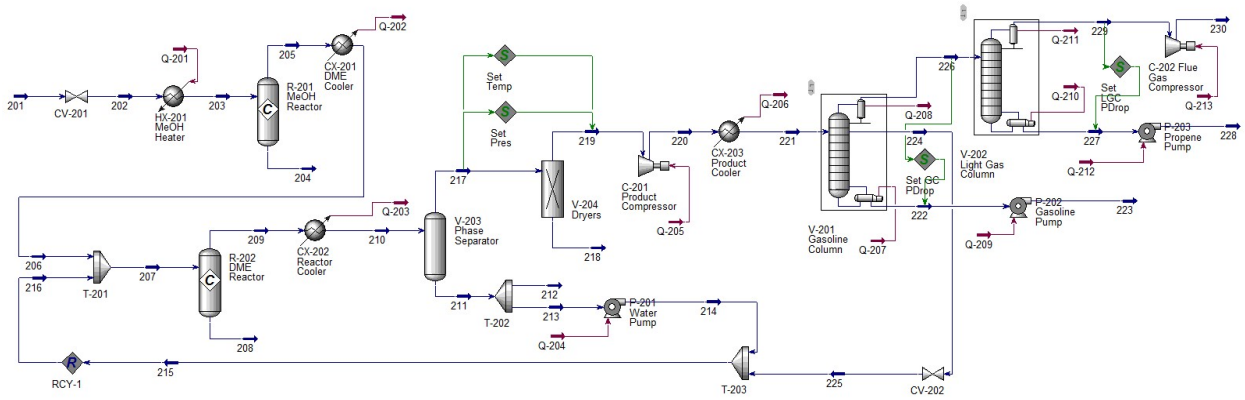


Figure 9 Process Flow Diagram of MTP Base Case.

The feed stream is depressurized with control valve CV-201 and heated with the MeOH Heaters (HX-201AB) to the appropriate pressure and temperature entering the MeOH Reactor (R-201). The MeOH Reactor was simulated with a conversion reactor. The MeOH conditions are consistent with what was found in the literature review. Afterwards, the MeOH Reactor product was cooled with DME Cooler (CX-201) and mixed with recycle streams. The combined stream entered the DME Reactor (R-202). The DME Reactor product was then cooled by Reactor Coolers (CX-202AB). The cooled DME Reactor product entered the Phase Separator (V-203). Water exited V-203 out the bottom. Some water was sent to be sold as process water, while the other part was pumped by Water Pump (P-201) and recycled back. Wet hydrocarbon gas was sent out the top of V-203. Dryers (V-204AB) separated the remaining water in the wet hydrocarbon gas stream. Separated water was assumed to be lost in the adsorbents used. The dry hydrocarbon gas stream was pressured by Product Compressor (C-201). The compressed dry hydrocarbon gas was cooled by Product Cooler (CX-203) and entered into the Gasoline Column (V-201). Heavy hydrocarbons (gasoline-grade) exited out the bottoms and pumped by Gasoline Pump (P-202) to be sold. A cut from V-201, containing mostly DME, was recycled and depressurized by control valve CV-202. Then, light hydrocarbons from V-201 was sent to the

Light Gas Column (V-202). Flue gas was vent out the top of V-202 and pressurized to battery limits conditions by Flue Gas Compressor (C-202). Polymer-grade propylene exited V-202 out the bottom and pressurized by Propene Pump (P-203) to battery limits. The process stream data is shown in Table 43:

Table 43 MTP Base Case Process Streams

Stream No.	**201**	**202**	**203**	**204**	**205**	**206**	**207**	**208**	**209**	**210**
Vapour Fraction	0.016	0.045	1.000	0.000	1.000	1.000	1.000	0.000	1.000	0.257
Temperature (K)	318.1	317.5	698.1	998.1	998.1	698.1	621.0	710.8	710.8	293.0
Pressure (kPa)	7556.7	218.9	184.5	184.5	184.5	150.0	150.0	150.0	150.0	115.5
Molar Flow (kmol/hr)	9024.9	9024.9	9024.9	0.0	11522.4	11522.4	12445.6	0.0	12445.6	12445.6
Mass Flow (kg/hr)	288200	288200	288200	0	288201	288201	304832	0	304832	304832
Acetone	0.00005	0.00005	0.00005	0.00004	0.00004	0.00004	0.00004	0.00004	0.00004	0.00004
n-Butane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00313	0.00312	0.00312
1-Butanol	0.00014	0.00014	0.00014	0.00011	0.00011	0.00011	0.00010	0.00010	0.00010	0.00010
1-Butene	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.02108	0.02103	0.02103
CO	0.03100	0.03100	0.03100	0.03148	0.03144	0.03144	0.02911	0.02920	0.02911	0.02911
CO2	0.00423	0.00423	0.00423	0.00331	0.00331	0.00331	0.00307	0.00308	0.00307	0.00307
DME	0.00004	0.00004	0.00004	0.06947	0.06945	0.06945	0.06430	0.01715	0.01712	0.01712
Ethane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00695	0.00695	0.00695
Hydrogen	0.00000	0.00000	0.00000	0.01431	0.01431	0.01431	0.01325	0.00000	0.00000	0.00000
Methane	0.00236	0.00236	0.00236	0.00172	0.00185	0.00185	0.00171	0.00281	0.00281	0.00281
Methanol	0.96180	0.96180	0.96180	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Nitrogen	0.00016	0.00016	0.00016	0.00013	0.00013	0.00013	0.00012	0.00012	0.00012	0.00012
1-Pentene	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.01984	0.01980	0.01980
Propane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00209	0.00209
Propene	0.00000	0.00000	0.00000	0.20248	0.20244	0.20244	0.18743	0.14690	0.14660	0.14660
H2O	0.00021	0.00021	0.00021	0.67695	0.67691	0.67691	0.70088	0.74961	0.74806	0.74806

Table 43 Continued

Stream No.	**211**	**212**	**213**	**214**	**215**	**216**	**217**	**218**	**219**	**220**
Vapour Fraction	0.000	0.000	0.000	0.000	0.000	0.000	1.000	0.932	1.000	1.000
Temperature (K)	293.0	293.0	293.0	293.0	293.0	293.0	293.0	376.9	293.0	346.7
Pressure (kPa)	115.5	115.5	115.5	150.0	150.0	150.0	115.5	115.5	115.5	334.5
Molar Flow (kmol/hr)	9245.9	8321.3	924.6	924.6	924.6	923.2	3199.7	64.3	3135.4	3135.4
Mass Flow (kg/hr)	166568	149911	16657	16657	16657	16631	138264	1158	137106	137106
Acetone	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00015	0.00000	0.00015	0.00015
n-Butane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.01213	0.00000	0.01238	0.01238
1-Butanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00039	0.00000	0.00040	0.00040
1-Butene	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.08181	0.00000	0.08348	0.08348
CO	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.11320	0.00000	0.11552	0.11552
CO2	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.01191	0.00000	0.01216	0.01216
DME	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.06658	0.00000	0.06794	0.06794
Ethane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.02704	0.00000	0.02759	0.02759
Hydrogen	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Methane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.01092	0.00000	0.01114	0.01114
Methanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Nitrogen	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00045	0.00000	0.00046	0.00046
1-Pentene	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.07701	0.00000	0.07859	0.07859
Propane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00812	0.00000	0.00829	0.00829
Propene	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.57019	0.00000	0.58189	0.58189
H2O	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.02009	1.00000	0.00000	0.00000
Stream No.	**221**	**222**	**223**	**224**	**225**	**226**	**227**	**228**	**229**	**230**
Vapour Fraction	0.266	0.000	0.000	0.000	0.014	1.000	0.000	0.000	1.000	1.000
Temperature (K)	240.0	272.8	275.4	245.0	242.4	227.1	231.1	233.8	170.8	276.9
Pressure (kPa)	300.0	167.6	4238.2	166.5	150.0	140.0	128.9	4238.2	101.3	446.1
Molar Flow (kmol/hr)	3135.4	834.6	834.6	0.0	0.0	2300.9	1768.8	1768.8	532.1	532.1
Mass Flow (kg/hr)	137106	47259	47259	0	0	89847	74448	74448	15399	15399
Acetone	0.00015	0.00058	0.00058	0.00006	0.00006	0.00000	0.00000	0.00000	0.00000	0.00000
n-Butane	0.01238	0.04651	0.04651	0.00847	0.00847	0.00000	0.00000	0.00000	0.00000	0.00000
1-Butanol	0.00040	0.00149	0.00149	0.00016	0.00016	0.00000	0.00000	0.00000	0.00000	0.00000
1-Butene	0.08348	0.31365	0.31365	0.07196	0.07196	0.00000	0.00000	0.00000	0.00000	0.00000
CO	0.11552	0.00000	0.00000	0.00000	0.00000	0.15742	0.00000	0.00000	0.68073	0.68073
CO2	0.01216	0.00000	0.00000	0.00000	0.00000	0.01656	0.00000	0.00000	0.07163	0.07163
DME	0.06794	0.25508	0.25508	0.23886	0.23886	0.00007	0.00008	0.00008	0.00000	0.00000
Ethane	0.02759	0.00000	0.00000	0.00000	0.00000	0.03760	0.00000	0.00000	0.16259	0.16259
Hydrogen	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Methane	0.01114	0.00000	0.00000	0.00000	0.00000	0.01518	0.00000	0.00000	0.06565	0.06565
Methanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Nitrogen	0.00046	0.00000	0.00000	0.00000	0.00000	0.00063	0.00000	0.00000	0.00274	0.00274
1-Pentene	0.07859	0.29527	0.29527	0.03444	0.03444	0.00000	0.00000	0.00000	0.00000	0.00000
Propane	0.00829	0.02184	0.02184	0.10436	0.10436	0.00337	0.00438	0.00438	0.00003	0.00003
Propene	0.58189	0.06558	0.06558	0.54168	0.54168	0.76916	0.99554	0.99554	0.01663	0.01663
H2O	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

5.3 MTP Heat Integration Design

A heat integrated analysis was completed to create a new MTP case and find energy savings. This analysis was done following the techniques in El-Halwagi's *Sustainable Design Through Process Integration*.

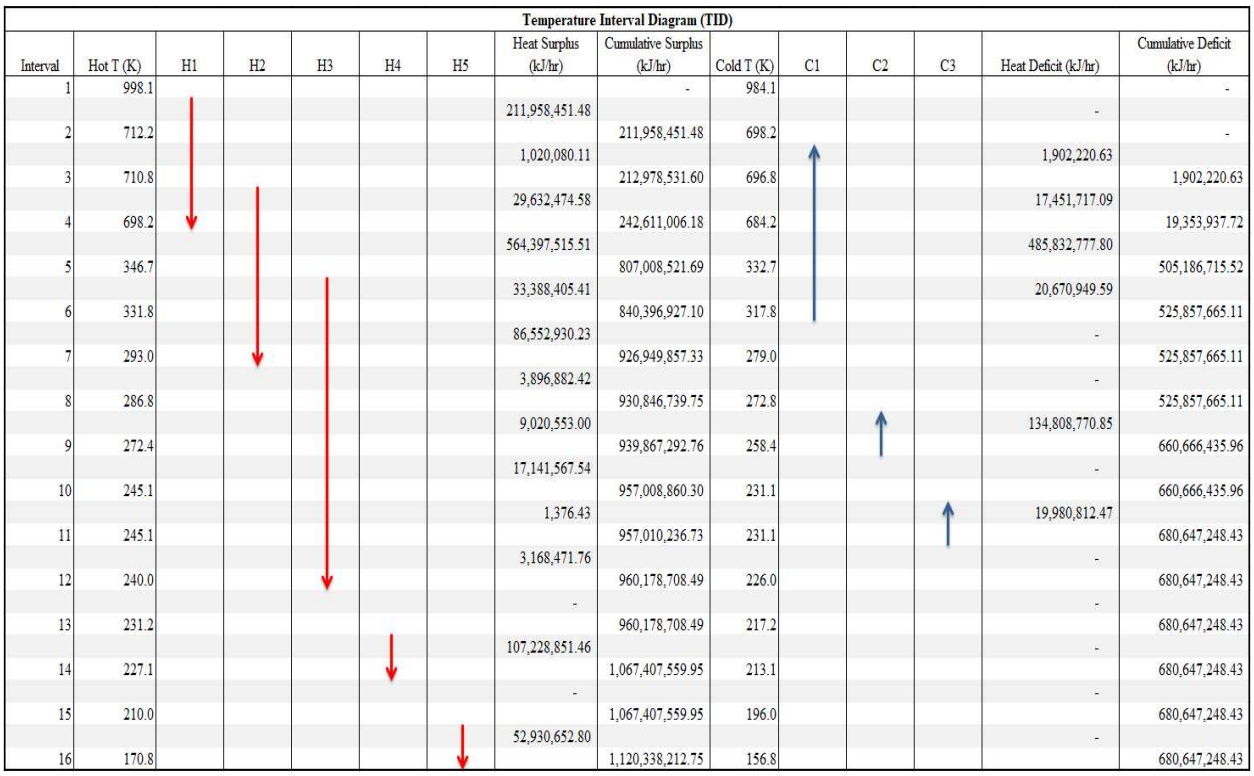
5.3.1 Heat Integration Analysis

First, the potential heat integrated streams were found and listed in the Table 44:

Table 44 Potential Heat Integration Streams

Stream	Description	Supply Temp. (K)	Target Temp. (K)	Heat Flow (kJ/hr)	Thermal Capacity (kJ/hr-K)
H1	CX-201	998.1	698.2	-222,337,146.09	741,335.33
H2	CX-202	710.8	293.0	-670,935,836.33	1,605,977.97
H3	CX-203	346.7	240.0	-66,905,726.07	626,959.46
H4	CX-204	231.2	227.1	-107,228,851.46	26,130,118.68
H5	CX-205	210.0	170.8	-52,930,652.80	1,348,441.37
C1	HX-201	317.8	698.2	525,857,665.11	1,382,424.12
C2	HX-202	258.4	272.8	134,808,770.85	9,369,673.19
C3	HX-203	231.1	231.1	19,980,812.47	9,101,181,082.58

These streams were found around heat exchanged equipment (i.e. heaters, coolers, reboilers, and condensers). The data was then reassigned into a Temperature Interval Diagram (TID), shown in Figure 10:



Temperature Interval Diagram (TID)

Interval	Hot T (K)	H1	H2	H3	H4	H5	Heat Surplus (kJ/hr)	Cumulative Surplus (kJ/hr)	Cold T (K)	C1	C2	C3	Heat Deficit (kJ/hr)	Cumulative Deficit (kJ/hr)
1	998.1							-	984.1					-
							211,958,451.48						-	
2	712.2							211,958,451.48	698.2					-
							1,020,080.11						1,902,220.63	
3	710.8							212,978,531.60	696.8					1,902,220.63
							29,632,474.58						17,451,717.09	
4	698.2							242,611,006.18	684.2					19,353,937.72
							564,397,515.51						485,832,777.80	
5	346.7							807,008,521.69	332.7					505,186,715.52
							33,388,405.41						20,670,949.59	
6	331.8							840,396,927.10	317.8					525,857,665.11
							86,552,930.23						-	
7	293.0							926,949,857.33	279.0					525,857,665.11
							3,896,882.42						-	
8	286.8							930,846,739.75	272.8					525,857,665.11
							9,020,553.00						134,808,770.85	
9	272.4							939,867,292.76	258.4					660,666,435.96
							17,141,567.54						-	
10	245.1							957,008,860.30	231.1					660,666,435.96
							1,376.43						19,980,812.47	
11	245.1							957,010,236.73	231.1					680,647,248.43
							3,168,471.76						-	
12	240.0							960,178,708.49	226.0					680,647,248.43
							-						-	
13	231.2							960,178,708.49	217.2					680,647,248.43
							107,228,851.46						-	
14	227.1							1,067,407,559.95	213.1					680,647,248.43
							-						-	
15	210.0							1,067,407,559.95	196.0					680,647,248.43
							52,930,652.80						-	
16	170.8							1,120,338,212.75	156.8					680,647,248.43

Figure 10 Temperature Interval Diagram (TID).

The TID clearly showed where heat integrated and savings can occur, solely by stream interactions. The hot and cold streams were broken down into components along with their associated enthalpy values, shown in Table 45 and Table 46:

Table 45 Hot Stream Components

Stream	Temp (K)	Enthalpy (kJ/hr)	Cumulative Enthalpy (kJ/hr)
	170.8	0	0
H5	210.0	52,930,652.80	52,930,652.80
	227.1	0	52,930,652.80
H4	231.2	107,228,851.46	160,159,504.26
	240.0	0	160,159,504.26
H3	293.0	33,228,851.16	193,388,355.42
H2+H3	346.7	119,941,335.64	313,329,691.06
H2	698.2	564,397,515.51	877,727,206.57
H1+H2	710.8	29,632,474.58	907,359,681.15
H1	998.1	212,978,531.60	1,120,338,212.75

Table 46 Cold Stream Components

Stream	Temp (K)	Enthalpy (kJ/hr)	Cumulative Enthalpy (kJ/hr)	Shifted Temp. (K)	Shifted C. Enthalpy (kJ/hr)
	231.05	0.00	0	245.05	226,712,432.72
C3	231.06	19980812	19,980,812.47	245.06	246,693,245.20
	258.40	0.00	19,980,812.47	272.40	246,693,245.20
C2	272.78	134808770	154,789,583.32	286.78	381,502,016.04
	317.76	0.00	154,789,583.32	331.76	381,502,016.04
C1	698.15	525857665	680,647,248.43	712.15	907,359,681.15

The enthalpy values were summed together in parts to find the cumulative enthalpy at each temperature. The cumulative enthalpies of both the hot and cold streams were plotted at their respective temperatures to create hot and cold composite curves, as shown below in Figure 11 and Figure 12:

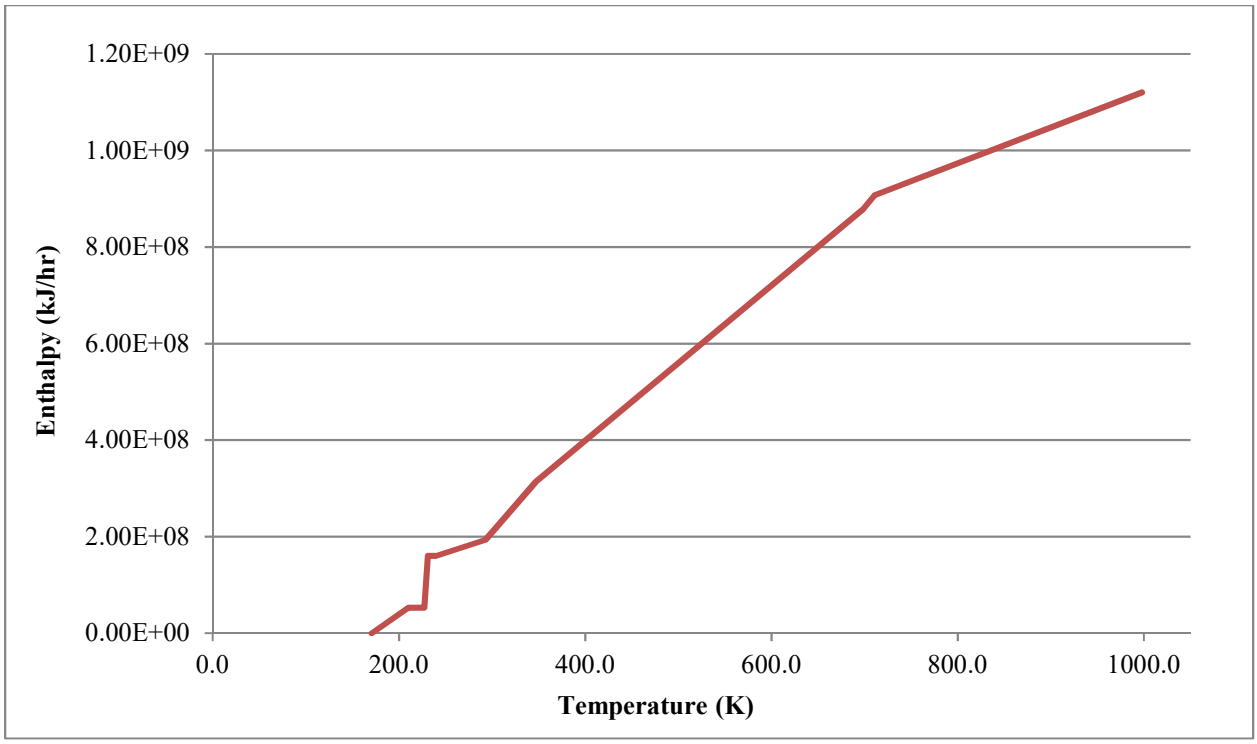


Figure 11 Hot Composite Curve.

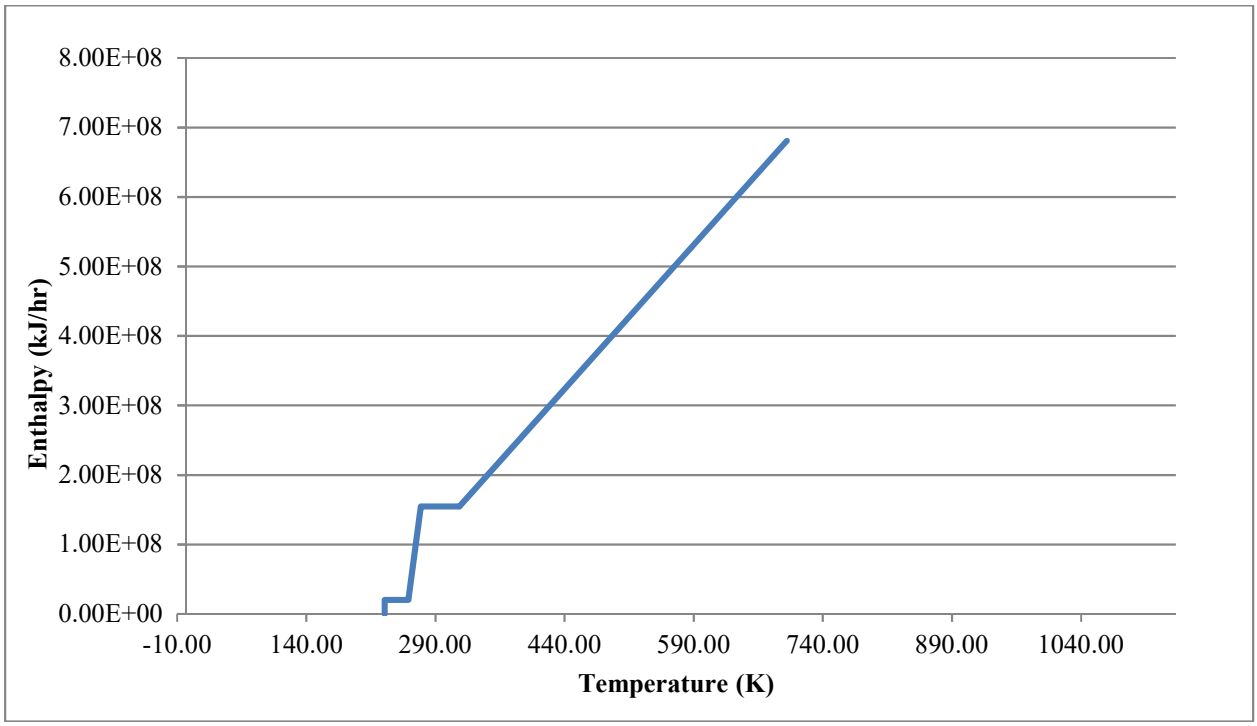


Figure 12 Cold Composite Curve.

The hot and cold composite curves were combined to find the combined composite curve, shown in Figure 13:

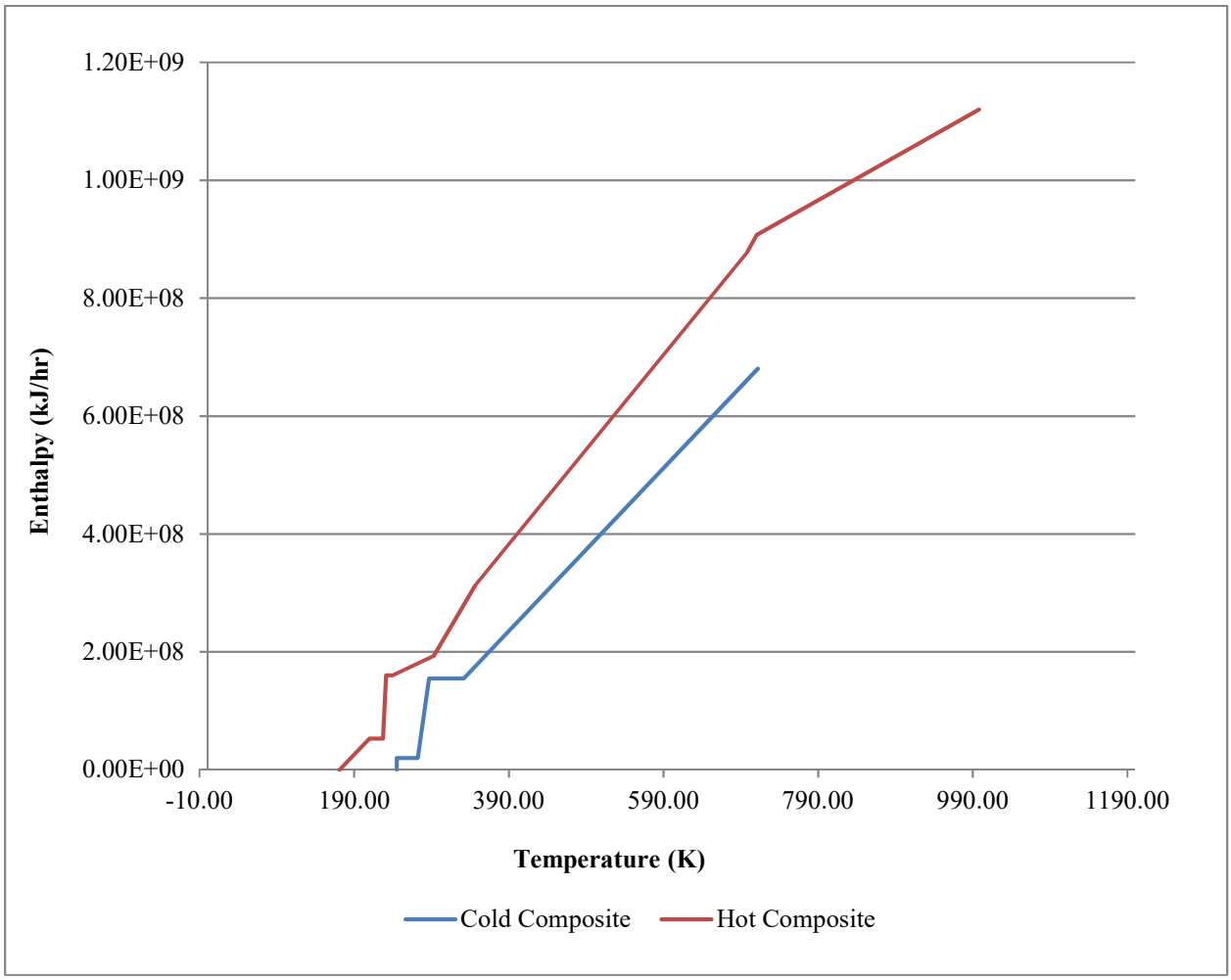


Figure 13 Combined Composite Curve.

The cold composite curve was adjusted in the combined composite curve until the pinch temperature was found, as shown below in Figure 14:

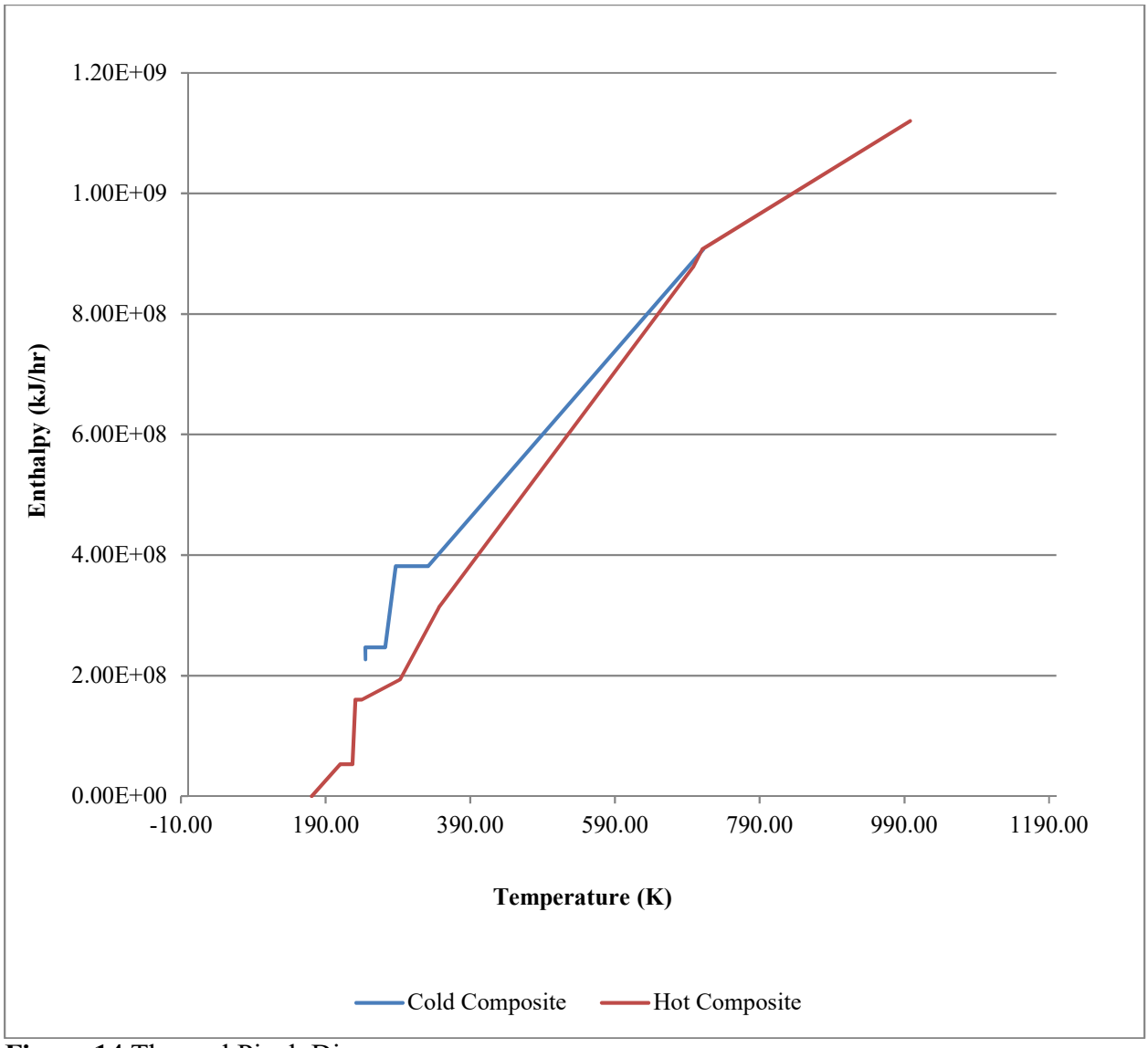


Figure 14 Thermal Pinch Diagram.

Now that the thermal pinch was found, the cold composite curve was adjusted by the minimum approach to find the overall minimum heating and cooling utilities, shown in Figure 15.

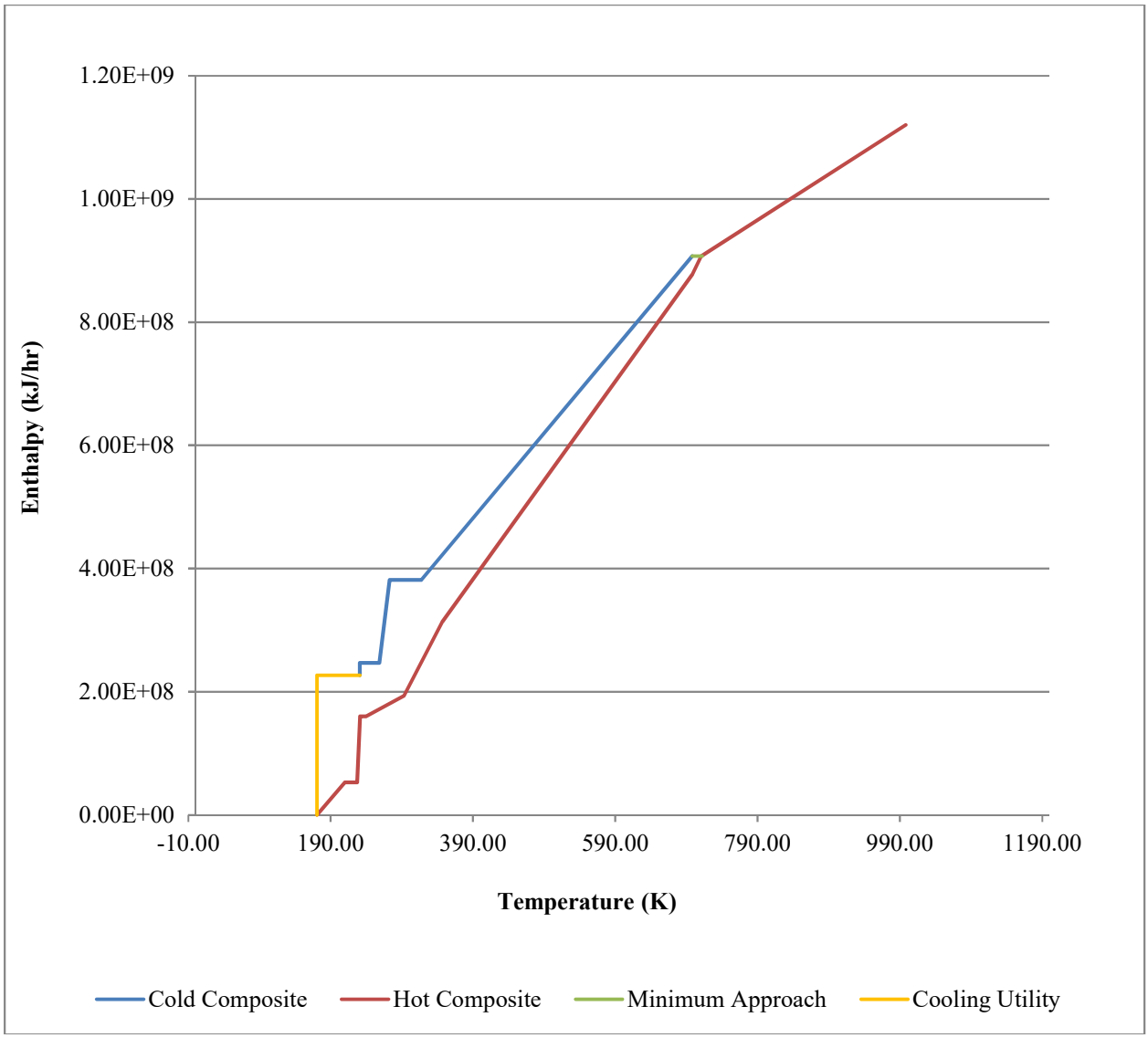


Figure 15 Thermal Pinch Diagram with Minimum Approach.

The values of the thermal pinch, minimum heating utility, and minimum cooling utility are shown in Table 47:

Table 47 Minimum Utilities and Pinch Temperature

Cooling Utility	226,712,432.72 kJ/hr
Heating Utility	0.00 kJ/hr
Pinch Temperature	710.8 K

With the data found in the heat analysis, heat integrated opportunities were found and can be selected. The minimum utilities can also be used as the maximum utility savings any alternate MTP projects can achieve.

5.3.2 Assumptions

The heat integrated case followed the same assumptions as the base case.

5.3.3 Integrated Case Process Flow Diagram

The MTP heat integrated case PFD is shown below in Figure 16:

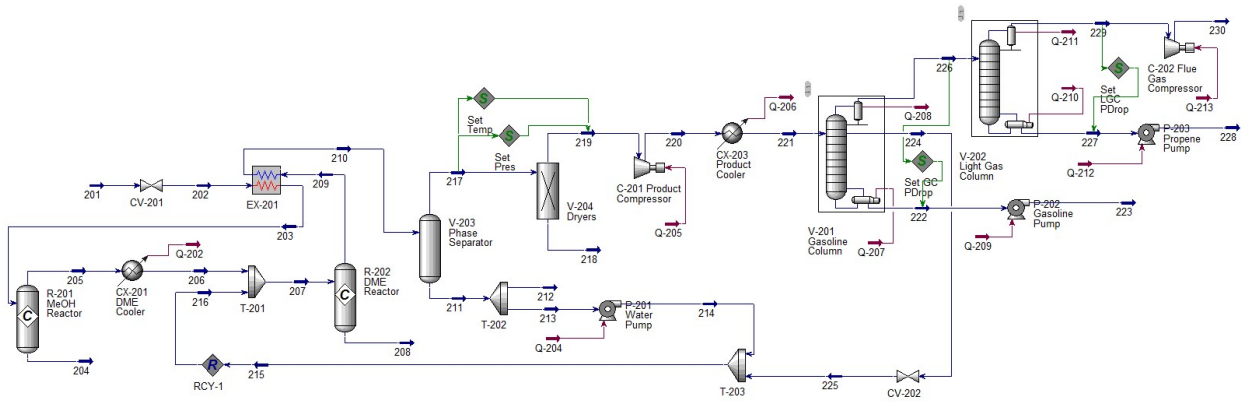


Figure 16 Process Flow Diagram of MTP Integrated Case

The heat integrated PFD flows a similar structure to the base case PFD except one key difference: the Feed Exchanger (EX-201). EX-201 substituted both MeOH Heaters (HX-201AB) and Reactor Coolers (CX-202AB). Various process changes occurred as a result, as shown in Table 48:

Table 48 MTP Integrated Case Process Streams

Stream No.	**201**	**202**	**203**	**204**	**205**	**206**	**207**	**208**	**209**	**210**
Vapour Fraction	0.016	0.045	1.000	0.000	1.000	1.000	1.000	0.000	1.000	0.446
Temperature (K)	318.1	317.5	698.1	998.1	998.1	698.1	645.8	735.0	735.0	353.9
Pressure (kPa)	7556.7	219.5	185.0	185.0	185.0	150.5	150.0	150.0	150.0	115.5
Molar Flow (kmol/hr)	9024.9	9024.9	9024.9	0.0	11522.4	11522.4	12198.2	0.0	12198.2	12198.2
Mass Flow (kg/hr)	288200	288200	288200	0	288201	288201	300376	0	300376	300376
Acetone	0.00005	0.00005	0.00005	0.00004	0.00004	0.00004	0.00004	0.00004	0.00004	0.00004
n-Butane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00319	0.00318	0.00318
1-Butanol	0.00014	0.00014	0.00014	0.00011	0.00011	0.00011	0.00010	0.00010	0.00010	0.00010
1-Butene	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.02150	0.02146	0.02146
CO	0.03100	0.03100	0.03100	0.03148	0.03144	0.03144	0.02970	0.02979	0.02970	0.02970
CO2	0.00423	0.00423	0.00423	0.00331	0.00331	0.00331	0.00313	0.00314	0.00313	0.00313
DME	0.00004	0.00004	0.00004	0.06947	0.06945	0.06945	0.06561	0.01750	0.01746	0.01746
Ethane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00708	0.00709	0.00709
Hydrogen	0.00000	0.00000	0.00000	0.01431	0.01431	0.01431	0.01352	0.00000	0.00000	0.00000
Methane	0.00236	0.00236	0.00236	0.00172	0.00185	0.00185	0.00175	0.00286	0.00286	0.00286
Methanol	0.96180	0.96180	0.96180	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Nitrogen	0.00016	0.00016	0.00016	0.00013	0.00013	0.00013	0.00012	0.00012	0.00012	0.00012
1-Pentene	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.02024	0.02020	0.02020
Propane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00213	0.00213
Propene	0.00000	0.00000	0.00000	0.20248	0.20244	0.20244	0.19123	0.14989	0.14957	0.14957
H2O	0.00021	0.00021	0.00021	0.67695	0.67691	0.67691	0.69481	0.74454	0.74295	0.74295
Stream No.	**211**	**212**	**213**	**214**	**215**	**216**	**217**	**218**	**219**	**220**
Vapour Fraction	0.000	0.000	0.000	0.000	0.000	0.000	1.000	0.982	1.000	1.000
Temperature (K)	353.9	353.9	353.9	353.9	353.9	353.9	353.9	376.9	353.9	409.9
Pressure (kPa)	115.5	115.5	115.5	150.0	150.0	150.0	115.5	115.5	115.5	334.5
Molar Flow (kmol/hr)	6756.1	6080.5	675.6	675.6	675.6	675.8	5442.1	2306.6	3135.5	3135.5
Mass Flow (kg/hr)	121713	109542	12171	12171	12171	12175	178663	41554	137109	137109
Acetone	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00009	0.00000	0.00015	0.00015
n-Butane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00713	0.00000	0.01238	0.01238
1-Butanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00023	0.00000	0.00040	0.00040
1-Butene	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.04810	0.00000	0.08348	0.08348
CO	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.06656	0.00000	0.11552	0.11552
CO2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00701	0.00000	0.01217	0.01217
DME	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.03914	0.00000	0.06794	0.06794
Ethane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.01590	0.00000	0.02759	0.02759
Hydrogen	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Methane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00642	0.00000	0.01114	0.01114
Methanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Nitrogen	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00027	0.00000	0.00046	0.00046
1-Pentene	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.04528	0.00000	0.07859	0.07859
Propane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00478	0.00000	0.00829	0.00829
Propene	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.33525	0.00000	0.58187	0.58187
H2O	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.42384	1.00000	0.00000	0.00000

Table 48 Continued

Stream No.	221	222	223	224	225	226	227	228	229	230
Vapour Fraction	0.267	0.000	0.000	0.000	0.014	1.000	0.000	0.000	1.000	1.000
Temperature (K)	240.0	272.8	275.4	245.0	242.4	227.1	231.1	233.8	170.8	276.9
Pressure (kPa)	300.0	167.6	4238.2	166.5	150.0	140.0	128.9	4238.2	101.3	446.1
Molar Flow (kmol/hr)	3135.5	834.6	834.6	0.0	0.0	2301.0	1768.8	1768.8	532.2	532.2
Mass Flow (kg/hr)	137109	47260	47260	0	0	89850	74447	74447	15402	15402
Acetone	0.00015	0.00058	0.00058	0.00006	0.00006	0.00000	0.00000	0.00000	0.00000	0.00000
n-Butane	0.01238	0.04651	0.04651	0.00847	0.00847	0.00000	0.00000	0.00000	0.00000	0.00000
1-Butanol	0.00040	0.00149	0.00149	0.00016	0.00016	0.00000	0.00000	0.00000	0.00000	0.00000
1-Butene	0.08348	0.31364	0.31364	0.07196	0.07196	0.00000	0.00000	0.00000	0.00000	0.00000
CO	0.11552	0.00000	0.00000	0.00000	0.00000	0.15742	0.00000	0.00000	0.68065	0.68065
CO2	0.01217	0.00000	0.00000	0.00000	0.00000	0.01659	0.00000	0.00000	0.07173	0.07173
DME	0.06794	0.25508	0.25508	0.23885	0.23885	0.00007	0.00008	0.00008	0.00000	0.00000
Ethane	0.02759	0.00000	0.00000	0.00000	0.00000	0.03760	0.00000	0.00000	0.16258	0.16258
Hydrogen	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Methane	0.01114	0.00000	0.00000	0.00000	0.00000	0.01518	0.00000	0.00000	0.06565	0.06565
Methanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Nitrogen	0.00046	0.00000	0.00000	0.00000	0.00000	0.00063	0.00000	0.00000	0.00274	0.00274
1-Pentene	0.07859	0.29527	0.29527	0.03444	0.03444	0.00000	0.00000	0.00000	0.00000	0.00000
Propane	0.00829	0.02184	0.02184	0.10436	0.10436	0.00337	0.00438	0.00438	0.00003	0.00003
Propene	0.58187	0.06558	0.06558	0.54170	0.54170	0.76913	0.99554	0.99554	0.01663	0.01663
H2O	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

5.4 Economic Analysis

An economic analysis was performed to calculate the plant economics within 5-10% accuracy. This analysis was done by using correlations and actual data found in the literature review.

5.4.1 MTP Base Case

Equipment used in the MTP base case PFD was used for analysis. The equipment, along with their respective size parameters, are listed in Table 49:

Table 49 MTP Base Case ISBL Cost Analysis

Fixed Capital Equipment	*S*	*S* Units	Jan. 2010 Cost	Lang Factor	ISBL Cost
C-201 Product Compressor	3,078	kW	$3,057,371.66	2.5	$7,643,429.15
C-202 Flue Gas Compressor	507.5	kW	$1,420,023.86	2.5	$3,550,059.66
CX-201 DME Cooler	853.9	m^2	$205,861.59	3.5	$720,515.57
CX-202A Reactor Cooler	852.5	m^2	$205,511.72	3.5	$719,291.01
CX-202B Reactor Cooler	852.5	m^2	$205,511.72	3.5	$719,291.01
CX-203 Product Cooler	886.3	m^2	$213,990.46	3.5	$748,966.60
CX-204A GC Condenser	514.4	m^2	$124,806.44	3.5	$436,822.54
CX-204B GC Condenser	514.4	m^2	$124,806.44	3.5	$436,822.54
CX-205 LGC Condenser	396.0	m^2	$98,733.96	3.5	$345,568.87
HX-201A MeOH Heater	668.2	m^2	$160,520.03	3.5	$561,820.10
HX-201B MeOH Heater	668.2	m^2	$160,520.03	3.5	$561,820.10
HX-202 GC Reboiler	300.1	m^2	$78,712.26	3.5	$275,492.91
HX-203 LGC Reboiler	37.37	m^2	$32,163.14	3.5	$112,571.01
P-201 Water Pump	5	L/s	$9,021.61	4	$36,086.43
P-202 Gasoline Pump	21	L/s	$11,717.14	4	$46,868.55
P-203 Propene Pump	34	L/s	$13,735.12	4	$54,940.47
V-201 Gasoline Column	56,360	kg	$382,967.81	4	$1,531,871.23
V-202 Light Gas Column	14,020	kg	$125,418.99	4	$501,675.96
V-203 Phase Separator	3,890	kg	$45,099.47	4	$180,397.89
V-204AB Dryers	1.842	m^2	$33,194.91	4	$132,779.65
VT-201 GC Trays	6.706	m	$13,653.44	2.5	$34,133.59
VT-202 LGC Trays	4.420	m	$6,515.76	2.5	$16,289.41
				Total	$19,367,514.24

The ISBL was then used to calculate the TCI. It was assumed that the ISBL made up 30% of the TCI. Similarly, OSBL and EEC was 30% of the TCI. The remaining 10% of the TCI made up the contingency cost.

Table 50 MTP Base Case Capital Costs

Capital Costs	Cost	%TCI
ISBL	$19,367,514.24	30%
OSBL	$19,367,514.24	30%
EEC	$19,367,514.24	30%
Contingency	$6,455,838.08	10%
TCI	$64,558,380.80	100%

The TCI cost listed above in Table 50 is the TCI without the reactor. The MTP reactor was calculated based off the FCC reactor cost, as shown in Table 51:

Table 51 FCC Plant Reactors Cost

FCC Plant Reactor (TCI)	S_R	Units for S_R	Jan. 2002 Cost
Plant Capacity	288,200	kg/hr	$100,796,901.23
No. Reactor & Regen.	2	----	**----**
		Total	$201,593,802.47

The FCC reactors cost and the TCI without the reactors cost was then summed to find the MTP base case TCI in Table 52:

Table 52 MTP Base Case Total Capital Investment

Year	January 2002	January 2010	November 2017
CEPCI	395.6	532.9	573.2
TCI Reactors & Regen.	$201,593,802.47		$292,096,985.78
Other Equipment TCI		$64,558,380.80	$69,440,540.20
		TCI Total	$361,537,525.98

The MTP base utilities were calculated in HYSYS V10 utilities analysis and listed in Table 53:

Table 53 MTP Base Case Utilities

Utility	Fluid	Rate		Unit Cost		Cost Rate	
Electricity	----	4377	kWh/hr	0.0775	$/kWh	339.19	$/hr
Cooling Water	Water	4785	m^3/hr	0.0317	$/$m^3$	151.68	$/hr
Refrigerant - Propane	Refrigerant	157.5	tonne/hr	0.0639	$/tonne	10.07	$/hr
Refrigerant - Ethane	Refrigerant	221.7	tonne/hr	0.0397	$/tonne	8.80	$/hr
Refrigerant - Freon 12	Refrigerant	4071	tonne/hr	0.1874	$/tonne	762.86	$/hr
Steam @100PSI	Steam	74.90	tonne/hr	17.946	$/tonne	1344.13	$/hr
					Total	2616.72	$/hr

Total Utility Cost = 21.1 $MM/yr

The MTP base case ROI was determined with the data above using a MACRS depreciation method over 7 years and a tax rate of 30%, summarized in Figure 17.

REVENUES AND PRODUCTION COSTS

	$MM/yr
Main product revenue	$ 570
Byproduct revenue	311.0
Raw materials cost	735.0
Utilities cost	21.1
Consumables cost	
VC	445.1
Salary and overheads	
Maintenance	
Interest	
Royalties	
FC	0.0

CAPITAL COSTS

	$MM
ISBL Capital Cost	109.0
OSBL Capital Cost	109.0
Engineering Costs	109.0
Contingency	35.0
Total Fixed Capital Cost	362.0
Working Capital	54.3

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	0.3	
Cost of debt		Depreciation method	MACRS	
Cost of capital		Depreciation period	7	years

CASH FLOW ANALYSIS

All figures in $MM unless indicated

Project year	Cap Ex	Revenue	Total Cost	Gr. Profit	Depren	Taxbl Inc	Tax Paid	Cash Flow	PV of CF	NPV
1	90.5	0.0	0.0	0.0	0.0	0.0	0.0	-90.5	-90.5	-90.5
2	325.8	0.0	0.0	0.0	0.0	0.0	0.0	-325.8	-325.8	-416.3
3	0.0	285.0	222.6	62.4	51.7	10.7	0.0	62.4	62.4	-353.9
4	0.0	570.0	445.1	124.9	88.7	36.2	3.2	121.7	121.7	-232.2
5	0.0	570.0	445.1	124.9	63.3	61.5	10.9	114.0	114.0	-118.2
6	0.0	570.0	445.1	124.9	45.2	79.6	18.5	106.4	106.4	-11.8
7	0.0	570.0	445.1	124.9	32.3	92.5	23.9	101.0	101.0	89.2
8	0.0	570.0	445.1	124.9	32.3	92.6	27.8	97.1	97.1	186.3
9	0.0	570.0	445.1	124.9	32.3	92.5	27.8	97.1	97.1	283.3
10	0.0	570.0	445.1	124.9	16.1	108.7	27.8	97.1	97.1	380.5
11	0.0	570.0	445.1	124.9	0.0	124.9	32.6	92.2	92.2	472.7
12	0.0	570.0	445.1	124.9	0.0	124.9	37.5	87.4	87.4	560.1
13	0.0	570.0	445.1	124.9	0.0	124.9	37.5	87.4	87.4	647.5
14	0.0	570.0	445.1	124.9	0.0	124.9	37.5	87.4	87.4	734.9
15	0.0	570.0	445.1	124.9	0.0	124.9	37.5	87.4	87.4	822.3
16	0.0	570.0	445.1	124.9	0.0	124.9	37.5	87.4	87.4	909.7
17	0.0	570.0	445.1	124.9	0.0	124.9	37.5	87.4	87.4	997.1
18	0.0	570.0	445.1	124.9	0.0	124.9	37.5	87.4	87.4	1084.5
19	0.0	570.0	445.1	124.9	0.0	124.9	37.5	87.4	87.4	1171.9
20	-54.3	570.0	445.1	124.9	1.0	123.9	37.5	141.7	141.7	1313.6

ECONOMIC ANALYSIS

Average cash flow	98.1	$MM/yr	NPV	10 years	380.5	$MM	IRR	10 years	15.8%
Simple pay-back period	4.244117	yrs		15 years	822.3	$MM		15 years	20.2%
Return on investment (10 yrs)	13.80%			20 years	1313.6	$MM		20 years	21.5%
Return on investment (15 yrs)	19.20%								
Return on investment (20 yrs)	21.88%								
			NPV to yr	21	1313.6	$MM			

Figure 17 MTP Base Case ROI Calculations.

For personal curiosity, a simple sensitivity analysis was done on different price ranges for methanol and propylene. Methanol in China is priced near $300 per tonne [54]. With methanol potentially this low and propylene varying between $900 and $1000 per tonne, Figure 18 was created with a $362 MM MTP Plant:

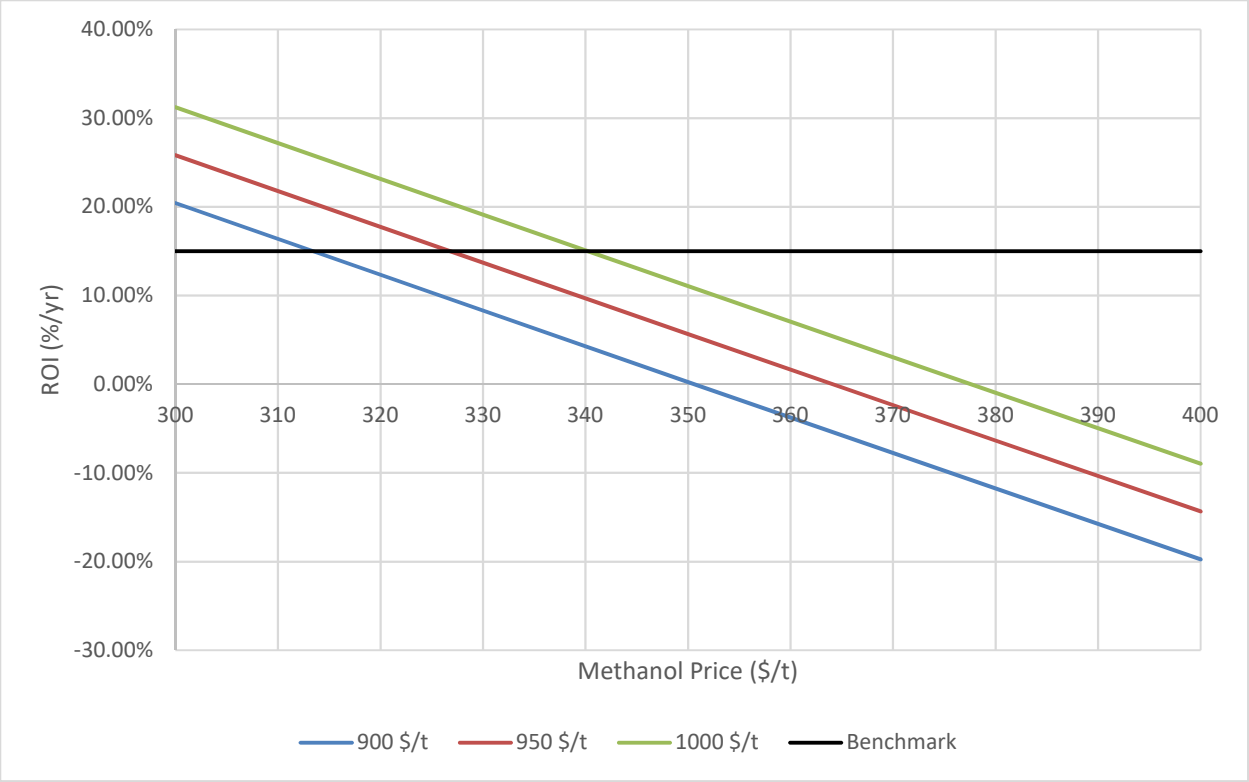


Figure 18 $362 MM Base MTP Plant ROI.

5.4.2 MTP Plant Comparison

The MTP plant found in the literature review was adjusted and compared to the base plant estimation to assess its cost accuracy, shown in Table 54.

Table 54 MTP Plant Comparison

Parameters	Value	Units
Capacity	520,000	t/a
Jan. 2002 CEPCI	395.6	----
Investment Cost	215	$MM
Case Study Capacity	600,000	t/a
Nov. 2017 CEPCI	573.2	----
Adjusted Investment Cost	344.3	$MM
Calculated TCI	362	$MM
Percent Difference	-5.128	%

The percent difference between the base case and the actual MTP plant (once adjusted for capacity and year) was approximately 5%. The estimated MTP plant from correlations was in the same ballpark as the actual MTP plant.

5.4.3 MTP Integrated Case

Equipment used in the MTP integrated case PFD was used for analysis. The equipment, along with their respective size parameters, are listed in Table 55:

Table 55 MTP Integrated Case ISBL Cost Analysis

Fixed Capital Equipment	*S*	*S* Units	Jan. 2010 Cost	Lang Factor	ISBL Cost
C-201 Product Compressor	3,931	kW	$3,449,008.41	2.5	$8,622,521.04
C-202 Flue Gas Compressor	507.6	kW	$1,420,123.17	2.5	$3,550,307.93
CX-201 DME Cooler	853.9	m^2	$205,861.59	3.5	$720,515.57
CX-202A Reactor Cooler	----	m^2	----	3.5	$0.00
CX-202B Reactor Cooler	----	m^2	----	3.5	$0.00
CX-203 Product Cooler	817.5	m^2	$196,802.58	3.5	$688,809.02
CX-204A GC Condenser	514.4	m^2	$124,806.44	3.5	$436,822.54
CX-204B GC Condenser	514.4	m^2	$124,806.44	3.5	$436,822.54
CX-205 LGC Condenser	396.1	m^2	$98,755.40	3.5	$345,643.89
HX-201A MeOH Heater	----	m^2	----	3.5	$0.00
HX-201B MeOH Heater	----	m^2	----	3.5	$0.00
HX-202 GC Reboiler	300.1	m^2	$78,712.26	3.5	$275,492.91
HX-203 LGC Reboiler	37.38	m^2	$32,164.48	3.5	$112,575.68
P-201 Water Pump	3	L/s	$8,645.09	4	$34,580.36
P-202 Gasoline Pump	21	L/s	$11,717.14	4	$46,868.55
P-203 Propene Pump	34	L/s	$13,735.12	4	$54,940.47
V-201 Gasoline Column	56,360	kg	$382,967.81	4	$1,531,871.23
V-202 Light Gas Column	14,020	kg	$125,418.99	4	$501,675.96
V-203 Phase Separator	5,570	kg	$57,552.03	4	$230,208.12
V-204AB Dryers	3.819	m^2	$50,070.66	4	$200,282.66
VT-201 GC Trays	6.706	m	$13,653.44	2.5	$34,133.59
VT-202 LGC Trays	4.420	m	$6,515.76	2.5	$16,289.41
EX-201 Feed Exchanger	730.85	m^2	$175,566.46	3.5	$614,482.61
				Total	$18,454,844.08

The ISBL was then used to calculate the TCI. It was assumed that the ISBL made up 30% of the TCI. Similarly, OSBL and EEC was 30% of the TCI. The remaining 10% of the TCI made up the contingency cost. All costs were listed in Table 56.

Table 56 MTP Integrated Case Capital Costs

Capital Costs	Cost	%TCI
ISBL	$18,454,844.08	30%
OSBL	$18,454,844.08	30%
EEC	$18,454,844.08	30%
Contingency	$6,151,614.69	10%
TCI	$61,516,146.95	100%

Since the operation of the MTP reactors did not change, the MTP reactors cost did not change as well. The FCC reactors cost and the TCI without the reactors cost was then summed to find the MTP integrated case TCI in Table 57:

Table 57 MTP Integrated Case Total Capital Investment

Year	January 2002	January 2010	November 2017
CEPCI	395.6	532.9	573.2
TCI Reactors & Regen.	$201,593,802.47		$292,096,985.78
Other Equipment TCI		$61,516,146.95	$66,168,240.63
		TCI Total	$358,265,226.41

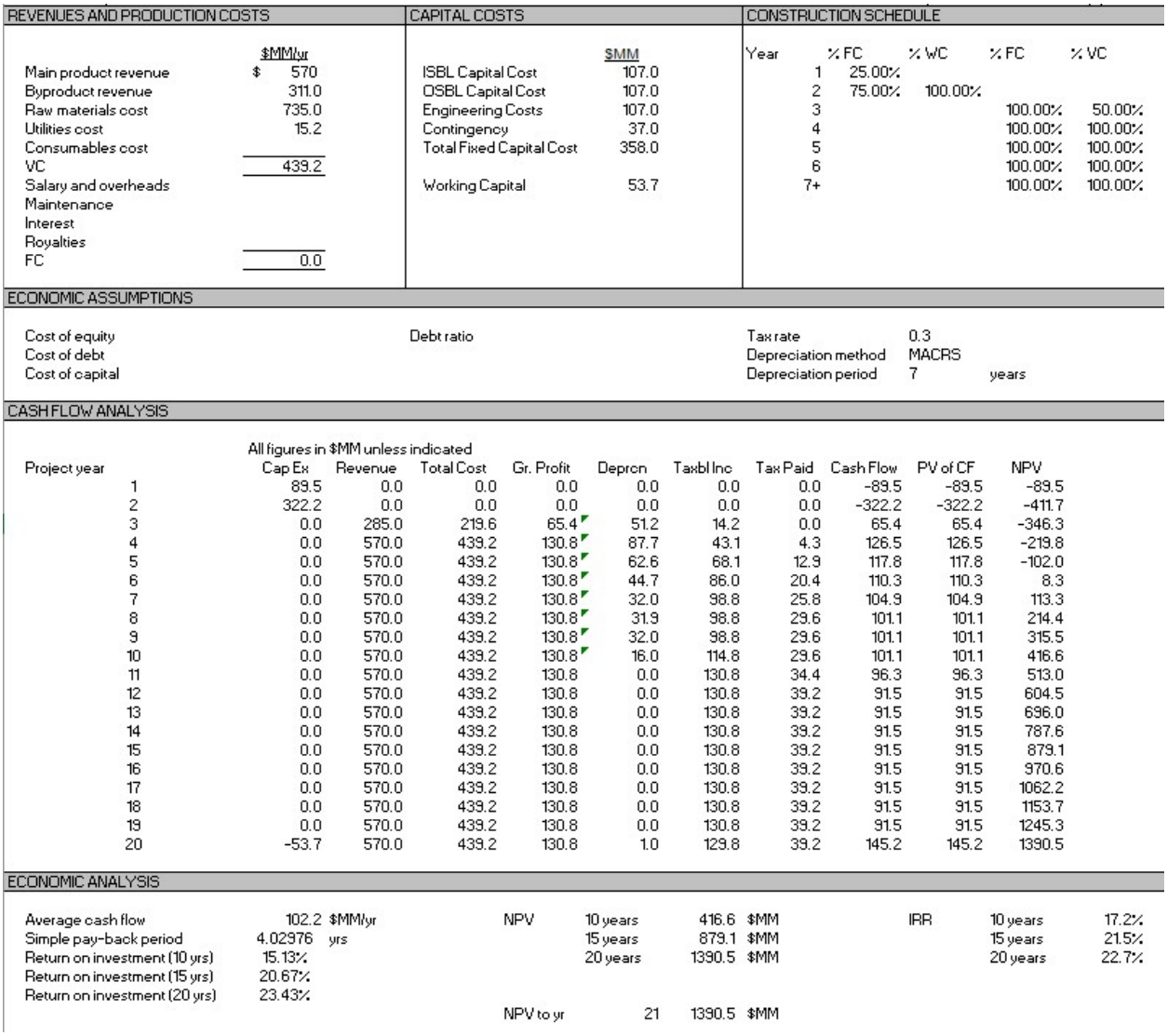
The MTP integrated case utilities were founded from Aspen HYSYS V10 utilities analysis and listed in Table 58:

Table 58 MTP Integrated Case Utilities

Utility	Fluid	Rate		Unit Cost		Cost Rate	
Electricity	----	4757	kWh/hr	0.0775	$/kWh	368.67	$/hr
Cooling Water	Water	4785	m^3/hr	0.0317	$/$m^3$	151.68	$/hr
Refrigerant - Propane	Refrigerant	194.1	tonne/hr	0.0639	$/tonne	12.41	$/hr
Refrigerant - Ethane	Refrigerant	221.7	tonne/hr	0.0397	$/tonne	8.80	$/hr
Refrigerant - Freon 12	Refrigerant	0	tonne/hr	0.1874	$/tonne	0.00	$/hr
Steam @100PSI	Steam	74.91	tonne/hr	17.946	$/tonne	1344.22	$/hr
					Total	1885.78	$/hr

Total Utility Cost = 15.2 $MM/yr

The MTP integrated case ROI was determined with the data above using a MACRS depreciation method over 7 years and a tax rate of 30%, summarized in Figure 19.



REVENUES AND PRODUCTION COSTS

	$MM/yr
Main product revenue	$ 570
Byproduct revenue	311.0
Raw materials cost	735.0
Utilities cost	15.2
Consumables cost	
VC	439.2
Salary and overheads	
Maintenance	
Interest	
Royalties	
FC	0.0

CAPITAL COSTS

	$MM
ISBL Capital Cost	107.0
OSBL Capital Cost	107.0
Engineering Costs	107.0
Contingency	37.0
Total Fixed Capital Cost	358.0
Working Capital	53.7

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	0.3	
Cost of debt		Depreciation method	MACRS	
Cost of capital		Depreciation period	7	years

CASH FLOW ANALYSIS

All figures in $MM unless indicated

Project year	Cap Ex	Revenue	Total Cost	Gr. Profit	Depron	Taxbl Inc	Tax Paid	Cash Flow	PV of CF	NPV
1	89.5	0.0	0.0	0.0	0.0	0.0	0.0	-89.5	-89.5	-89.5
2	322.2	0.0	0.0	0.0	0.0	0.0	0.0	-322.2	-322.2	-411.7
3	0.0	285.0	219.6	65.4	51.2	14.2	0.0	65.4	65.4	-346.3
4	0.0	570.0	439.2	130.8	87.7	43.1	4.3	126.5	126.5	-219.8
5	0.0	570.0	439.2	130.8	62.6	68.1	12.9	117.8	117.8	-102.0
6	0.0	570.0	439.2	130.8	44.7	86.0	20.4	110.3	110.3	8.3
7	0.0	570.0	439.2	130.8	32.0	98.8	25.8	104.9	104.9	113.3
8	0.0	570.0	439.2	130.8	31.9	98.8	29.6	101.1	101.1	214.4
9	0.0	570.0	439.2	130.8	32.0	98.8	29.6	101.1	101.1	315.5
10	0.0	570.0	439.2	130.8	16.0	114.8	29.6	101.1	101.1	416.6
11	0.0	570.0	439.2	130.8	0.0	130.8	34.4	96.3	96.3	513.0
12	0.0	570.0	439.2	130.8	0.0	130.8	39.2	91.5	91.5	604.5
13	0.0	570.0	439.2	130.8	0.0	130.8	39.2	91.5	91.5	696.0
14	0.0	570.0	439.2	130.8	0.0	130.8	39.2	91.5	91.5	787.6
15	0.0	570.0	439.2	130.8	0.0	130.8	39.2	91.5	91.5	879.1
16	0.0	570.0	439.2	130.8	0.0	130.8	39.2	91.5	91.5	970.6
17	0.0	570.0	439.2	130.8	0.0	130.8	39.2	91.5	91.5	1062.2
18	0.0	570.0	439.2	130.8	0.0	130.8	39.2	91.5	91.5	1153.7
19	0.0	570.0	439.2	130.8	0.0	130.8	39.2	91.5	91.5	1245.3
20	-53.7	570.0	439.2	130.8	1.0	129.8	39.2	145.2	145.2	1390.5

ECONOMIC ANALYSIS

Average cash flow	102.2	$MM/yr	NPV	10 years	416.6	$MM	IRR	10 years	17.2%
Simple pay-back period	4.02976	yrs		15 years	879.1	$MM		15 years	21.5%
Return on investment (10 yrs)	15.13%			20 years	1390.5	$MM		20 years	22.7%
Return on investment (15 yrs)	20.67%								
Return on investment (20 yrs)	23.43%								
			NPV to yr	21	1390.5	$MM			

Figure 19 MTP Heat Integrated ROI Calculations.

Similar to before, a simple sensitivity analysis was completed on the price ranges for methanol and propylene. The basis for this set of calculations was the $358 MM Integrated MTP Plant instead of the $362 MM Base MTP Plant in Figure 20:

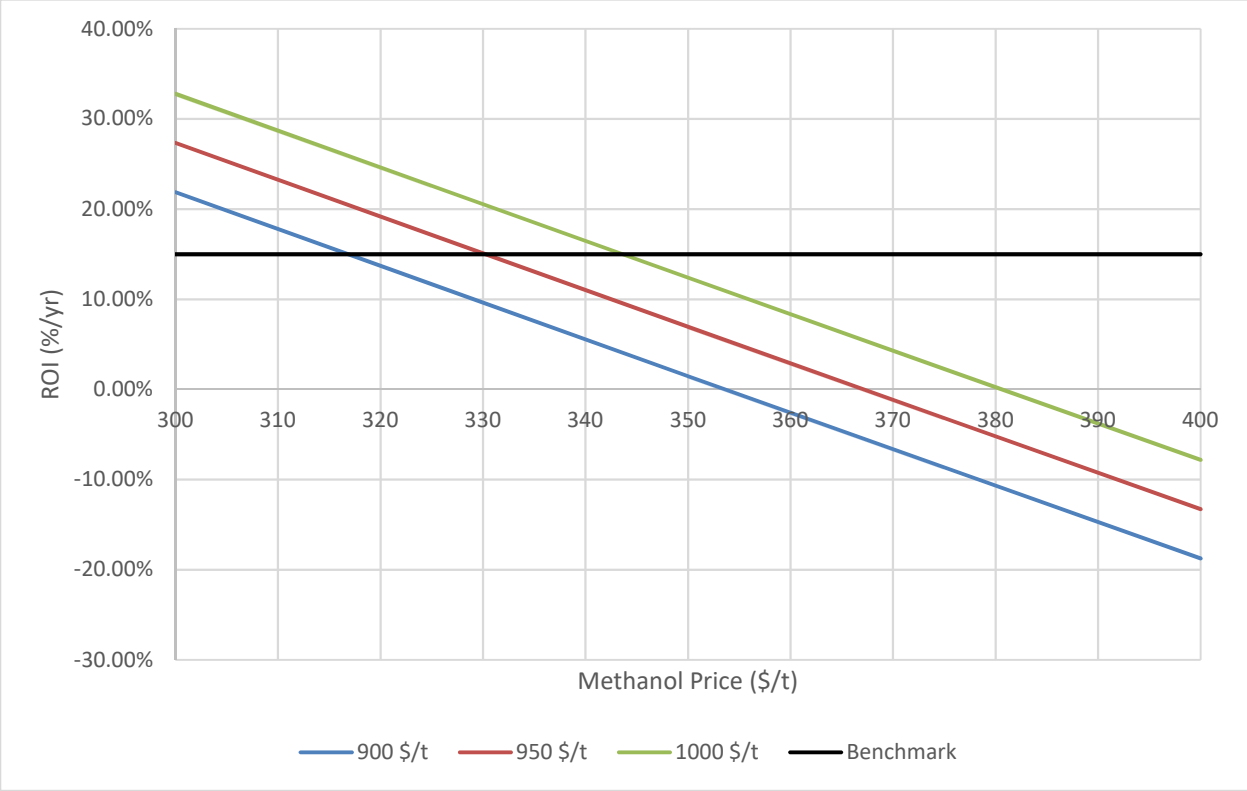


Figure 20 $358 MM Integrated MTP Plant ROI.

5.5 Environmental Analysis

An environmental analysis was performed to calculate the cases' environmental impact. This analysis was done by using correlations and actual data found in the literature review. The water reduction was found through the savings difference in cooling water and steam and listed in Table 59:

Table 59 MTP Water Reduction Analysis

Water Reduction	Base	Integrated	Units
Cooling Water	0.019	0.019	10^6 kg/h
Steam @ 100PSI	0.075	0.075	10^6 kg/h
Net	0.094260626	0.094260626	10^6 kg/h
Savings		0	10^6 kg/h

The ERCOT (Texas) ratio of CO_2 emissions and N2O emissions to power is 1142.8 lbm/MWh and 11.6 lbm/GWh respectively [55]. The electricity reduction was found through the savings difference in electricity usage and listed Table 60:

Table 60 MTP Electricity Reduction Analysis

Electricity Reduction	Base	Integrated	Units
Usage	4376.608	4757.006	kW
	4.377	4.757	MW
Savings		-0.380	MW

The fuel savings were calculated through the savings difference in heat flow usage and listed in Table 61:

Table 61 MTP Fuel Savings from Natural Gas Analysis

Fuel Savings (NG)	Base	Integrated	Units
HX-201	525911010.4	0	kJ/hr
HX-202	134808770.8	134812846.7	kJ/hr
HX-203	19980812.47	19987159.31	kJ/hr
Net	680700593.7	154800006	kJ/hr
	189.0834982	43.00000167	MW
Savings		146.0834966	MW

The emission factors for industrial heaters was provided by the U.S. EPA [56]. The carbon emissions were found through the sum of natural gas combustion, electricity consumption, and flaring waste streams and listed in Table 62:

Table 62 MTP Overall CO_2 Emissions Analysis

Overall CO_2 Emissions	**Base**	**Integrated**	**Units**
Natural Gas Combustion	343.1921607	78.04627912	10^3 tons/yr
Electricity Consumption	2.500793811	2.718153228	10^3 tons/yr
Flaring Waste Streams	0.030796934	0.030801189	10^3 tons/yr
Net	345.7237514	80.79523354	10^3 tons/yr
Savings		264.9285179	10^3 tons/yr

Similarly, the VOC emissions were found through the sum of natural gas combustion, electricity consumption, and flaring waste streams and listed in Table 63:

Table 63 MTP Overall VOC Emissions Analysis

Overall VOC Emissions	**Base**	**Integrated**	**Units**
Natural Gas Combustion	50.73524108	10.50559989	tons/yr
Electricity Consumption	2.53843E-05	2.75906E-05	tons/yr
Flaring Waste Streams	0	0	tons/yr
Net	50.73526647	10.50562748	tons/yr
Savings		40.22963899	tons/yr

Lastly, the refrigerant savings were found through the savings difference in refrigerant usage of propane, ethane, and Freon 12 and listed in Table 64:

Table 64 MTP Refrigerant Savings Analysis

Refrigerant Savings	Base	Integrated	Units
Refrigerant - Propane	0.157478341	0.194086101	10^6 kg/h
Refrigerant - Ethane	0.22168918	0.221699114	10^6 kg/h
Refrigerant - Freon 12	4.071176439	0	10^6 kg/h
Net	4.45034396	0.415785215	10^6 kg/h
Savings		4.034558745	10^6 kg/h

5.6 Safety Analysis

A safety analysis was performed to track the safety impact of each case. The means and indicators for PSI and PRI were found for each case and every stream. Water streams were neglected. A summary of the PSI and PRI values for each case are presented in Table 65:

Table 65 Safety Indicator Summary

Social	PSI	PRI
MTP Base Case	21.97	10.60
MTP Heat Integrated Case	22.90	10.17
PDH Base + WHR Case	48.29	60.17
PDH Integrated Case	56.61	43.46
PDH Integrated + Intensified Case	55.86	38.63
Targets	28.31	30.09

The target for these indicators are arbitrarily determined by the user of the study, since the safety comparison between cases is relative. The targets were selected as 50% of the worst case listed.

5.7 Social Analysis

Based on the chemicals listed in the literature review, the following chemicals were considered in the social analysis in Table 66 and Table 67:

Table 66 Oleflex PDH Chemicals List

Stream	Feed Treatment	Reactor/CCR	SHP	Dehydrogenation
Hydrogen	Sulfur Removal	DEH-16	Ni	UI-94
Methane	(H2S)	DEH-14	W	
Ethylene	(SO2)	(Pt-Al2O3)	Al2O3	
Ethane	(COS)	DMDS		
Propene	(CS2)	Coke		
Propane	(CO2)			
Propadiene	ADS-120			
m-Aceylene	Hg Removal			
i-Butane	(Hg)			
n-Butane	Arsine Removal			
Benzene	(As)			
Toluene	(AsH3)			
	GB-236 Abs.			
	GB-238 Ads.			
	(Cu)			
	(NH3)			
	Phosphine Removal			
	(PH3)			

Table 67 Lurgi MTP Chemicals List

Stream	Feed Treatment	Reactor	Dehydration
Hydrogen	S Removal	ZSM-5	UI-94
Water	(H2S)	(SiO2)	
Methane	(SO2)	(Al2O3)	
Nitrogen	(COS)	DME	
Ethane	(CS2)	Coke	
Propane	(CO2)		
CO	ADS-120		
Methanol	Hg Removal		
Butanol	(Hg)		
DME	Arsine Removal		
Acetone	(As)		
Oxygen	(AsH3)		
CO2	GB-236 Abs.		
Propene	GB-238 Ads.		
Propadiene	(Cu)		
	(NH3)		
	Phosphine Removal		
	(PH3)		

Next, the chemical toxicity was sought for in OSHA's PEL table and listed in Table 68 and Table 69:

Table 68 OEL-TWA List for Oleflex PDH Chemicals adapted from [57]

Chemical List	OSHA Name	PEL (ppm)	PEL (mg/M3)	MW	OELTWA (ppm)
m-Aceylene	Acetylene	(h)	---	---	30000
Al2O3	Aluminum metal and oxide (total dust)	---	10	101.961	2.4
NH3	Ammonia	25	18	---	25
As	Arsenic, organic compounds as As	---	0.2	74.922	0.07
AsH3	Arsine	0.05	0.2	---	0.05
Benzene	Benzene	1	---	---	1
i-Butane	Butane	800	1900	---	800
n-Butane	Butane	800	1900	---	800
CO2	Carbon dioxide	5000	9000	---	5000
CS2	Carbon disulfide	1	3	---	1
COS	Carbonyl sulfide	---	---	---	---
Coke	Coke oven emissions	---	0.15	12.011	0.31
Cu	Copper metal fume, as Cu	---	0.1	63.546	0.04
DMDS	Dimethyl disulfide	12.5	---	---	12.5
Ethane	Ethane	(h)	---	---	30000
Ethylene	Ethylene	(h)	---	---	30000
Hydrogen	Hydrogen	(h)	----	---	30000
H2S	Hydrogen sulfide	10	14	---	10
Hg	Mercury aryl compounds as Hg	---	0.01	200.59	0.0012
Methane	Methane	(h)	---	---	30000
Ni	Nickel metal, as Ni	---	0.5	58.693	0.21
PH3	Phosphine	0.3	0.4	---	0.3
Pt	Platinum metal, as Pt	---	1	195.08	0.13
Propadiene	Methylacetylene, propyne	1000	1650	---	1000
Propane	Propane	1000	1800	---	1000
Propene	Propylene	(h)	---	---	30000
SO2	Sulfur dioxide	2	5	---	2
Toluene	Toluene, toluol	10	37	---	10
W	Tungsten metal, as W	---	5	193.84	0.63

Table 69 OEL-TWA List for Lurgi MTP Chemicals adapted from [57]

Chemical List	OSHA Name	PEL (ppm)	PEL (mg/M3)	MW	OELTWA (ppm)
Acetone	Acetone	500	---	---	500
Al2O3	Aluminum metal and oxide (total dust)	---	10	101.961	2.4
Butanol	n-Butyl alcohol; 1-butanol	50	---	---	50
N2	Nitrogen	(h)	---	---	30000
NH3	Ammonia	25	18	---	25
As	Arsenic, organic compounds as As	---	0.2	74.922	0.07
AsH3	Arsine	0.05	0.2	---	0.05
CO2	Carbon dioxide	5000	9000	---	5000
CS2	Carbon disulfide	1	3	---	1
COS	Carbonyl sulfide	---	---	---	---
Coke	Coke oven emissions	---	0.15	12.011	0.31
Cu	Copper metal fume, as Cu	---	0.1	63.546	0.04
DME	Dimethyl ether	1000	---	---	1000
Ethane	Ethane	(h)	---	---	30000
Hydrogen	Hydrogen	(h)	----	---	30000
H2S	Hydrogen sulfide	10	14	---	10
Hg	Mercury aryl compounds as Hg	---	0.01	200.59	0.0012
Methane	Methane	(h)	---	---	30000
Methanol	Methanol	200	---	---	200
Oxygen	Oxygen	(h)	---	---	30000
PH3	Phosphine	0.3	0.4	---	0.3
Propadiene	Methylacetylene, propyne	1000	1650	---	1000
Propane	Propane	1000	1800	---	1000
Propene	Propylene	(h)	---	---	30000
SiO2	Silica, fused, respirable dust	---	0.1	60.083	0.0407
SO2	Sulfur dioxide	2	5	---	2
Water	Water (gas)	(h)	---	---	30000

(h)OSHA notes that for compounds like acetylene, methane, ethane, etc. “a number of gases and vapors, when present in high concentrations, act primarily as asphyxiants without other adverse effects.

A concentration limit is not included for each material because the limiting factor is the available oxygen. (Several of these materials present fire or explosion hazards.)” [57]. Therefore, it is assumed the OEL-TWA of these components is 30,000 ppm.

Air has an oxygen concentration of about 22.0 mol%. For an adult person, some unnoticeable adverse physiological effects appears when the oxygen concentration is 19.0 mol%. If the presence of a new chemical were to make up the 3 mol% difference, then it can be assumed the concentration for gases that cause asphyxiation is 30,000 ppm.

The chemicals listed above were used along with the EHI equations to determine the individual EHI_p. Table 70 lists the individual EHI calculations for the Oleflex PDH Base Case EHI Analysis:

Table 70 Oleflex PDH Base Case EHI Analysis

Chemicals	OELTWA (ppm)	ED (min)	N	Control Measure	MI_i	PI_i	TI_i	EI_i	PDI_i	EHI_i
m-Aceylene	30000	65.8823529	0	CM2	0.18	0.42	0.80	0.1478	0.92	0.110
Al2O3	2.4	23.5294118	1	CM3	0.39	0.61	13.74	0.0504	0.76	0.528
NH3	25	23.5294118	1	CM3	0.39	0.61	6.78	0.0504	0.76	0.261
As	0.07	23.5294118	1	CM3	0.39	0.61	39.81	0.0504	0.76	1.529
AsH3	0.05	23.5294118	1	CM3	0.39	0.61	44.05	0.0504	0.76	1.692
Benzene	1	65.8823529	1	CM3	0.39	0.61	17.88	0.1478	0.76	2.014
i-Butane	800	65.8823529	0	CM2	0.18	0.42	2.39	0.1478	0.92	0.327
n-Butane	800	65.8823529	0	CM2	0.18	0.42	2.39	0.1478	0.92	0.327
CO2	5000	65.8823529	0	CM2	0.18	0.42	1.38	0.1478	0.92	0.188
CS2	1	65.8823529	1	CM3	0.39	0.61	17.88	0.1478	0.76	2.014
Coke	0.31	23.5294118	1	CM3	0.39	0.61	25.43	0.0504	0.76	0.977
Cu	0.04	23.5294118	1	CM3	0.39	0.61	47.11	0.0504	0.76	1.810
DMDS	12.5	65.8823529	1	CM3	0.39	0.61	8.36	0.1478	0.76	0.942
Ethane	30000	65.8823529	0	CM2	0.18	0.42	0.80	0.1478	0.92	0.110
Ethylene	30000	65.8823529	0	CM2	0.18	0.42	0.80	0.1478	0.92	0.110
Hydrogen	30000	65.8823529	0	CM2	0.18	0.42	0.80	0.1478	0.92	0.110
H2S	10	65.8823529	1	CM3	0.39	0.61	8.94	0.1478	0.76	1.007
Hg	0.0012	23.5294118	2	CM3	0.60	0.61	135.38	0.0504	0.63	4.327
Methane	30000	65.8823529	0	CM2	0.18	0.42	0.80	0.1478	0.92	0.110
Ni	0.21	23.5294118	1	CM3	0.39	0.61	28.60	0.0504	0.76	1.099
PH3	0.3	65.8823529	1	CM3	0.39	0.61	25.69	0.1478	0.76	2.894
Pt	0.13	23.5294118	1	CM3	0.39	0.61	33.04	0.0504	0.76	1.269
Propadiene	1000	65.8823529	0	CM2	0.18	0.42	2.23	0.1478	0.92	0.305
Propane	1000	65.8823529	0	CM2	0.18	0.42	2.23	0.1478	0.92	0.305
Propene	30000	65.8823529	0	CM2	0.18	0.42	0.80	0.1478	0.92	0.110
SO2	2	65.8823529	1	CM3	0.39	0.61	14.51	0.1478	0.76	1.635
Toluene	10	65.8823529	0	CM2	0.18	0.42	8.94	0.1478	0.92	1.221
W	0.63	23.5294118	1	CM3	0.39	0.61	20.54	0.0504	0.76	0.789
									EHI_p	28.119

Table 71 lists the individual EHI calculations for the Oleflex PDH Integrated Case EHI Analysis:

Table 71 Oleflex PDH Integrated Case EHI Analysis

Chemicals	OELTWA (ppm)	ED (min)	N	Control Measure	MI_i	PI_i	TI_i	EI_i	PDI_i	EHI_i
m-Aceylene	30000	62.3529412	0	CM2	0.18	0.42	0.80	0.1397	0.92	0.104
Al2O3	2.4	23.5294118	1	CM3	0.39	0.61	13.74	0.0504	0.76	0.528
NH3	25	23.5294118	1	CM3	0.39	0.61	6.78	0.0504	0.76	0.261
As	0.07	23.5294118	1	CM3	0.39	0.61	39.81	0.0504	0.76	1.529
AsH3	0.05	23.5294118	1	CM3	0.39	0.61	44.05	0.0504	0.76	1.692
Benzene	1	62.3529412	1	CM3	0.39	0.61	17.88	0.1397	0.76	1.903
i-Butane	800	62.3529412	0	CM2	0.18	0.42	2.39	0.1397	0.92	0.309
n-Butane	800	62.3529412	0	CM2	0.18	0.42	2.39	0.1397	0.92	0.309
CO2	5000	62.3529412	0	CM2	0.18	0.42	1.38	0.1397	0.92	0.178
CS2	1	62.3529412	1	CM3	0.39	0.61	17.88	0.1397	0.76	1.903
Coke	0.31	23.5294118	1	CM3	0.39	0.61	25.43	0.0504	0.76	0.977
Cu	0.04	23.5294118	1	CM3	0.39	0.61	47.11	0.0504	0.76	1.810
DMDS	12.5	62.3529412	1	CM3	0.39	0.61	8.36	0.1397	0.76	0.890
Ethane	30000	62.3529412	0	CM2	0.18	0.42	0.80	0.1397	0.92	0.104
Ethylene	30000	62.3529412	0	CM2	0.18	0.42	0.80	0.1397	0.92	0.104
Hydrogen	30000	62.3529412	0	CM2	0.18	0.42	0.80	0.1397	0.92	0.104
H2S	10	62.3529412	1	CM3	0.39	0.61	8.94	0.1397	0.76	0.952
Hg	0.0012	23.5294118	2	CM3	0.60	0.61	135.38	0.0504	0.63	4.327
Methane	30000	62.3529412	0	CM2	0.18	0.42	0.80	0.1397	0.92	0.104
Ni	0.21	23.5294118	1	CM3	0.39	0.61	28.60	0.0504	0.76	1.099
PH3	0.3	62.3529412	1	CM3	0.39	0.61	25.69	0.1397	0.76	2.735
Pt	0.13	23.5294118	1	CM3	0.39	0.61	33.04	0.0504	0.76	1.269
Propadiene	1000	62.3529412	0	CM2	0.18	0.42	2.23	0.1397	0.92	0.289
Propane	1000	62.3529412	0	CM2	0.18	0.42	2.23	0.1397	0.92	0.289
Propene	30000	62.3529412	0	CM2	0.18	0.42	0.80	0.1397	0.92	0.104
SO2	2	62.3529412	1	CM3	0.39	0.61	14.51	0.1397	0.76	1.545
Toluene	10	62.3529412	0	CM2	0.18	0.42	8.94	0.1397	0.92	1.154
W	0.63	23.5294118	1	CM3	0.39	0.61	20.54	0.0504	0.76	0.789
									EHP_p	27.359

Table 72 lists the individual EHI calculations for the Oleflex PDH Integrated & Intensified Case EHI Analysis:

Table 72 Oleflex PDH Integrated & Intensified Case EHI Analysis

Chemicals	OELTWA (ppm)	ED (min)	N	Control Measure	MI_i	PI_i	TI_i	EI_i	PDI_i	EHI_i
m-Aceylene	30000	63.7647059	0	CM2	0.18	0.42	0.80	0.1430	0.92	0.106
Al2O3	2.4	23.5294118	1	CM3	0.39	0.61	13.74	0.0504	0.76	0.528
NH3	25	23.5294118	1	CM3	0.39	0.61	6.78	0.0504	0.76	0.261
As	0.07	23.5294118	1	CM3	0.39	0.61	39.81	0.0504	0.76	1.529
AsH3	0.05	23.5294118	1	CM3	0.39	0.61	44.05	0.0504	0.76	1.692
Benzene	1	63.7647059	1	CM3	0.39	0.61	17.88	0.1430	0.76	1.948
i-Butane	800	63.7647059	0	CM2	0.18	0.42	2.39	0.1430	0.92	0.316
n-Butane	800	63.7647059	0	CM2	0.18	0.42	2.39	0.1430	0.92	0.316
CO2	5000	63.7647059	0	CM2	0.18	0.42	1.38	0.1430	0.92	0.182
CS2	1	63.7647059	1	CM3	0.39	0.61	17.88	0.1430	0.76	1.948
Coke	0.31	23.5294118	1	CM3	0.39	0.61	25.43	0.0504	0.76	0.977
Cu	0.04	23.5294118	1	CM3	0.39	0.61	47.11	0.0504	0.76	1.810
DMDS	12.5	63.7647059	1	CM3	0.39	0.61	8.36	0.1430	0.76	0.911
Ethane	30000	63.7647059	0	CM2	0.18	0.42	0.80	0.1430	0.92	0.106
Ethylene	30000	63.7647059	0	CM2	0.18	0.42	0.80	0.1430	0.92	0.106
Hydrogen	30000	63.7647059	0	CM2	0.18	0.42	0.80	0.1430	0.92	0.106
H2S	10	63.7647059	1	CM3	0.39	0.61	8.94	0.1430	0.76	0.974
Hg	0.0012	23.5294118	2	CM3	0.60	0.61	135.38	0.0504	0.63	4.327
Methane	30000	63.7647059	0	CM2	0.18	0.42	0.80	0.1430	0.92	0.106
Ni	0.21	23.5294118	1	CM3	0.39	0.61	28.60	0.0504	0.76	1.099
PH3	0.3	63.7647059	1	CM3	0.39	0.61	25.69	0.1430	0.76	2.798
Pt	0.13	23.5294118	1	CM3	0.39	0.61	33.04	0.0504	0.76	1.269
Propadiene	1000	63.7647059	0	CM2	0.18	0.42	2.23	0.1430	0.92	0.295
Propane	1000	63.7647059	0	CM2	0.18	0.42	2.23	0.1430	0.92	0.295
Propene	30000	63.7647059	0	CM2	0.18	0.42	0.80	0.1430	0.92	0.106
SO2	2	63.7647059	1	CM3	0.39	0.61	14.51	0.1430	0.76	1.581
Toluene	10	63.7647059	0	CM2	0.18	0.42	8.94	0.1430	0.92	1.181
W	0.63	23.5294118	1	CM3	0.39	0.61	20.54	0.0504	0.76	0.789
									EHI_p	27.663

Table 73 lists the individual EHI calculations for the Lurgi MTP Base Case EHI Analysis:

Table 73 Lurgi MTP Base Case EHI Analysis

Chemicals	OELTWA (ppm)	ED (min)	N	Control Measure	MI_i	PI_i	TI_i	EI_i	PDI_i	EHI_i
Acetone	500	65.8823529	0	CM2	0.18	0.42	2.75	0.1478	0.92	0.376
Al2O3	2.4	23.5294118	1	CM3	0.39	0.61	13.74	0.0504	0.76	0.528
Butanol	50	65.8823529	0	CM2	0.18	0.42	5.51	0.1478	0.92	0.752
N2	30000	65.8823529	0	CM2	0.18	0.42	0.80	0.1478	0.92	0.110
NH3	25	23.5294118	1	CM3	0.39	0.61	6.78	0.0504	0.76	0.261
As	0.07	23.5294118	1	CM3	0.39	0.61	39.81	0.0504	0.76	1.529
AsH3	0.05	23.5294118	1	CM3	0.39	0.61	44.05	0.0504	0.76	1.692
CO2	5000	65.8823529	0	CM2	0.18	0.42	1.38	0.1478	0.92	0.188
CS2	1	65.8823529	1	CM3	0.39	0.61	17.88	0.1478	0.76	2.014
Coke	0.31	23.5294118	1	CM3	0.39	0.61	25.43	0.0504	0.76	0.977
Cu	0.04	23.5294118	1	CM3	0.39	0.61	47.11	0.0504	0.76	1.810
DME	1000	65.8823529	0	CM2	0.18	0.42	2.23	0.1478	0.92	0.305
Ethane	30000	65.8823529	0	CM2	0.18	0.42	0.80	0.1478	0.92	0.110
Hydrogen	30000	65.8823529	0	CM2	0.18	0.42	0.80	0.1478	0.92	0.110
H2S	10	65.8823529	1	CM3	0.39	0.61	8.94	0.1478	0.76	1.007
Hg	0.0012	23.5294118	2	CM3	0.60	0.61	135.38	0.0504	0.63	4.327
Methane	30000	65.8823529	0	CM2	0.18	0.42	0.80	0.1478	0.92	0.110
Methanol	200	65.8823529	0	CM2	0.18	0.42	3.63	0.1478	0.92	0.496
Oxygen	30000	65.8823529	0	CM2	0.18	0.42	0.80	0.1478	0.92	0.110
PH3	0.3	65.8823529	1	CM3	0.39	0.61	25.69	0.1478	0.76	2.894
Propadiene	1000	65.8823529	0	CM2	0.18	0.42	2.23	0.1478	0.92	0.305
Propane	1000	65.8823529	0	CM2	0.18	0.42	2.23	0.1478	0.92	0.305
Propene	30000	65.8823529	0	CM2	0.18	0.42	0.80	0.1478	0.92	0.110
SiO2	0.0407	23.5294118	2	CM3	0.60	0.61	46.86	0.0504	0.63	1.498
SO2	2	65.8823529	1	CM3	0.39	0.61	14.51	0.1478	0.76	1.635
Water	30000	65.8823529	0	CM2	0.18	0.42	0.80	0.1478	0.92	0.110
									EHI_p	23.669

Table 74 lists the individual EHI calculations for the Lurgi MTP Integrated Case EHI Analysis:

Table 74 Lurgi MTP Integrated Case EHI Analysis

Chemicals	OELTWA (ppm)	ED (min)	N	Control Measure	MI_i	PI_i	TI_i	EI_i	PDI_i	EHI_i
Acetone	500	62.3529412	0	CM2	0.18	0.42	2.75	0.1397	0.92	0.356
Al2O3	2.4	23.5294118	1	CM3	0.39	0.61	13.74	0.0504	0.76	0.528
Butanol	50	62.3529412	0	CM2	0.18	0.42	5.51	0.1397	0.92	0.711
N2	30000	62.3529412	0	CM2	0.18	0.42	0.80	0.1397	0.92	0.104
NH3	25	23.5294118	1	CM3	0.39	0.61	6.78	0.0504	0.76	0.261
As	0.07	23.5294118	1	CM3	0.39	0.61	39.81	0.0504	0.76	1.529
AsH3	0.05	23.5294118	1	CM3	0.39	0.61	44.05	0.0504	0.76	1.692
CO2	5000	62.3529412	0	CM2	0.18	0.42	1.38	0.1397	0.92	0.178
CS2	1	62.3529412	1	CM3	0.39	0.61	17.88	0.1397	0.76	1.903
Coke	0.31	23.5294118	1	CM3	0.39	0.61	25.43	0.0504	0.76	0.977
Cu	0.04	23.5294118	1	CM3	0.39	0.61	47.11	0.0504	0.76	1.810
DME	1000	62.3529412	0	CM2	0.18	0.42	2.23	0.1397	0.92	0.289
Ethane	30000	62.3529412	0	CM2	0.18	0.42	0.80	0.1397	0.92	0.104
Hydrogen	30000	62.3529412	0	CM2	0.18	0.42	0.80	0.1397	0.92	0.104
H2S	10	62.3529412	1	CM3	0.39	0.61	8.94	0.1397	0.76	0.952
Hg	0.0012	23.5294118	2	CM3	0.60	0.61	135.38	0.0504	0.63	4.327
Methane	30000	62.3529412	0	CM2	0.18	0.42	0.80	0.1397	0.92	0.104
Methanol	200	62.3529412	0	CM2	0.18	0.42	3.63	0.1397	0.92	0.468
Oxygen	30000	62.3529412	0	CM2	0.18	0.42	0.80	0.1397	0.92	0.104
PH3	0.3	62.3529412	1	CM3	0.39	0.61	25.69	0.1397	0.76	2.735
Propadiene	1000	62.3529412	0	CM2	0.18	0.42	2.23	0.1397	0.92	0.289
Propane	1000	62.3529412	0	CM2	0.18	0.42	2.23	0.1397	0.92	0.289
Propene	30000	62.3529412	0	CM2	0.18	0.42	0.80	0.1397	0.92	0.104
SiO2	0.0407	23.5294118	2	CM3	0.60	0.61	46.86	0.0504	0.63	1.498
SO2	2	62.3529412	1	CM3	0.39	0.61	14.51	0.1397	0.76	1.545
Water	30000	62.3529412	0	CM2	0.18	0.42	0.80	0.1397	0.92	0.104
									EHI_p	23.062

A summary of the project EHI to each case is shown below in Table 75.

Table 75 Project EHI Results

Case	$\mathbf{EHI}_p$
PDH Base	28.12
PDH Integrated	27.36
PDH Integrated & Intensified	27.66
MTP Base	23.67
MTP Integrated	23.06

The EHI Analysis followed the following assumptions: (1) There are O_1 occasions in which workers work with absorbents and catalysts per year for t_1 hours at a time. (2) Stream

components follow the previous assumption and O_2 other occasions for t_2 hours each. (3) No managerial measures are implemented for feed components. (4) There is at least a minimum of one managerial measure for catalysts and absorbents. (5) Feed components follow CM2, while catalysts and absorbents follow CM3.

Table 76 EHI Assumptions between Cases

Case	O_1	t_1 (hr)	O_2	t_2 (hr)
PDH Base	20	5	60	3
PDH Integrated	20	5	55	3
PDH Integrated & Intensified	20	5	57	3
MTP Base	20	5	60	3
MTP Integrated	20	5	55	3

In Table 76, the variation between cases occurs based on the number of occasions workers will be exposed with stream components. It is assumed that all integrated cases will require less occasions than base cases.

Wang *et al.* provides a list of recommended EHI values for various industries. EHI values for chemical processing pulled from their table is listed below in Table 77:

Table 77 EHI for Chemical Industries adapted from [20]

Chemical Industry	EHI Value
Plastic products manufacturing (n = 37)	43.47
Petroleum products manufacturing (n = 7)	35.54
Chemical materials manufacturing (n = 94)	21.66
Chemical products manufacturing (n = 16)	14.06

It is understood that petroleum products manufacturing refers to early chemical refinement, chemical materials manufacturing refers to initial chemical production, and chemical products

manufacturing refers to final chemical production for consumers. The target for this case study is 21.66 for chemical materials manufacturing.

5.8 Integrated Analysis

An integrated analysis was completed to accurately find the SASWROIM for each case. A summary of the economic metrics used for SASWROIM is shown below in Table 78:

Table 78 Economic Metrics for Cases

Description	**10-yr AEP**	**TCI**	**ROI (10-yr)**
Units	$/yr	$MM	%/yr
---	---	---	---
MTP Base Case	50	362	13.80
MTP Heat Integrated Case	54	358	15.13
---	---	---	---
PDH Base + WHR Case	67	643	10.38
PDH Integrated Case	79	645	12.29
PDH Integrated + Intensified Case	104	536	19.45

A summary of the environmental metrics used for SASWROIM is shown below in Table 79:

Table 79 Environmental Metrics for Cases

Description	WRM	EES	FSM	CER	VRM	RSM	Environmental Indicator Summation
Units	10^6 kg/h	MW	MW	10^3 tons/yr	tons/yr	10^6 kg/h	---
Weights	0.1	0.1	0.07	0.25	0.05	0.07	---
---	---	---	---	---	---	---	---
MTP Targets	0.094	4.38	189	345.7	50.7	4.45	---
MTP Base Case	0	0	0	0	0	0	0.00
MTP Heat Integrated Case	0	-0.38	146	80.1	40.3	4.03	0.21
---	---	---	---	---	---	---	---
PDH Targets	45.08	36	159	1013	32.7	0.25	---
PDH Base + WHR Case	0	0	0	101.4	4.6	0	0.03
PDH Integrated Case	25.6	0	87	192.3	8.8	0	0.16
PDH Integrated + Intensified Case	38.7	-14.5	87	481.4	24.9	0	0.24

A summary of the social metrics used for SASWROIM is shown below in Table 80:

Table 80 Social Metrics for Cases

Description	EHI for Occupational Health	Jobs Created	Social Indicator Summation
Units	---	jobs	---
Weights	0.1	0.1	---
---	---	---	---
MTP Targets	21.66	130	---
MTP Base Case	23.67	118	0.00
MTP Heat Integrated Case	23.06	118	0.03
---	---	---	---
PDH Targets	21.66	130	---
PDH Base + WHR Case	28.12	96	0.00
PDH Integrated Case	27.36	107	0.04
PDH Integrated + Intensified Case	27.66	119	0.07

A summary of the safety metrics used for SASWROIM is shown below in Table 81:

Table 81 Safety Metrics for Cases

Description	**PSI**	**PRI**	**Safety Indicator Summation**
Units	---	---	---
Weights	0.1	0.1	---
---	---	---	---
MTP Targets	28.31	30.09	---
MTP Base Case	21.97	10.60	0.00
MTP Heat Integrated Case	22.90	10.17	0.01
---	---	---	---
PDH Targets	28.31	30.09	---
PDH Base + WHR Case	48.29	60.17	0.00
PDH Integrated Case	56.61	43.46	0.01
PDH Integrated + Intensified Case	55.86	38.63	0.03

The SASWROIM for each case was calculated and shown below in Table 82:

Table 82 Integrated Metric for Cases

Description	**ROI (10-yr)**	**Environmental Indicator Summation**	**Social Indicator Summation**	**Safety Indicator Summation**	**SASWROIM**
Units	%/yr	---	---	---	%/yr
MTP Base Case	13.80	0.00	0.00	0.00	13.80
MTP Heat Integrated Case	15.13	0.21	0.03	0.01	18.90
PDH Base + WHR Case	10.38	0.03	0.00	0.00	10.71
PDH Integrated Case	12.29	0.16	0.04	0.01	14.92
PDH Integrated + Intensified Case	19.45	0.24	0.07	0.03	26.24

The weights for each indicator was selected from Agarwal *et al.* and Guillen-Cuevas *et al.* papers. A graph was created to visually represent the effect of each indicator, shown below in Figure 21:

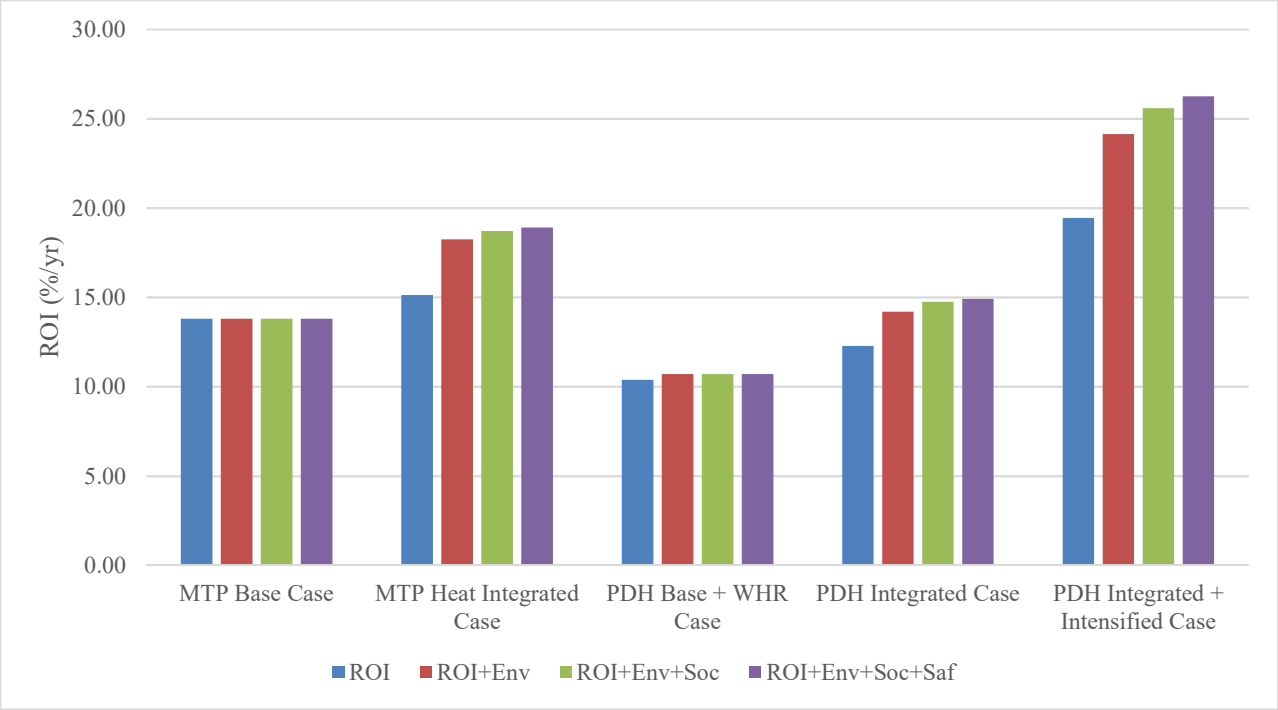


Figure 21 Weight Effect on ROI.

Decision-makers can use this figure to compare the different cases and their respective economic, environmental, social, and safety impacts. If the decision-maker only wants projects that are above 15% ROI, then the MTP Heat Integrated Case and the PDH Integrated + Intensified Case are both acceptable given all their impacts.

6. CONCLUSIONS

Two case studies were conducted to examine the application of social indicators on process selection and the application of SASWROIM with a society-impact focus with on-purpose propylene plants.

6.1 Social Indicators Case Study

This paper found, applied, and verified objective social indicators through a case study of biomass versus shale gas routes. Biomass routes can create more jobs than shale gas routes. However, this claim is a weak conclusion. The results found were not compared to actual data on number of jobs created. The case study shows the approach works, but the results of the case study are meaningless.

6.2 On-Purpose Propylene Case Study

This paper provided a systematic method based around SASWROIM for on-purpose propylene production. The models and analysis demonstrated the impacts of each case on the environmental, society, and safety of individuals. The economics of the MTP plants were within 5% error of actual MTP plants. Lastly, the approach was validated.

6.3 Research Justifications and Limitations

The knowledge of this research benefits academia and industry. The systematic method is an extension of previous research incorporating sustainability and safety in decision-making (i.e. SASWROIM) by including social indicators. Furthermore, it can be applied to various marketable products and projects beyond process design.

In the first case study, it does not account for actual mass yields, selectivity of products, market factors, and more. The results are strongly influenced by feed compositions. Only five routes were studied.

In the second case study, it does not account for pressure changes in MTP reactions. Since moles of vapor are generated via the MTP reactions, pressure plays a heavy role in the conversion of methanol to propylene. It also does not account for side reactions. Lastly, the model only measure a light feed composition instead of a heavy feed composition.

Unfortunately, one paper cannot sufficiently address all problems associated with decision-making. Not all indicators and metrics found in the literature review was used, since some require company-specific information, e.g. indirect community benefit per unit value-added. Therefore, only some of the indicators that was determined from process data was used. The work was also only limited to on-purpose propylene production and not studies of other product productions.

6.4 Suggestions for Improvement

In the first case study, the actual yield of propylene from the chemicals used in the social indicators case study could be used instead of theoretical yields. Same things can be done for selectivity of products. More research could be done towards the market factors and how they play a role in creating more jobs. More intense sensitivity analysis can be done on the composition to jobs created. Lastly, incorporating different metrics or feed compositions than what was used in the study could improve it.

In the second case study, a more intense sensitivity analysis can be done on methanol and propylene market cost. Another sensitivity analysis could be done on the weights for the SASWROIM. The analysis would then provide the appropriate range in which environmental, social, and safety factors should be used when paired together. Other improvements would be to incorporate different metrics into the study, to improve integration and/or intensification of the MTP process, and to improve accuracy of the models. Lastly, and probably most importantly, a

better representation of the reaction network to create MTP should be used to accurate gauge and track the conversion of methanol to propylene.

6.5 Final Remarks

In the end, models are only as good as the data in which it is based off of. With more time and effort, the models could be further improved and changed to fit different scenarios. Nonetheless, the approaches for each case study were validated as reasonable methods for decision-making. Hopefully, future engineers will gladly utilize these approach in their engineering design efforts.

Thank you for taking time to read this thesis. May it be what you had hoped and be beneficially to you in your future endeavors.

8. REFERENCES

[1] D. S. Rogers, A. K. Duraiappah, C. D. Antons, P. Munoz, X. Bai, M. Fragkias and H. Gutscher, "A vision for human well-being: transition to social sustainability," *Current Opinion in Environmental Sustainability,* vol. 4, pp. 61-73, 2012.

[2] M. M. El-Halwagi, Sustainable Design Through Process Integration, Oxford: Elsevier Inc., 2012.

[3] D. A. Crowl and J. F. Louvar, Chemical Process Safety: Fundamentals with Applications, Boston: Prentice Hall, 2011.

[4] IChemE, "The sustainability metrics: Sustainable development progress metrics recommended for use in the process industries," 2002. [Online]. Available: http://nbis.org/nbisresources/metrics/triple_bottom_line_indicators_process_industries.pdf. [Accessed 9 January 2018].

[5] G. Towler and R. Sinnott, Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design, Amsterdam: Elsevier Ltd., 2013.

[6] R. A. Meyers, "Lurgi MTP Technology," in *Handbook of Petrochemicals Production Processes*, Boston, McGraw-Hill Professional, 2005.

[7] Nexant, "Equipment Design and Cost Estimation for Small Modular Biomass Systems, Synthesis Gas Cleanup, and Oxygen Separation Equipment," National Renewable Energy Laboratory, May 2006. [Online]. Available: https://www.nrel.gov/docs/fy06osti/39943.pdf. [Accessed 5 March 2018].

[8] M. Narodoslawsky and C. Krotscheck, "The sustainable process index (SPI): evaluating processes according to environmental compatibility," *Journal of Hazardous Materials,* vol. 41, no. 2-3, pp. 383-397, 1995.

[9] J. Schwarz, B. Beloff and E. Beaver, "Use Sustainability Metrics to Guide Decision-Making," July 2002. [Online]. Available: https://pdfs.semanticscholar.org/b29a/e01b85d8ef7c72150a7e938823c02a4ee685.pdf. [Accessed 9 January 2018].

[10] A. Agarwal, D. Sengupta and M. M. El-Halwagi, "A Sustainable Process Design Approach for On-Purpose Propylene Production and Intensification," 18 December 2017. [Online]. Available: http://pubs.acs.org/doi/abs/10.1021/acssuschemeng.7b03854. [Accessed 10 January 2018].

[11] F. I. Khan and P. R. Amyotte, "Integrated inherent safety index (I2SI): A tool for inherent safety evaluation," *Process Safety Progress,* vol. 23, no. 2, pp. 136-148, 2004.

[12] C. T. Leong and A. M. Shariff, "Inherent safety index module (ISIM) to assess inherent safety level during preliminary design stage," *Process Safety and Environmental Protection,* vol. 86, no. 2, pp. 113-119, 2008.

[13] C. T. Leong and A. M. Shariff, "Process route index (PRI) to assess level of explosiveness for inherent safety quantification," *Journal of Loss Prevention in the Process Industries,* vol. 22, no. 2, pp. 216-221, 2009.

[14] D. Zaini, A. M. Shariff and C. T. Leong, "Three-Tier Inherent Safety Quantification (3-TISQ) For Toxic Release At Preliminary Design Stage," *Applied Mechanics and Materials,* vol. 625, pp. 426-430, 2014.

[15] A. M. Shariff, C. T. Leong and D. Zaini, "Using process stream index (PSI) to assess inherent safety level during preliminary design stage," *Safety Science,* vol. 50, no. 4, pp. 1098-1103, 2012.

[16] H. A. Becker, "Social impact assessment," *European Journal of Operational Research,* vol. 128, no. 2, pp. 311-321, 2001.

[17] K. Magis, "Community Resilience: An Indicator of Social Sustainability," *Society & Natural Resources,* vol. 23, no. 5, pp. 401-416, 2010.

[18] M. S. Peters, K. D. Timmerhaus and R. E. West, Plant Design and Economics for Chemical Engineers, Boston: McGraw Hill, 2003.

[19] C. C. K. Wang, OSHA Compliance and Management Handbook, New Jersey: Noyes Publications, 1993.

[20] S.-M. Wang, T.-N. Wu, Y.-J. Juang, Y.-T. Dai, P.-J. Tsai and C.-Y. Chen, "Developing a Semi-Quantitative Occupational Risk Prediction Model for Chemical Exposures and Its Applications to a National Chemical Exposure Databank," *International Journal of Environmental Research and Public Health,* vol. 10, pp. 3157-3171, 2013.

[21] M. M. El-Halwagi, "A return on investment metric for incorporating sustainability in process integration and improvement projects," *Clean Technology Environmental Policy,* vol. 19, pp. 611-617, 2017.

[22] K. Guillen-Cuevas, A. P. Ortiz-Espinoza, E. Ozinan, A. Jimenez-Gutierrez, N. K. Kazantzis and M. M. El-Halwagi, "Incorporation of Safety and Sustainability in Conceptual Design via a Return on Investment Metric," *Sustainable Chemistry & Engineering,* vol. 6, no. 1, pp. 1411-1416, 2018.

[23] Platts, "Global Polymer Pricing Analysis," October 2017. [Online]. Available: https://www.platts.com/news-feature/2016/petrochemicals/global-polymer-pricing-analysis/lldpe. [Accessed 2 March 2018].

[24] ICIS, "US July ethylene contracts settle down 1.25 cents/lb, not market-wide," 3 August 2017. [Online]. Available: https://www.icis.com/resources/news/2017/08/03/10062158/us-july-ethylene-contracts-settle-down-1-25-cents-lb-not-market-wide/. [Accessed 2 March 2018].

[25] M. M. B. Noureldin, N. O. Elbashir and M. M. El-Halwagi, "Optimization and Selection of Reforming Approaches for Syngas Generation from Natural/Shale Gas," *Industrial & Engineering Chemistry Research I&EC,* vol. 53, pp. 1841-1855, 2013.

[26] M. M. B. Noureldin and M. M. El-Halwagi, "Synthesis of C-H-O Symbiosis Networks," *American Institute of Chemical Engineers AIChE,* vol. 61, no. 4, pp. 1242-1262, 2015.

[27] "Refiner Gasoline Prices by Grade and Sales Type," U.S. Energy Information Administration (EIA), July-December 2017. [Online]. Available: https://www.eia.gov/dnav/pet/pet_pri_refmg_dcu_nus_m.htm. [Accessed 5 March 2018].

[28] "Indicative Chemical Prices A-Z," ICIS, 6 February 2017. [Online]. Available: https://www.icis.com/chemicals/channel-info-chemicals-a-z/. [Accessed 3 January 2018].

[29] Methanex, "Methanex posts regional contract methanol prices for North America, Europe and Asia," 1 March 2018. [Online]. Available: https://www.methanex.com/our-business/pricing. [Accessed 2 March 2018].

[30] "United States Natural Gas Industrial Price," U.S. Energy Information Administration, 29 December 2017. [Online]. Available: https://www.eia.gov/dnav/ng/hist/n3035us3m.htm. [Accessed 3 January 2018].

[31] U. EIA, "Wholesale Propane Weekly Heating Oil and Propane Prices (October-March)," October 2017. [Online]. Available: https://www.eia.gov/dnav/pet/pet_pri_wfr_a_EPLLPA_PWR_dpgal_w.htm. [Accessed 2 March 2018].

[32] Platts, "S&P Global Platts Petrochemical Pricing Index (PGPI)," 8 December 2017. [Online]. Available: https://www.platts.com/news-feature/2014/petrochemicals/pgpi/propylene. [Accessed 2 March 2018].

[33] J. Gregor and D. Wei, "UOP OLEFLEX Process," in *Handbook of Petrochemicals Production Processes*, Boston, McGraw-Hill, 2005, p. Section 10.3.

[34] S. Jasper and M. M. El-Halwagi, "A Techno-Economic Comparison between Two Methanol-to-Propylene Processes," *Processes,* vol. 3, pp. 684-698, 2015.

[35] V. M. Ehlinger, K. J. Gabriel, M. M. B. Noureldin and M. M. and El-Halwagi, "Process Design and Integration of Shale Gas to Methanol," *ACS Sustainable Chemical Engineering,* vol. 2, pp. 30-37, 2014.

[36] O. Onel, A. M. Niziolek and C. A. Floudas, "Optimal Production of Light Olefins from Natural Gas via the Methanol Intermediate," *Industrial & Engineering Chemistry Research,* vol. 55, pp. 3043-3063, 2016.

[37] J. Gotro, "Bio-Based Polypropylene: Multiple Synthetic Routes Under Investigation," Polymer Innovation Blog, 30 April 2018. [Online]. Available:

https://polymerinnovationblog.com/bio-based-polypropylene-multiple-synthetic-routes-under-investigation/. [Accessed 12 February 2018].

[38] R. McGill, "Carbonation Advice," Real Beer New Zealand, 30 March 2012. [Online]. Available: http://www.forum.realbeer.co.nz/forum/topics/carbonation-advice?commentId=1500433%3AComment%3A208231. [Accessed 12 February 2018].

[39] L. D. Dung, K. Morishita and T. Takarada, "Catayltic Decomposition of Biomass Tars at Low-Temperature," 30 April 2013. [Online]. Available: https://www.intechopen.com/books/biomass-now-sustainable-growth-and-use/catalytic-decomposition-of-biomass-tars-at-low-temperature. [Accessed 12 February 2018].

[40] "Biofuels," Centre for Industry Education Collaboration: University of York, 5 April 2014. [Online]. Available: http://www.essentialchemicalindustry.org/materials-and-applications/biofuels.html. [Accessed 12 February 2018].

[41] "What reactions are used in MTP (methanol to propylene) process?," Research Gate, May 2017. [Online]. Available: https://www.researchgate.net/post/What_reactions_is_used_in_MTPmethanol_to_propylene_process. [Accessed 24 February 2018].

[42] "Methanol Synthesis," Global Syngas Technologies Council, 2018. [Online]. Available: http://www.globalsyngas.org/applications/methanol-synthesis/. [Accessed 12 February 2018].

[43] A. Behr, N. Rentmeister, T. Seidensticker, T. A. Fabach, S. Peitz and D. Maschmeyer, "Nickel catalyzed dimerization reactions of vinylidene compounds: Head-to-head couplings

and catalyst stabilization," *Journal of Molecular Catalysis A: Chemical,* vol. 395, pp. 355-363, 2014.

[44] T. I. Bhuiyan, P. Arudra, M. N. Akhtar, A. M. Aitani, R. H. Abudawoud, M. A. Al-Yami and S. S. Al-Khattaf, "Metathesis of 2-butene to propylene over W-mesoporous molecular sieves: A comparative study between tungsten containing MCM-41 and SBA-15," *Applied Catalysis A: General,* vol. 467, pp. 224-234, 2013.

[45] A. Witsuthammakul and T. Sooknoi, "Selective hydrodeoxygenation of bio-oil derived products: acetic acid to propylene over hybrid CeO2-Cu/zeolite catalysts," *Catalysis Science & Technology,* vol. 6, pp. 1737-1745, 2016.

[46] M. M. El-Halwagi, Sustainable Design Through Process Integration, Amsterdam: Elsevier, 2017.

[47] H. H. Mardihiah, H. C. Ong, H. H. Masjuki, S. Lim and H. V. Lee, "A review on latest developments and future prospects of heterogeneous catalyst in biodiesel production from non-edible oils," *Renewable and Sustainable Energy Reviews,* vol. 67, pp. 1225-1236, 2017.

[48] S. K. Hoekman, A. Broch, C. Robbins, E. Ceniceros and M. and Natarajan, "Review of biodiesel composition, properties, and specifications," *Renewable and Sustainable Energy Reviews,* vol. 16, pp. 143-169, 2012.

[49] "2012 Census Highlights: Farm Demographics," United States Department of Agriculture, May 2014. [Online]. Available: https://www.agcensus.usda.gov/Publications/2012/Online_Resources/Highlights/Farm_Demographics/. [Accessed 12 February 2018].

[50] "Chemical elements listed by atomic mass," Lenntech, [Online]. Available: https://www.lenntech.com/periodic/mass/atomic-mass.htm. [Accessed 12 February 2018].

[51] "Densities and molecular weights of some common gases," The Engineering Toolbox, [Online]. Available: https://www.engineeringtoolbox.com/gas-density-d_158.html. [Accessed 4 January 2017].

[52] J. Tomczyk, "A Look At Compressor Discharge Temperatures," Air Condition, Heating & Refrigeration News, 27 February 2002. [Online]. Available: https://www.achrnews.com/articles/88734-a-look-at-compressor-discharge-temperatures. [Accessed 6 March 2018].

[53] M. Wen, J. Ding, C. Wang, Y. Li, G. Zhao, Y. Liu and Y. Lu, "High-performance SS-fiber@HZSM-5 core-shell catalyst for methanol-to-propylene: A kinetic and modeling study," *Microporous and Mesoporous Materials,* vol. 221, pp. 187-196, 2015.

[54] K. Chong, "China Methanol import prices surpass $300/tonne mark," ICIS, 25 August 2017. [Online]. Available: https://www.icis.com/resources/news/2017/08/25/10136944/china-methanol-import-prices-surpass-300-tonne-mark/. [Accessed 6 March 2018].

[55] U. EPA, "eGrid 2014 Summary Tables," 2014. [Online]. Available: https://www.epa.gov/sites/production/files/2017-02/documents/egrid2014_summarytables_v2.pdf. [Accessed 8 March 2018].

[56] U. EPA, "AP-42: Compilation of Air Emission Factors | Air Emissions Factors and Quantification," 14 December 2009. [Online]. Available: https://www.epa.gov/air-

emissions-factors-and-quantification/ap-42-compilation-air-emissions-factors#Proposed/. [Accessed 8 March 2018].

[57] "Permissible Exposure Limits for Chemical Contaminants," Occupational Safety and Health Administration, 2018.