

**PROCESS SIMULATION AND EVALUATION OF ALTERNATIVE SOLVENTS
FOR *JATROPHA CURCAS L.* SEED OIL EXTRACTION IN BIODIESEL
PRODUCTION**

A Thesis

by

MING-HAO CHIOU

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

MASTER OF SCIENCE

August 2011

Major Subject: Chemical Engineering

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Approved by:

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ABSTRACT

Process Simulation and Evaluation of Alternative Solvents for *Jatropha Curcas L.* Seed Oil Extraction in Biodiesel Production. (August 2011)

Ming-Hao Chiou, B.S., National Chung Hsing University

Chair of Advisory Committee: Dr. Mahmoud M. El-Halwagi

Jatropha curcas L. is a drought-resistant plant which can be grown in poor soil and marginal lands. The use of *Jatropha* seed oil to produce biodiesel has been widely studied in recent years. Results showed that it is one of the most promising alternatives for conventional petro-diesel. Currently, hexane is still the most commonly used solvent for commercial oil extraction. However, the increasing price and flammability properties of hexane are motivating industry to seek alternative solvents. The objectives of this study are to design and analyze the *Jatropha* seed oil extraction for use in biodiesel production, and to provide a systematic safety-economic analysis of alternative solvents that can be used in *Jatropha* seed oil extraction. First, a base-case flowsheet is synthesized for oil extraction. Then, the base-case extraction process and each solvent are evaluated by Dow's Fire and Explosion Index (F&EI) and the Solvent Safety Index (SSI). Eight solvents, including n-heptane, toluene, xylene, dichloromethane, chloroform, 1,2-dichloroethane, methanol and ethanol are selected for candidates by comparing these results to those for hexane. Two cases are developed to evaluate the economic potential of these candidates. Furthermore, heat integration is applied to the process to minimize energy usage. Finally, a comprehensive solvent comparison is developed based on F&EI, SSI, solvent makeup cost, utilities cost, and capital investment. The results show that chloroform is the optimal solvent, while dichloromethane is the next best.

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NOMENCLATURE

Actual MPPD	Actual Maximum Probable Property Damage
AIChE	American Institute of Chemical Engineers
AEOE	Aqueous Enzymatic Oil Extraction
AOE	Aqueous Oil Extraction
Base MPPD	Base Maximum Probable Property Damage
CC	Cost of Cooling Utility
CH	Cost of Heating Utility
Cp	Specific Heat of Jatropha Seed (kJ/kg-K)
$F_u C_{p_u}$	Heat Capacity for u^{th} Process Hot Stream
$f_v C_{p_v}$	Heat Capacity for v^{th} Process Cold Stream
F&EI	Fire and Explosion Index
GHG	Greenhouse Gases
$HC_{v,z}$	Heat Exchange at u^{th} Cold Stream
HC_z^{Total}	Total Cooling Loads
HCU_v^{Total}	Total Cooling Utility
$HH_{u,z}$	Heat Exchange at u^{th} Hot Stream
HH_z^{Total}	Total Heating Loads
HHU_z^{Total}	Total Heating Utility
I_{LC50}	Priority Index Value for LC ₅₀
I_{NFPA}	Priority Index Value for NFPA 704 Health
I_{VD}	Priority Index Value for Vapor Density
ISI	Inherent Safety Index
I2SI	Integrated Inherent Safety Index
LC ₅₀	Lethal Concentration 50
MF	Material Factor
M	Weight Percentage of Moisture Containing in Jatropha Seed

NFPA	National Fire Protection Association
PIIS	Prototype Index of Inherent Safety
R	Exposure Radius
SI	Safety Index
r_{z-1}	Residual Heat Entering the z^{th} Interval
r_z	Residual Heat Leaving the z^{th} Interval
SCE	Supercritical Carbon Dioxide Extraction
SSI	Solvent Safety Index
T_{z-1}	Hot Stream Supply Temperature for z^{th} Interval
T_z	Hot Stream Target Temperature for z^{th} Interval
t_{z-1}	Cold Stream Supply Temperature for z^{th} Interval
t_z	Cold Stream Target Temperature for z^{th} Interval
ΔT^{min}	Minimum Heat Exchange Driving Force
u	Process Hot Streams
v	Process Cold Streams
WF_{LC50}	Weighting Factor for the Corresponding LC ₅₀
WF_{NFPA}	Weighting Factor for the Corresponding NFPA 704
WF_{VD}	Weighting Factor for the Corresponding Vapor Density
ρ	Jatropha Seed Density (kg/m ³)
z	Temperature Interval

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CHAPTER I

INTRODUCTION

For many years, fossil fuels have supplied the majority of energy for industrial and personal use. The availability, convenience and relative low price of fossil fuels was lack of concern from the government and community. However, the quickly expanding economies of developing countries such as China and India require more energy to support their growth. Meanwhile, developed countries also need more energy to improve their quality of life. The increasing demand for fossil fuels forces the price higher and higher. However, the large amounts of greenhouse gases (GHG) emitted from the combustion of fossil fuels is threatening our environment. In fact, current emissions of GHG are nearly 10 billion tons of carbon dioxide equivalents per year and could have significant negative impacts to climate change (Makkar and Becker, 2009).

The use of vegetable oils and animal fats to produce biodiesel as the replacement to conventional fossil fuels is one of the most promising options to reduce GHG emissions. Many edible oils, such as soybean oil, cotton oil and palm oil are being used for biodiesel production. However, the competition with food products forces scientists and engineers to continuously look for other alternatives (Nazir et al., 2009). An oil-bearing plant, *Jatropha Curcas* L. is currently attracting interest as a feedstock for the production of biodiesel. It can be grown in marginal and waste lands. Its seeds are toxic for humans and animals and will, therefore not compete with food sources.

The aim of this study is to analyze the safety and economics of the *Jatropha Curcas* L. seed oil extraction process. A systematic approach to evaluate the process of *Jatropha* seed oil extraction is developed. Computer-aided simulation is also applied to model the process. In order to assess the safety of the extraction process and extraction solvents, Dow's Fire and Explosion Index (F&EI) is incorporated to evaluate the risks

and hazards of the extraction process, and Solvent Safety Index (SSI) is constructed to analyze the risks and hazards of extraction solvents.

CHAPTER II

BACKGROUND AND LITERATURE REVIEW

2.1 *Jatropha curcas* L.: A Promising Biofuel Plant

Jatropha curcas L. (*Jatropha*) is a plant from the family Euphorbiaceae. It is a drought-resistant perennial that grows well in poor soil and marginal lands, and is easy to establish and produce seeds for over 50 years (Chhetri et al., 2008). The high environmental adaptability allowed *Jatropha* to become widespread in arid, semi-arid, and tropical region in the world, as shown in Figure 2-1. Furthermore, its deep root system allows it to store carbon, maintain soil quality, and manage water and nutrients conservatively. The deep roots can prevent landslides and the shallow can defend soil erosion caused by wind or water. Figure 2-2 shows the images of *Jatropha*. Moreover, scientists believe that toxins in the seed and plant makes *Jatropha* non-edible; thus it will not compete with food (King et al., 2009).

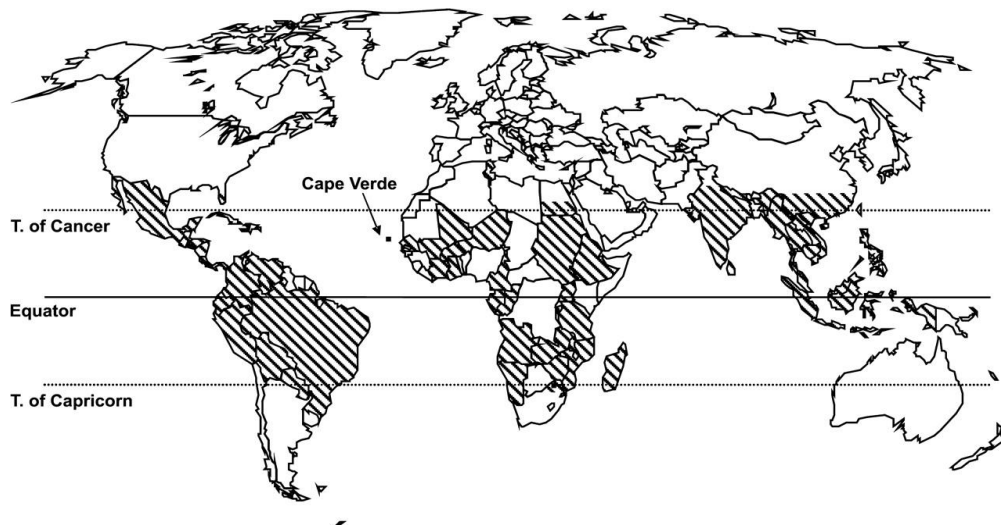


Figure 2-1 Approximate global distribution of *Jatropha curcas* L. (King et al., 2009)

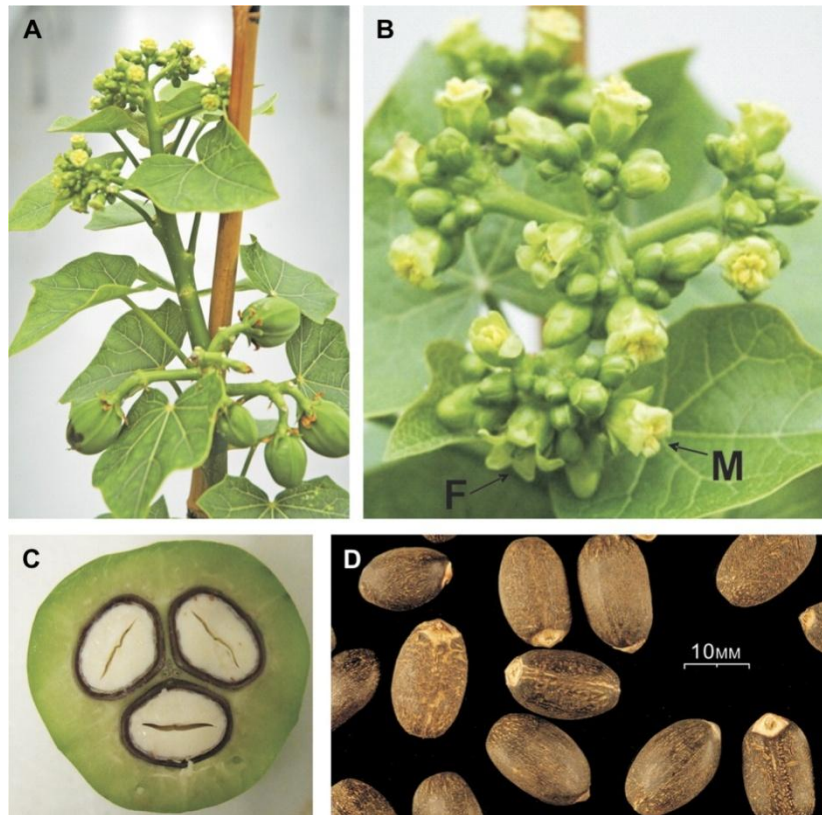


Figure 2-2 Images of Jatropha (A) young Jatropha plant with both flowers and developing seed pods. (B) Jatropha inflorescence containing both male staminate flowers (M) and female pistillate flowers (F). (C) cross-section of a Jatropha seed pod containing three developing seeds. (D) mature seeds of Jatropha. (King et al., 2009)

Recent research shows that Jatropha is one of the best candidates for biodiesel production. Jatropha oil can be blended with petro-diesel directly or followed by transesterification to produce biodiesel. For most vegetable oils, the high viscosity causes the formation of gums, injector deposits, ring sticking, and incompatibility with conventional lubricating oils (Ryan et al., 1984). One must reduce the viscosity of vegetable oils before they can be used as alternatives fuels in a diesel engine. However, the high viscosity of Jatropha oil is decreased by blending it with diesel, and after this

process, *Jatropha* oil significantly improved engine performance compared to other vegetable oils (Pramanik, 2003). Forson (Forson et al., 2004) concluded that a 97.4:2.6 volumetric ratio fuel blend yielded the highest cetane number. Furthermore, Staubmann (Staubmann et al., 1997) reported that residues such as husks from seeds and meals from extraction can be used for direct combustion and biogas production.

However, *Jatropha* seed yield and price are still unknown because systematic yield monitoring began recently. Although some data have been reported by Openshaw (Openshaw, 2000), a comprehensive analysis is still limited. One expectation is that the price of *Jatropha* seed should be lower than the price of soybean because it does not compete with food, but the value of residuals (cakes or meal) might be lower due to toxic component content. Figure 2-3 shows the historic prices of soybean, soy oil, and soy meal over the past twenty years. The price of soybeans started to climb in 2000 and reached an apex in 2008. The World Bank reported (Mitchell, 2008) that the use of foods as biofuel sources is an important contributor to higher prices and caused a food price crisis during 2007 to 2008.

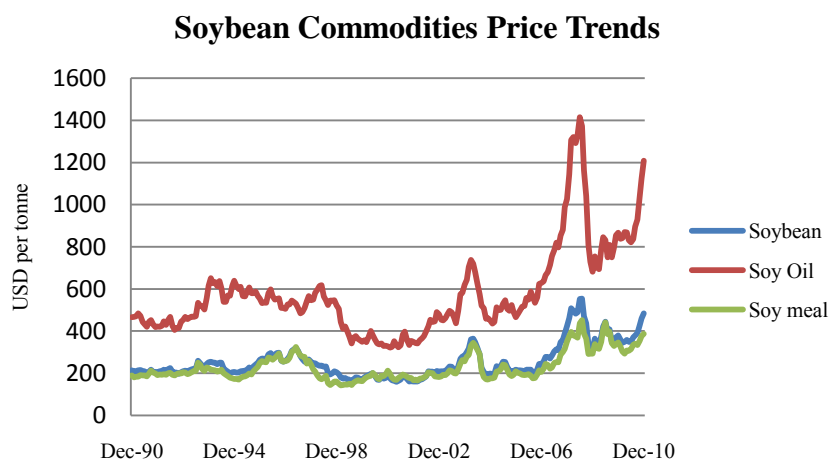


Figure 2-3 History price of soybean, soy oil and soy meal (Index Mundi, 2011)

The oil content in *Jatropha* has been reported to be 30-50 weight percentage of the seed and 40-60 weight percentage of the kernel (Chhetri et al., 2008). The chemical composition is shown in Figure 2-4. However, it is important to note that the composition of *Jatropha* seed varies widely between different regions and climates.

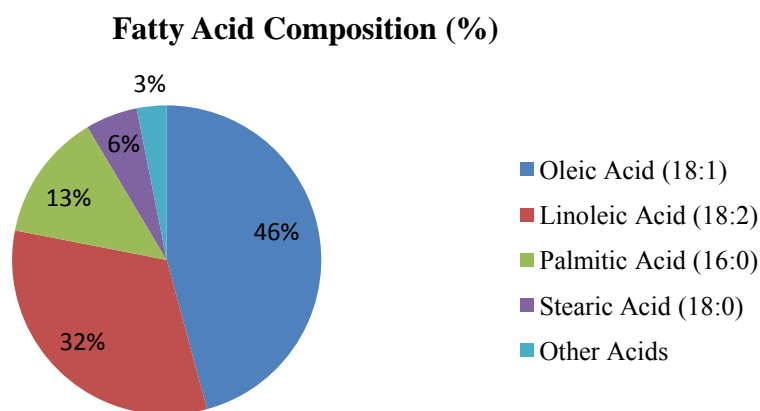


Figure 2-4 Fatty acid composition of *Jatropha* oil (Chhetri et al., 2008)

2.2 Oil Extraction

The first step of biodiesel production is to produce oil from oil seeds. Two primary methods are identified: mechanical pressing and solvent extraction. In the early 20th century (before 1950's), mechanical pressing was the primary method to extract oil. However, the poor efficiency of oil recovery and high temperature generated during pressing forced engineers to seek other methods to extract oil. Therefore, solvent extraction was developed to successfully extract more oil at lower temperature (Tzia and Liadakis, 2003). After World War II, the large demand of vegetable oils and technology improvement caused solvent extraction to become more attractive for commercial use. Adriaans (Adriaans, 2006) concluded that solvent extraction is the only economical

method when the throughput of seeds is over 200 tons per day. Figure 2-5 presents the Jatropha oil extraction process.

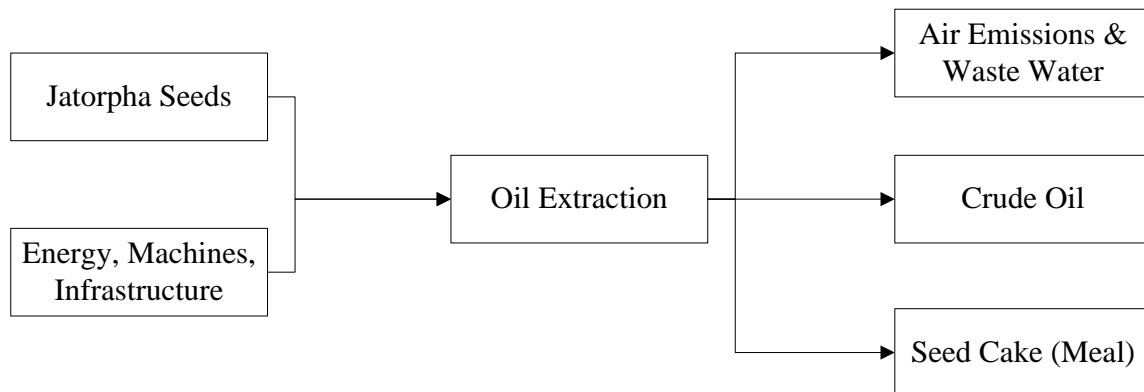


Figure 2-5 Input and output of the Jatropha oil extraction unit process (Achten et al., 2008)

2.2.1 Mechanical Pressing

A typical oil extraction process begins with seed preparation. The preparation consists of a series of treatments, such as cleaning, breaking, grinding and cooking, which produces a feed material in the optimum condition for subsequent extraction (Tzia and Liadakis, 2003). Henning (Henning, 2000) and Tobin (Lam et al., 2009) reported that Jatropha seeds must be dried before extraction. This procedure can be performed via oven or sunlight. The feed for the pressing step can be seeds or kernels or a mix of both, but common practice is to use whole seeds. The temperature for the pressing step is about 60°C (Nazir et al., 2009). The pressing step is carried out using a manual ram press or an engine driven screw press. Figure 2-6 shows a typical engine screw press machine. However, the extraction efficiency of mechanical pressing is quite low and seed cakes still contain some oil. Henning (Henning, 2000) stated that engine driven screws extract

75-80% of the available oil and manual ram presses only achieved 60-65%, but a good pretreatment of seeds might increase the yield of screw pressing up to 91%.

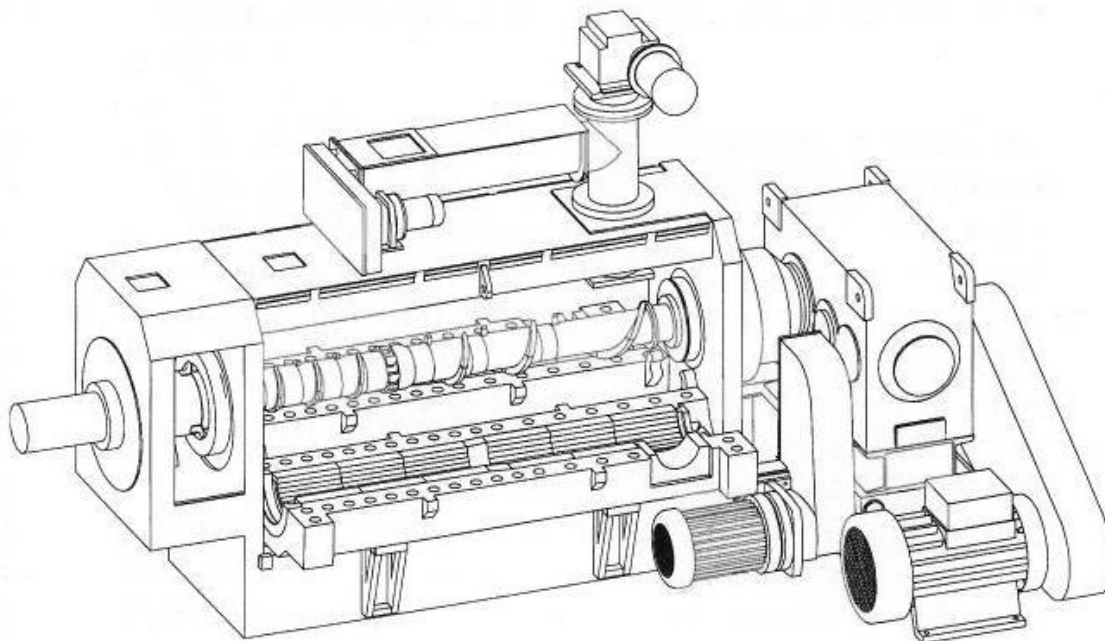


Figure 2-6 A typical engine screw press machine (Tzia and Liadakis, 2003)

2.2.2 Chemical Extraction

Various studies (Chen et al., 2009; Gubitz et al., 1999; Min et al., 2010; Qian et al., 2010; Shah et al., 2004, 2005; Sharma et al., 2002) have been reported for the chemical extraction of *Jatropha* oil, including organic solvent extraction, aqueous extraction, three-phase partitioning extraction and supercritical fluid extraction. In Table 2-1, a summary of different chemical extraction methods is presented.

Table 2-1 Summary of different method for Jatropha oil extraction

Extraction method	Reference	Temperature (°C)	Pressure (bar)	pH	Time (hr)	Oil yield (%)
n-hexane oil extraction	(Gubitz et al., 1999)	-			8	95-99
Aqueous oil extraction (AOE) with 10 min ultrasonication pretreatment	(Shah et al., 2005)	50	-	9	6	67
Aqueous enzymatic oil extraction (AEOE) with 5 min ultrasonication pretreatment	(Shah et al., 2005)	50	-	9	6	74
Three-phase partitioning	(Shah et al., 2004)	25	-	9	2	97
Supercritical carbon dioxide extraction	(Min et al., 2010)	55	400	-	-	92
	(Chen et al., 2009)	60	350	-	5	98

The use of n-hexane as the solvent for oil extraction is still the most common method and results in the highest oil yield. Gubitz (Gubitz et al., 1999) stated that n-hexane can recover 98% (mass percentage of original oil in the seed and kernels) of oil from Jatropha seeds. Furthermore, Jatropha oil from two-phase solvent extraction was investigated by Qian (Qian et al., 2010). Experimental results showed that the optimal conditions were a methanol/n-hexane volume ratio of 60:40 at 35°C. Moreover, small amounts of dissolved n-hexane in methanol can be used as co-solvent to increase the reaction rate later in the transesterification reaction, and the cost of biodiesel could be reduced (Shah et al., 2005).

The use of aqueous enzymatic oil extraction has emerged as one of the most popular methods for extraction oil from plant materials. Its main advantages are that it is environmentally friendly and does not emit volatile toxic solvent (Shah et al., 2005). However, one disadvantage for aqueous enzymatic extraction is the long process time which is necessary for enzymes to liberate oil bodies (Shah et al., 2005). Shah (Shah et al., 2005) reported that the use of ultrasonication as a pretreatment step before aqueous oil extraction and aqueous enzymatic oil extraction is useful in oil extraction from *Jatropha* seeds. The use of ultrasonication for 10 minutes at pH 9.0 followed by aqueous oil extraction gave a yield of 67%, and a maximum yield of 74% was obtained by ultrasonication for 5 minutes followed by aqueous enzymatic oil extraction using an alkaline protease at pH 9.0. Use of ultrasonication also resulted in reducing the process time from 18 to 6 hours (Shah et al., 2005).

Three phase partitioning is a method generally used for protein separation (Sharma et al., 2002). It has been evaluated for oil extraction from *Jatropha* seeds by Sharma (Shah et al., 2004). This technique consists of adding an organic solvent (usually *t*-butanol) to a salt solution (ammonium sulphate). Sharma (Shah et al., 2004) stated that three-phase partitioning extraction with enzyme pretreatment and sonication increased the oil yield to 97% and also reduced the time for extraction.

Supercritical carbon dioxide extraction (SCE) has been extensively used in the extraction of natural products (Min et al., 2010). The advantages of using SCE are that the high quality of oil does not need to be refined and the high oil recovery is achieved without using any organic solvent. However, intensive energy consumption and technical challenge for continuous operation restricted it to be used only in small amounts and for high value products. Min (Min et al., 2010) reported that the maximum recovery of 92% can be obtained at 328K and 40 MPa. A maximum yield of 97.6% was obtained by Chen (Chen et al., 2009) at 333K and 350 bar.

2.3 Alternative Solvents for Oil Extraction

Since the 1950's, hexane has become the major solvent for oil extraction because of high stability, low evaporation loss, low corrosivity, low greasy residue, and better odor and flavor of mill products. Nearly all known oil seed extraction plants are currently using hexane (Johnson and Lusas, 1983). However, its extreme flammability causes serious fire and explosion risks, increasing price and environmental regulation are pushing industry to seek other solvents. Although numerous studies for alternative extraction solvents have been examined in the past, various degrees of toxicity of these solvents made them unlikely to be used as replacements for hexane. However, because of toxins contained in *Jatropha* seeds and meal, the products and residuals cannot be used as edible sources for humans or animals. Therefore, the option of using toxic solvents for oil extraction became available. Several properties for selecting ideal solvents for oil extraction have been concluded by Johnson (Johnson and Lusas, 1983), as shown follows:

1. High solvent power for triglycerides at elevated temperature is the most important properties of a solvent.
2. To reduce the hazard of fire and explosions, nonflammability or low flammability are preferred.
3. The solvent should be non-toxic to humans or animals when the meal or products are used as feed or food.
4. The solvent should be easily removed from oil and meal.
5. Extraction solvents should be stable to heat, light, and water.
6. Ideal solvents should not react with oil, meal and, equipment.
7. High purity is desired for extracting solvents.
8. The ideal solvent would be available at a low price.

Various alternative solvents for oil extraction have also been reviewed by Hron (Hron et al., 1982) and Johnson (Johnson and Lusas, 1983) and shown in Table 2-2.

Table 2-2 Possible alternative solvents for oil extraction (Johnson and Lusas, 1983)

Petroleum fractions		Halogenated Hydrocarbons	
1	Gasoline (diesel medium)	20	Dichloromethane
2	Petroleum ether	21	Ethyl chloride
3	Pentanes	22	Chloroform
4	Methyl pentanes	23	Carbon tetrachloride
5	Hexanes	24	1,2-Dichloroethane
6	Heptanes	25	1,2-Dichloroethylene
7	Cyclohexane	26	1,1,1-Trichloroethane
Alkanes		27	1,2,2-Trichloroethylene
8	n-Propane	28	1,1,2,2-Tetrachloroethylene
9	n-Butane	29	1,2-Dichloropropane
10	n-Pentane	30	1,1,2-Trichloro-1,2,2-trifluoroethane
11	Isopentane	Alcohols	
12	n-Hexane	31	Methanol
13	Isohexane	32	Ethanol
14	n-Heptane	33	n-Propanol
Cycloparafins		34	Isopropanol
15	Cyclopentane	35	n-Butanol
16	Cyclohexane	36	Isobutanol
Aromatic Hydrocarbons		37	Allyl alcohol
17	Benzene	38	Furfuryl alcohol
18	Toluene	Aldehydes	
19	Xylene	39	Furfural

Table 2-2 continued

Possible alternative solvents for oil extraction (Johnson and Lusas, 1983)

Ketones		52	Pyridine
40	Acetone	Other solvents	
41	Methyl ethyl ketone	53	Carbon disulfide
Esters		Solvent mixtures	
42	Methyl acetate	54	Hexane/acetic acid (96:4)
43	Ethyl acetate	55	Hexane/methanol (75:25)
Ethers		56	Hexane/ethanol (79:21)
44	Ethyl ether	57	Hexane/isopropanol (77:23)
45	Isopropyl ether	58	Hexane/allyl alcohol (95:5)
46	Dioxan	59	Aromatic hydrocarbon/ethanol (90:10)
47	Ethylene glycol monomethyl ether	60	Ethanol/water (96:4)
48	Ethylene glycol monoethyl ether	61	Isopropanol/water (87.7:12.3)
		62	Methanol/trichloroethylene (75:25)
49	Ethanolamine	63	Ethanol/trichloroethylene (75:25)
50	(Tert) Butylamine	65	Acetone/water (90:10)
51	Triethylamine	65	Acetone/hexane/water (54:44:2)

2.4 Safety Evaluation

Safety considerations have critically issue for process design. The traditional method for minimizing process risks is to provide layer of protection between the hazard and people, property, or the environment. However, costly construction and maintenance of protection system, and continued existence of hazard may lead to an accident during protection failure (Abedi and Shahriari, 2005). Therefore, hazards should be eliminated during preliminary design, rather than accepted hazards and implementing protection systems to control them (Rahman et al., 2005).

Several methods for inherent safety evaluation of process design have been developed recently, including Dow's Fire and Explosion Index (F&EI); The Mond Fire, Explosion and Toxicity Index; and inherent safety index. F&EI identifies fire and explosion damage and equipment contributing to an accident. The latest version, published in 1994, also provides a systematic approach to evaluate the potential loss caused by the damage of fire or explosion. The Mond Fire, Explosion and Toxicity Index (Mond F&EI) is a modified version of F&EI which includes the hazards of toxic chemicals in the process (Abedi and Shahriari, 2005). Various studies were developed to evaluate the inherent safety of chemical processes. Edwards (Edwards and Lawrence, 1995) developed a prototype index of inherent safety (PIIS) to analyze the selection of process route (Abedi and Shahriari, 2005). Heikkilä (Heikkila, 2000) provided an inherent safety index (ISI) for preliminary chemical process design. The index is divided into two categories: chemical and process. The chemical inherent safety index describes the inherent safety of chemicals in the process. The process inherent safety index expresses safety of the process itself (Heikkila, 2000). Khan(Khan and Amyotte, 2004) proposed a conceptual framework for an integrated inherent safety index (I2SI). It considered the life cycle of the process with economic evaluation and hazard potential identification. Pokoo-Aikins et al. (Pokoo-Aikins et al., 2010) developed a new safety metric index for analyzing the hazards of oil extraction. The inherent safety of extraction solvents and extraction process are both evaluated in this study. A summary of

advantages and disadvantages for these indices is concluded by Abedi (Abedi and Shahriari, 2005) and presented in Table 2-3.

Table 2-3 Advantages and disadvantages of inherently safety evaluation methods (Abedi and Shahriari, 2005)

Method	Design for	Advantages	Disadvantages
Dow F&EI	Damage quantification of fire and explosion Identification of equipment contribution in an accident for operation involving in storing, handling, process flammable and combustible material	Good coverage of risks and hazards in a chemical plant	Needs more detailed information for the process
Mond E&EI	Modification of Dow F&EI	Good coverage of risks and hazards in a chemical plant	Needs more detail information for the process
PIIS	Selection of process route	Requires less information. Suitable for early design.	All aspects relevant to inherent safety are not evaluated (other parts of the process e.g. equipment and piping). Not flexible enough to apply additional data.
ISI	Classification of process alternatives during the preliminary process design	Requires less information. Suitable for early design.	Selection of the scores and weighting factors is a subjective and knowledge based process. The results will not be reproducible. Not flexible enough to apply additional data.
I2IS	Inherent Safety evaluation by hazard potential identification as well as economic evaluation	Good applicability in the initial phase of process design.	Necessitates subjective judgment to estimate the sub-indices.

CHAPTER III

PROBLEM STATEMENT AND APPROACH

Figure 3-1 shows the approach for this research. The goals for this study are to design and analyze the Jatropha seed oil extraction process for use in biodiesel production and provide a systematic safety-economics evaluation of alternative solvents for the extraction process. The detailed procedures of this work are presented as follows:

- Synthesize a base-case seed oil extraction process flowsheet
- Generate Safety Index to determine alternative solvents for the extraction process through Fire and Explosion Index and Solvent Safety Index
- Model feedstock materials' thermodynamic properties and develop process flow diagrams in ASPEN Plus
- Analyze extraction process and evaluate process performance associated with each selected candidate solvent using ASPEN Plus simulation
- Incorporate heat integration to minimize energy consumption and utilities costs
- Estimate cost of oil extraction process
- Assess hazards and risks of alternative solvents for Jatropha seed oil extraction process

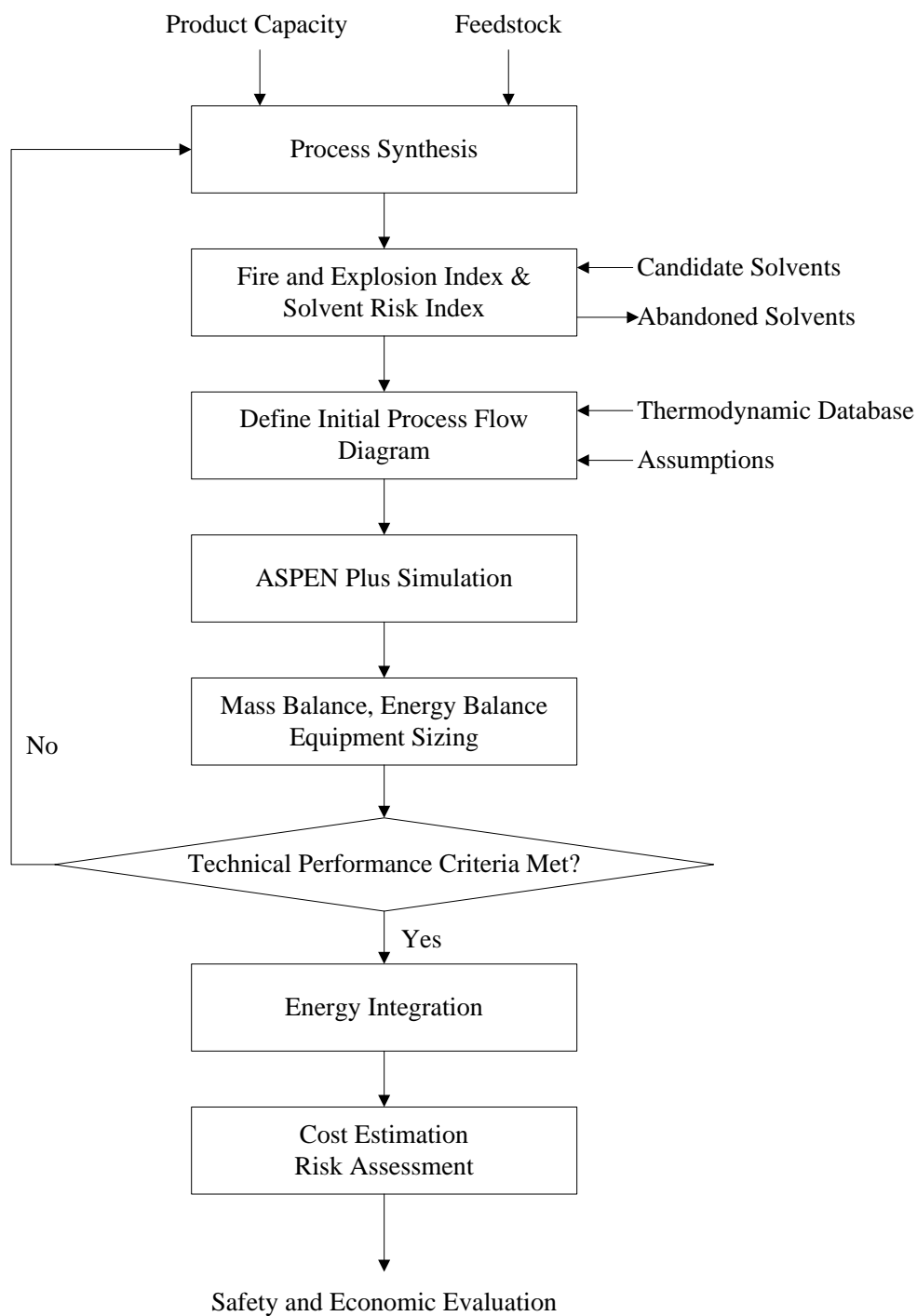


Figure 3-1 Schematic of study approach

CHAPTER IV

PROCESS OVERVIEW

The extraction process consists of five operations: extraction, evaporation, solvent recovery, desolventizing-toasting, and drying. Figure 4-1 presents an overview of the Jatropha seed oil extraction process.

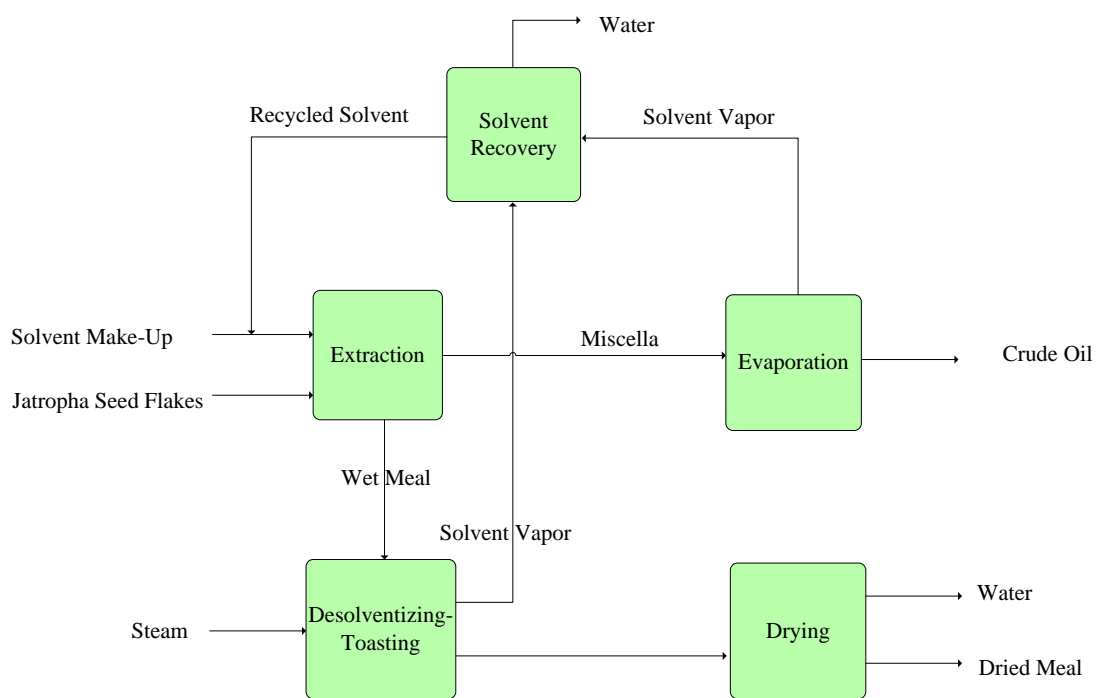


Figure 4-1 Process overview of Jatropha seed oil extraction

4.1 Extraction

In this study, the oil extraction plant's capacity is based on 8,400 tons of seed per day (350,000 kg/hr) fed to the system producing approximately 3,360 tons (22,971 barrels) of crude oil per day. The extraction solvent feed is the same as seed feed. Seventeen solvents have been selected based on Johnson's recommendation (Johnson and Lusas, 1983), as shown in Table 4-1. Furthermore, all solvents are assumed to have the same mutual solubility with *Jatropha* seed oil and are able to extract 98 wt% oil from *Jatropha* seeds. Before extraction, *Jatropha* seeds are cracked to form thin flakes. Thermal treatment and moisturization are performed to increase the solvent extraction efficiency. After heating to 80°C and increasing 12% moisture by weight, seed flakes are conveyed to the extractor (Tzia and Liadakis, 2003). After extraction, the miscella is sent to the evaporator and the solid material (wet meal) is transported to the desolventizer-toaster.

Table 4-1 Candidate solvents for oil extraction

No.	Solvent	No.	Solvent
1	n-Hexane	10	1,1,2-Trichloroethylene
2	n-Heptane	11	Methanol
3	Cyclohexane	12	Ethanol
4	Benzene	13	Isopropanol
5	Toluene	14	n-Butanol
6	Xylene	15	Acetone
7	Dichloromethane	16	Methyl ethyl ketone
8	Chloroform	17	Ethyl acetate
9	1,2-Dichloroethane		

4.2 Evaporation

Following extraction, the miscella is heated and sent to evaporators to remove solvent and water. The purpose of miscella evaporation is to separate solvent from crude oil. Solvent vapors are then condensed in the condenser. During evaporation, evaporators may maintain negative pressure to increase efficiency and reduce energy consumption (Hamm and Hamilton, 2000). After solvent separation, the crude oil can be blended with diesel directly or used as a feedstock for a transesterification or hydrogenation process.

4.3 Desolventizing-Toasting and Drying

In the desolventizer-toaster, residual solvent is removed by steam injection. Once the meal exits the desolventizer-toaster, most of the solvent has been evaporated. The meal discharged from the desolventizer-toaster may contain considerable moisture; thus it must be further dried for final moisture adjustment (Hamm and Hamilton, 2000). The desolventized and toasted meal is passed to the dryer, where excess moisture is removed by heat.

4.4 Solvent Recovery

Solvent recycled from the miscella and meal may contain a considerable amount of water, thereby reducing the extraction efficiency. Therefore, water contained in the solvent must be separated before the recovered solvent can be recycled to the extractor. A decanter is equipped to recover solvents that are immiscible with water. However, a distillation column is required for water-miscible solvents.

4.5 Properties of Jatropha Seed

4.5.1 Chemical Composition

As noted earlier, Jatropha seeds contain oil about 40 percent by weight. In ASPEN Plus, Jatropha seed oil is modeled as a mixture of four fatty acids: palmitic acid, stearic acid, oleic acid, and linoleic acid. Each of these components is available in the ASPEN Plus databank. Besides oil contained in the seed, the remainder of the seed is treated as “nonconventional solid” in ASPEN Plus. Table 4-2 shows the component names and weight percentages of fatty acid in the feed (Chhetri et al., 2008).

Table 4-2 Chemical composition of Jatropha seed and oil (Chhetri et al., 2008)

Jatropha seed composition	wt%
Oil (fatty acid)	40
Others (Nonconventional Solid)	60
Fatty acid composition	wt%
Palmitic acid	14.26
Stearic acid	5.75
Oleic acid	45.79
Linoleic acid	34.2

4.5.2 Physical Properties

The only properties calculated in ASPEN Plus for nonconventional solid components are enthalpy and density. In addition, component diameter is also required if the particle size distribution is involved in the simulation. Jatropha seed enthalpy, density and mean diameter are affected by moisture content. Increases in enthalpy, density, and mean diameter vary with an increase in moisture content. The mean

diameter of Jatropha seed at 12 wt% moisture is given as 13 mm by Garnayak et al. (Garnayak et al., 2008) and the density is described by a linear equation as follows (Garnayak et al., 2008):

$$\rho = 668.55 + 5.15M \quad 4-1$$

where

ρ is the density of Jatropha seed (kg/m³)

M is the weight percentage of moisture in Jatropha seed.

Specific heat of Jatropha seed is required for ASPEN plus to calculate enthalpy because thermal treatments of Jatropha seeds and meal are also involved in heating, desolventizing-toasting, and drying. Unfortunately, values for specific heat of Jatropha seed were not available for this work. Therefore, it was assumed that the specific heat of Jatropha seed is 20% higher than the specific heat of soybean and is calculated by following equation (Deshpande and Bal, 1999):

$$C_p = 1.7328 \times (1 + 4.06 \times 10^{-2} \times M) \quad 4-2$$

where

C_p is the specific heat of Jatropha seed (kJ/kg-K)

M is the weight percentage of moisture containing in Jatropha seed.

4.6 Heat Integration

In the chemical process, there are always requirements for heating cold streams and cooling hot streams. The use of external cooling and heating is not cost effective (El-Halwagi, 2006). In the extraction process, including pretreatment, evaporation, desolventizing-toasting, drying, and solvent recovery, energy consumption is known as one of the highest expenses in the operation cost. Therefore, integration of heating and cooling may plays a significant role in energy cost savings.

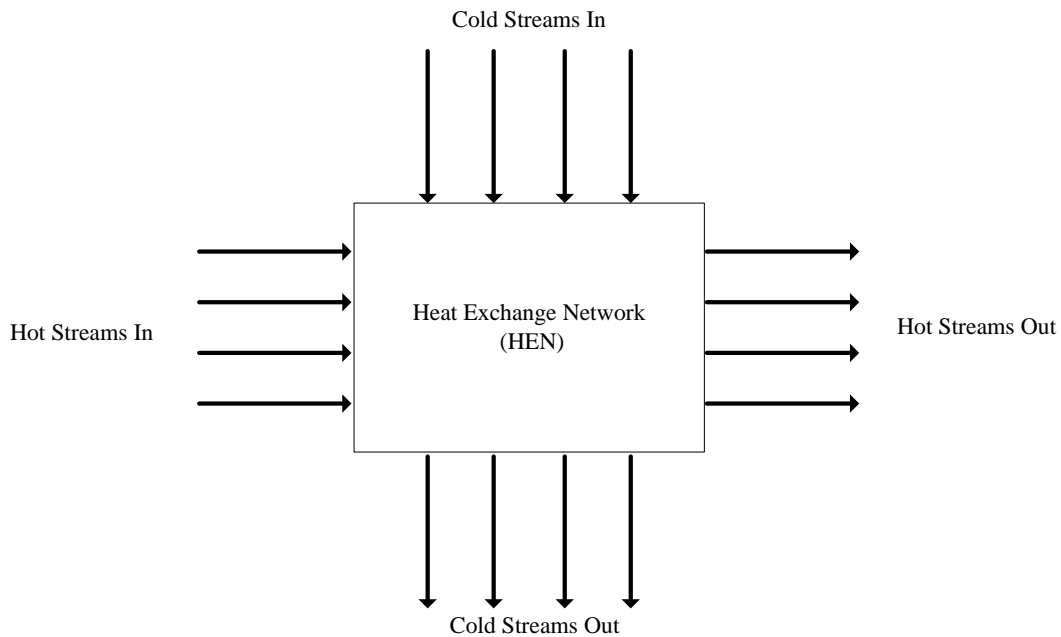


Figure 4-2 Synthesis of heat exchange network (HEN) (Seider, 2009)

Since the 1970s the techniques used for heat exchange network integration have been greatly expanded as shown in Figure 4-2, including graphical method (pinch diagram), temperature interval method (algebraic method), and mathematical approaches (linear programming method). In this study, both temperature interval method and mathematical approach are introduced to determine minimum energy requirement.

Consider a process with N_H hot streams and H_C cold streams. The heat of exchangeable hot loads at u th stream is defined as (El-Halwagi, 2006):

$$HH_{u,z} = F_u Cp_u (T_{z-1} - T_z) \quad 4-3$$

where

u represents the process hot streams, $u = 1, 2, \dots, N_H$

z is the temperature interval, $z = 1, 2, \dots, n$

$F_u C_{p_u}$ is heat capacity for u th process hot stream

T_{z-1} is the supply temperature for z th interval

T_z is the target temperature for z th interval

$HH_{u,z}$ is heat exchange at u th hot stream.

On the other hand, the heat of exchangeable cold loads at v th stream is determined as follows (El-Halwagi, 2006):

$$HC_{v,z} = f_v C_{p_v} (t_{z-1} - t_z) \quad 4-4$$

where

v represents the process cold streams, $v = 1, 2, \dots, N_C$

$f_v C_{p_v}$ is heat capacity for v th process cold stream

t_{z-1} is the supply temperature for z th interval

t_z is the target temperature for z th interval

$HC_{v,z}$ is heat exchange at v th cold stream.

Figure 4-3 shows an example to construct a temperature interval diagram (TID). The heads of vertical arrows represent stream target temperatures and the tails represent stream supply temperature. To ensure thermodynamic feasibility, a minimum heat exchange driving force ΔT^{\min} between the hot streams and cold streams is given (El-Halwagi, 2006).

$$T_z = t_z + \Delta T^{\min} \quad 4-5$$

Interval	Hot Stream	Cold Stream
	H_{P1} T_{H1}^{in}	$T_{H1}^{in} - \Delta T^{min}$
1	$T_{C1}^{in} + \Delta T^{min}$	T_{C1}^{out}
2	$T_{C2}^{out} + \Delta T^{min}$	T_{C2}^{out}
3	H_{P2} T_{H2}^{in}	$T_{H2}^{in} - \Delta T^{min}$
4	T_{H1}^{out}	T_{C1}^{in}
5	$T_{C2}^{out} + \Delta T^{min}$	T_{C2}^{out} C_{P1}
6	H_{P3} T_{H3}^{in}	$T_{H3}^{in} - \Delta T^{min}$
7	$T_{C2}^{in} + \Delta T^{min}$	T_{C2}^{in}
8	T_{H2}^{out}	T_{C3}^{out} C_{P2}
9	$T_{C3}^{in} + \Delta T^{min}$	T_{C3}^{in}
10	T_{H3}^{out}	$T_{H3}^{out} - \Delta T^{min}$ C_{P3}
...
...	T_{CN}^{in}
N	T_{HN}^{out}	

Figure 4-3 Temperature Interval Diagram (El-Halwagi, 2006)

Furthermore, the total heating loads and cooling loads capacity can be represented as (El-Halwagi, 2006):

$$HH_z^{Total} = \sum_{u \text{ passes through interval } z} HH_{u,z} \quad \text{where } u=1,2,\dots,N_H \quad 4-6$$

and

$$HC_z^{Total} = \sum_{v \text{ passes through interval } z} HC_{v,z} \quad \text{where } v=1,2,\dots,N_C \quad 4-7$$

For temperature interval z , the total heating and cooling utility is given by HHU_z^{Total} and HCU_v^{Total} , respectively. As shown in Figure 4-4, the energy balance for the z th interval can be expressed as:

$$HH_z^{\text{Total}} - HC_z^{\text{Total}} = HHU_z^{\text{Total}} - HCU_v^{\text{Total}} + r_{z-1} - r_z \quad 4-8$$

where

$$r_z \geq 0, z = 1, 2, \dots, n$$

r_{z-1} is the residual heat entering the z th interval

r_z is the residual heat leaving the z th interval

r_0 is zero, since no process stream exits above the first interval.

The object of heat integration is to minimize the heating and cooling utilities cost.

$$\text{Minimum } \sum_{z=1}^n CH \times HHU_z^{\text{Total}} + \sum_{z=1}^n CC \times HCU_v^{\text{Total}} \quad 4-9$$

where

CH is the cost of heating utility

CC is the cost of cooling utility.

To address the minimum heating and cooling utilities, an optimization modeling software, LINGO, is applied.

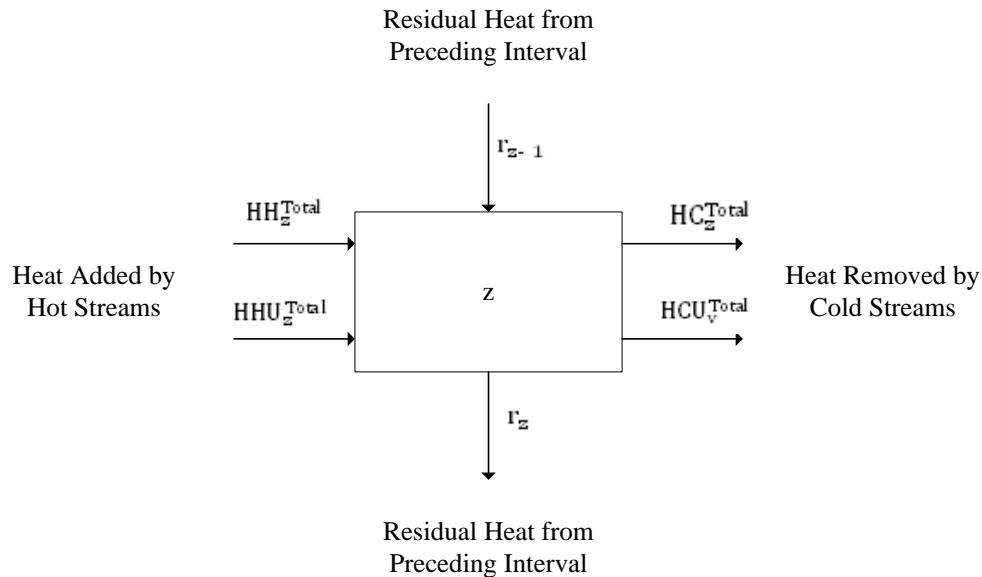


Figure 4-4 Heat balance around temperature interval z (El-Halwagi, 2006)

4.7 Process Design and Simulation

Two oil extraction processes are designed to evaluate the performance of alternative solvents in Jatropha seed oil extraction. Both processes are carried out by ASPEN plus process simulator. UNIQUAC properties are used throughout the simulation.

Case 1: Extraction solvents are immiscible in water

Case 2: Extraction solvents are miscible in water

4.7.1 Case 1: Extraction Solvents Are Immiscible in Water

In this case, shown in Figure 4-5, solvents which are immiscible in water are used for the extraction solvent. Table 4-3 shows process units for case 1. First, Jatropha seeds are conveyed to the crusher (E-101), then heated to 80 °C (HEX-101) before entering to the extractor (E-102). Makeup solvent and recycled solvent are mixed and pumped to E-102.

After extraction, the miscella including solvent and oil is transported to the evaporators (E-201, E-202, and E-203) to separate solvent and oil. The wet Jatropha meal which contains approximately 30 wt% solvent is sent to the desolventizer-toaster (E-301) to recover solvent.

In the evaporation unit, three evaporators (E-201, E-202 and E-203) are installed to recover solvent from the oil. The temperatures are controlled to be able to recover 90 wt% solvent from E-201, 96 wt% from E-202, and 99.8 wt% from E-203. Furthermore, due to thermal decomposition of Jatropha oil start at 203°C, operation temperature for all process units will not be over 203°C (Freire et al., 2009). Solvent vapors from these evaporators are condensed in HEX-205 and pumped to the decanter (E-402). Jatropha oil remaining at the bottom of E-203 is cooled to 45°C (HEX-204) and transported to the storage tank.

To recover solvent from Jatropha meal, 100°C saturated steam is injected into the bottom of the desolventizer-toaster (E-301). Vapors containing water and solvent remaining at the top of the tower are condensed before entering to E-402. After desolventizing, wet meal which contains water enters the dryers (E-302 and E-303) to remove water.

Most of the solvent is recycled in the decanter (E-402) because solvent is immiscible with water. The water-rich stream from the decanter containing small amounts of solvent is pumped to a flash evaporator (E-403) to recover remaining solvent. The recycled solvent then returns to E-102, where it is mixed with the solvent makeup stream.

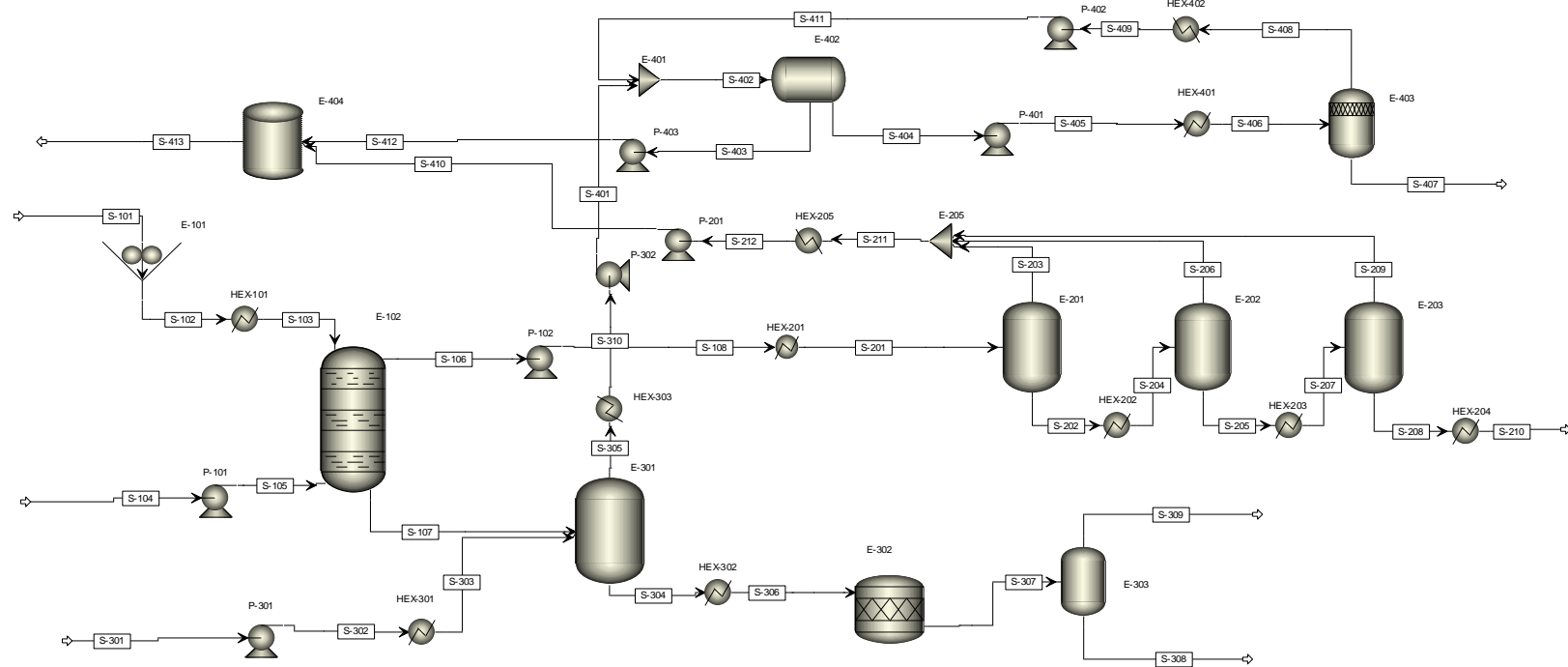


Figure 4-5 Process flow diagram for case 1

Table 4-3 Process units for case 1

E-101	HEX-101	P-101	E-102	E-201	E-202	E-203	HEX-201	HEX-202	HEX-203	HEX-204	HEX-205	P-301
Crusher	Pretreatment Heater	Solvent Feed Pump	Extractor	Evaporator I	Evaporator II	Evaporator III	Evaporator I Heater	Evaporator II Heater	Evaporator III Heater	Crude Oil Cooler	Solvent Condenser	Water Feed Pump
HEX-301	E-301	HEX-302	HEX-303	E-302	E-303	E-401	E-402	HEX-401	HEX-402	E-403	E-404	
Heater	Desolventizer - Toaster	Dryer Heater	Solvent Condenser	Dryer	Dryer	Mixer	Decanter	Reboiler	Condenser	Separator	Solvent Recovery Tank	

4.7.2 Case 2: Extraction Solvents Are Miscible in Water

As shown in Figure 4-6, this case is designed for alcohol solvents. Table 4-4 shows process units for case 1. The mutual solubility of oil and alcohols is low at room temperature, but increases with increasing temperature to be completely miscible before boiling point (Magne and Skau, 1953).

Pretreatment of *Jatropha* seeds is similar to the first case. However, solvents are heated (HEX-102) before entering to the extractor (E-102). During extraction, 50 wt% moisture contained in flakes is also extracted by solvents. The miscella left from the extractor is cooled to room temperature and sent to the decanter (E-201). The wet meal containing approximately 30 wt% solvent is conveyed to the desolventizer-toaster (E-301) to recover solvent.

In E-201, liquid is separated into two phases, oil and aqueous. The aqueous phase is an alcohol-water mixture and the oil phase contains only a small amount of alcohol. The oil phase is pumped to the evaporator (E-202) to recover remaining alcohol. The aqueous stream from E-201 is heated and sent to a distillation column (E-402).

The vapors from the E-301 are sent to a distillation column (E-304). Distillation columns E-304 and E-402 produce a solvent concentration of 94 wt%. Solvent recovered from E-304 and E-402 and E-202 are mixed and then return to E-102.

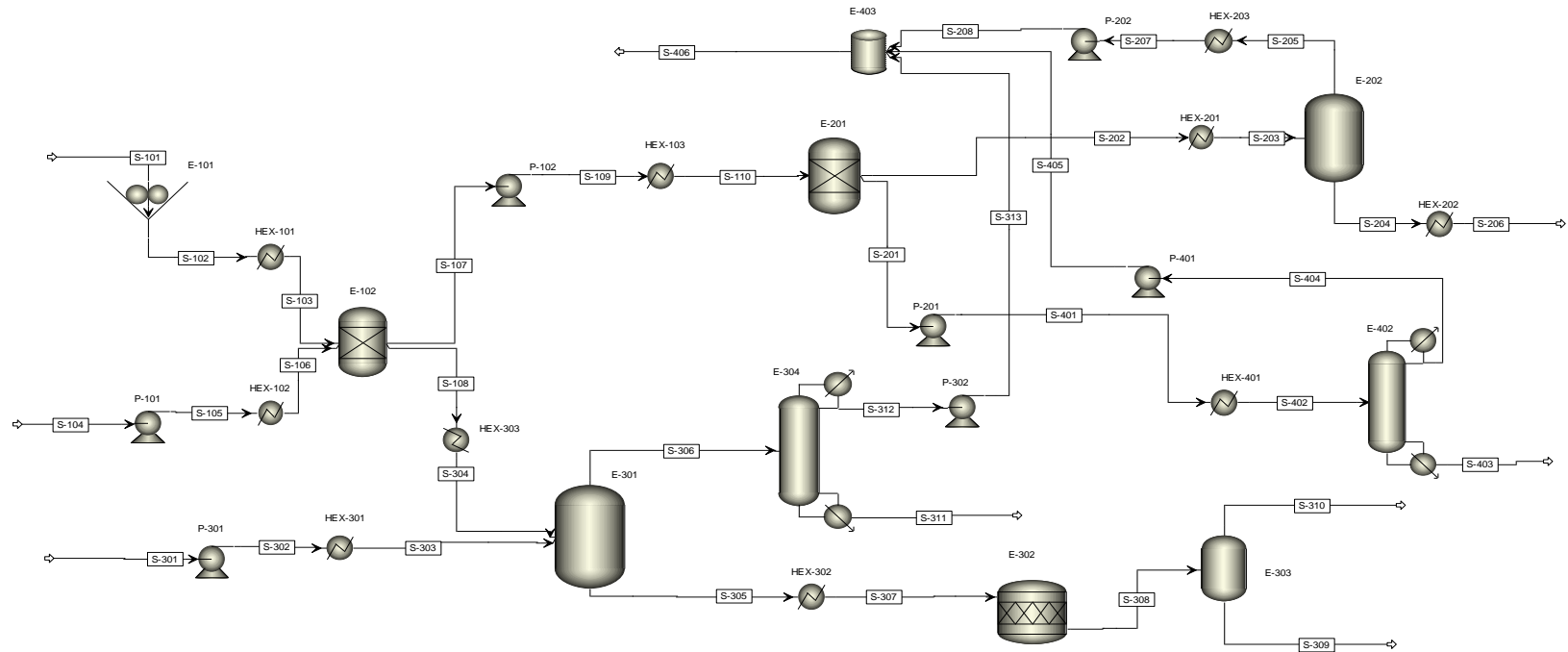


Figure 4-6 Process flow diagram for case 2

Table 4-4 Process units for case 2

E-101	HEX-101	HEX-102	P-101	E-102	P-102	E-201	P-201	E-202	HEX-201	HEX-202	HEX-203	P-202	P-301
Crusher	Pretreatment Heater	Solvent Heater	Solvent Feed Pump	Oil Extractor	Pump	Decanter	Pump	Evaporator	Evaporator Heater	Crude Oil Cooler	Solvent Condenser	Pump	Water Feed Pump
HEX-301	HEX-304	E-301	HEX-302	E-302	E-303	E-304	HEX-303	P-302	E-401	HEX-401	E-304	P-301	E-403
Heater	Heater	Desolventizer-Toaster	Dryer Heater	Dryer	Dryer	Distillation Tower I	Heater	Pump	Mixer	Heater	Distillation Tower II	Pump	Recovered Solvent Tank

CHAPTER V

PROCESS RISK ASSESSMENT AND EXTRACTION SOLVENT SELECTION

Figure 5-1 shows the procedure to evaluate risks associated with the extraction solvent. The first step is to calculate the Fire and Explosion Index (F&EI). F&EI is a process hazard indicator from Dow's Fire and Explosion Index published by the American Institute of Chemical Engineers (AIChE). It is based on historical data and potential energy of the evaluated material. Table 5-1 presents process hazards and their corresponding penalties for calculating F&EI.

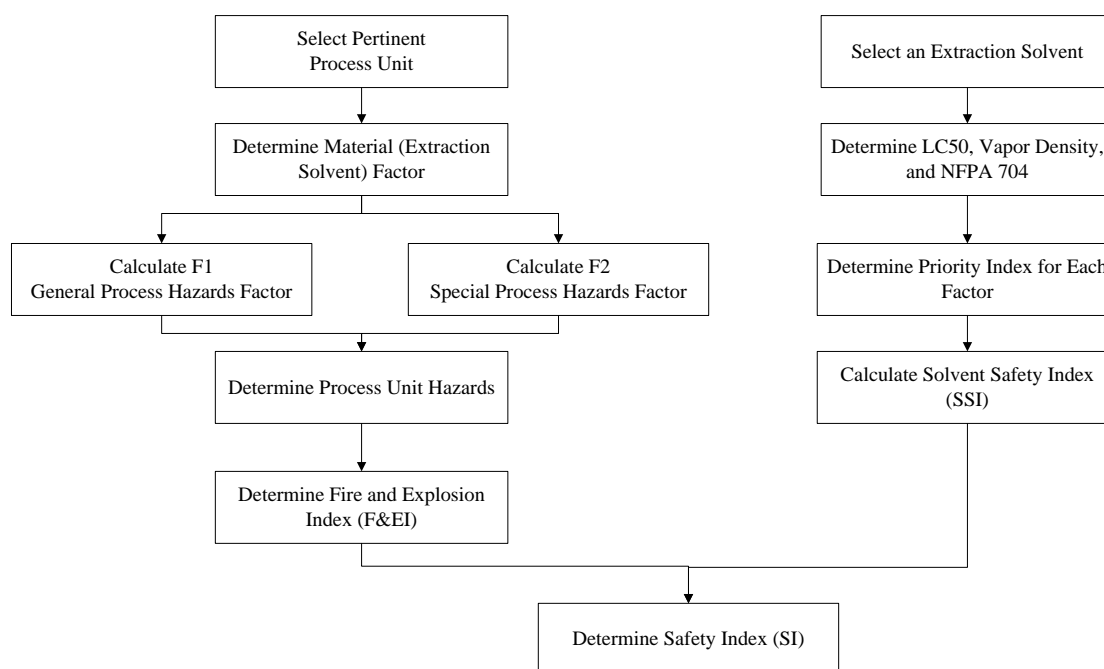


Figure 5-1 Procedure for calculating Safety Index (American Institute of Chemical Engineers., 1994)

Table 5-1 Table for calculating fire and explosion index (American Institute of Chemical Engineers., 1994)

1. General Process Hazards		Penalty Factor Range	Penalty Factor Used
Base Factor		1.00	
A. Exothermic Chemical Reactions		0.30-1.25	
B. Endothermic Process		0.20-0.40	
C. Material Handling Transfer		0.25-1.05	
D. Enclosed or Indoor Process Units		0.25-0.90	
E. Access		0.20-0.35	
F. Drainage and Spill Control gal or cum.		0.25-0.50	
General Process Hazards Factor (F1)			
2. Special Process Hazards			
Base Factor		1.00	
A. Toxic Material(s)		0.20-0.80	
B. Sub-Atmospheric Pressure (<500 mmHg)		0.50	
C. Operation In or Near Flammable Range		Inerted	Not Inerted
1. Tank Farms Storage Flammable Range		0.50	
2. Process Upset or Purge Failure		0.30	
3. Always in Flammable		0.80	
D. Dust Explosion		0.25-2.00	
E. Pressure			
Operating Pressure			psig
Relief Setting			psig
F. Low Temperature		0.20-0.30	
G. Quantity of Flammable/Unstable Material			
Quantity			lb
Hc =			BTU/lb
1. Liquids or Gases in Process			
2. Liquids or Gases in Storage			
H. Corrosion and Erosion		0.10-0.75	
I. Leakage-Joints and Packing		0.10-1.5	
J. Use of Fired Equipment		0.10-1.00	
K. Hot Oil Heat Exchange System		0.15-1.15	
L. Rotating Equipment		0.50	
Special Process Hazards Factor (F2)			
Process Unit Hazards Factor (F1 x F2) = F3			
Material Factor (MF)			
Fire and Explosion Index (F3 x MF = F&EI)			

To calculate F&EI, process units that are considered for key importance to the extraction process and that would have the greatest impact on the magnitude of a potential fire and explosion are selected to participate in the evaluation (American Institute of Chemical Engineers., 1994). The second step is to determine the material factor (MF), which is the basis of F&EI. After the general process hazards factor (F1) and special process hazards factor (F2) are calculated, the process unit hazards (F3) is determined by the product of F1 and F2. Then, the F&EI is calculated as the product of F3 and MF (American Institute of Chemical Engineers., 1994).

After F&EI, solvent hazards and risks are evaluated by the Solvent Safety Index (SSI). To determine SSI, three properties for candidate solvents are used: LC₅₀, vapor density and NFPA 704. The next step is to estimate the index value for each property. The value assigned depends on the solvent safety index metric. After that, the SSI for each solvent is found by applying a weighting factor to each sub-index. Finally, the Safety Index (SI) of the extraction process can be determined.

5.1 Fire and Explosion Index

5.1.1 Material Factor

The material factor is a measure of the intrinsic rate of energy release from burning, explosion, or chemical reaction (American Institute of Chemical Engineers., 1994). Values for candidate solvents are given in Dow's Fire and Explosion Index and are presented in Appendix A. Moreover, the guide also provides a procedure for calculating values for unlisted chemicals.

5.1.2 Process Unit Hazards

5.1.2.1 General Process Hazards

A. Exothermic Chemical Reactions:

This penalty is taken if a chemical reaction takes place. The penalty varies from 0.3 to 1.25. No penalty is taken for no chemical reaction in the process.

B. Endothermic Processes:

A penalty of 0.2 is selected for any endothermic process that occurs in the reactor. The value increases to 0.4 if the reactor's energy is provided by the combustion of a solid, liquid, or gaseous fuel. No penalty is taken in the absence of endothermic reaction.

C. Material Handling and Transfer:

This subsection evaluates the potential for fire involving process units during the handling, transfer, and storage of materials. The penalty varies from 0.2 for non-flammable and low flammable solvent, to 0.8 for high flammable solvents. Detailed penalty information is presented in Appendix B.

D. Enclosed or Indoor Process Units:

This category is used to identify the additional hazards of inadequate or non-existent ventilation. In this work, it is assumed that facilities are constructed in open areas and no penalty is taken.

E. Access:

Process units must have at least two access points for emergency equipment. Processes which do not have adequate access are penalized. In this analysis, two side access points are assumed in the design and no penalty is taken.

F. Drainage and Spill Control:

This factor gives a penalty for design condition that could cause large spills of flammable or combustible liquids near process equipment. A design that gives sufficient drainage and spill control is assumed and no penalty is applied.

Once the general process hazards have been evaluated, General Process Hazard (F1) is calculated by the sum of all the factors in this subsection.

5.1.2.2 Special Process Hazards

A. Toxic Material(s):

Toxic materials will prevent or inhibit emergency response personnel from handling an incident. Penalties are calculated by multiplying 0.2 and by the health value in NFPA 704. However, one important note is that these factors are only intended to represent emergency response limitations which can cause additional loss by toxic materials (American Institute of Chemical Engineers., 1994). Detailed penalty information is presented in Appendix B.

B. Sub-Atmospheric Pressure (< 500 mmHg):

This penalty allows for the hazard which is caused by air leakage. A 0.50 penalty is given due to negative pressure in the evaporator.

C. Operation In or Near Flammable Range:

This factor includes three operating conditions: flammable liquids storage in tank, process equipment or process storage tanks that could be in or near flammable range, and processes or operations that are by nature always in or near the flammable range. However, if a penalty is applied in subsection B, do not add a penalty for this subsection. For this study, no penalty is taken in this section (American Institute of Chemical Engineers., 1994).

D. Dust Explosion:

A penalty is given if any process unit involves dust handling operations, such as transferring, blending, grinding, bagging, etc. During the extraction process, particle size of Jatropha seed flakes and meal are believed too heavy to be suspended in air, and moisture in flake and meal also make it more difficult for them to float. Therefore, no penalty is given.

E. Pressure:

If operating pressures are above atmospheric, a penalty will be given for the risk posed by flammable materials potentially released from the process. No penalty is taken because all process units operate at or below atmospheric pressure.

F. Low Temperature:

If operation temperature is lower than transition temperature, it can increase material brittleness. In this study, operating temperatures are above the materials' transition temperature for all units. Therefore, no penalty is taken.

G. Quantity of Flammable/Unstable Material:

This penalty indicates the hazard and risk of large amounts of hazardous materials in the process. Three categories are covered in this subsection: liquids or gases in the process, liquids or gases in storage, and combustible solids in storage. Only one of them needs to be applied for the entire subsection. The first category, liquid or gases in the process, is chosen for this analysis and the penalty for each solvent is calculated by equation 5-1. The amount of solvent in the process is assumed to be equivalent to the amount of feedstock solvent. X is the amount of feedstock solvent and Y is the penalty that will be received.

$$\begin{aligned} \text{Log } Y = & 0.17179 + 0.42988(\text{Log } X) - 0.37244 (\text{Log } X^2) - 0.177112 (\text{Log } X^3) \\ & -0.029984 (\text{Log } X^4) \end{aligned} \quad 5-1$$

H. Corrosion and Erosion:

A good design can prevent corrosion and erosion in the system, although they still occur under certain conditions, such as when using highly corrosive materials and during severe weather conditions. Prevention of corrosion and erosion is assumed to be designed in the process; thus, a minimum penalty of 0.1 is given.

I. Leakage Joints and Packing:

This subsection considers the possibility of leakage from gaskets, seals of joints, and shafts and packing. A minimum penalty of 0.1 is used in this factor.

J. Use of Fired Equipment:

This penalty applies to the presence of heating equipment, such as boilers and furnaces, heated by combustion. In this study, steam is assumed to supply all heating requirements and the boiler is assumed to be far away from other process units. Therefore, a minimum penalty of 0.1 is taken.

K. Hot Oil Heat Exchange System:

This term gives a penalty for hot oil fluids used in heat exchangers. Since steam is the only heating transfer in the process, no penalty is received in this subsection.

L. Rotating Equipment:

This factor recognizes the hazard from large pieces of rotating equipments, such as compressors and centrifuges. No penalty is applied because no large rotating equipment is used.

Once all special process hazards have been evaluated, Special Process Hazards (F2) is estimated from the sum of penalty factors applied in this subsection.

5.2 Solvent Safety Index

F&EI provides a method to evaluate process hazard. However, it does not include consideration of material hazard to humans and animals in the surrounding area. Therefore, a Solvent Safety Index (SSI) for evaluating the hazard of extracting solvents is developed to complement F&EI. In this study, three factors are considered to evaluate the SSI: LC_{50} , vapor density and the health subsection in NFPA 704.

5.2.1 LC_{50}

Lethal concentration 50, also known as LC_{50} , is the concentration of a material in the surrounding medium such as air or water that will kill half of the sample population of test subjects (mice or rats) in a certain amount of time (1 or 4 hours). This value gives an idea of the relative toxicity of an inhalable material. In here, 4-hour inhalation exposure for rat is used as the measure.

5.2.2 Vapor Density

Vapor density is the relative weight of a gas or vapor with respect to air. Substances lighter than air have a vapor density less than 1.0, and substances heavier than air have a vapor density higher than 1.0. The value of the vapor density of a chemical implies the potential hazard to personnel and the environment. High vapor density substances disperse closer to the ground, accumulate in a smaller area, and can affect the surrounding population more quickly than low vapor density substances (Pokoo-Aikins et al., 2010).

5.2.3 NFPA 704

NFPA704 is the standard system for the identification of material hazard for emergency response. As shown in Figure 5-2, its colored diamond shape gives an immediate indication to emergency personnel to quickly identify the hazards of nearby materials. The blue HEALTH subsection is used to produce the SSI. Its level is rated on a scale from 0 (no hazard; normal substance) to 4 (can be lethal) .

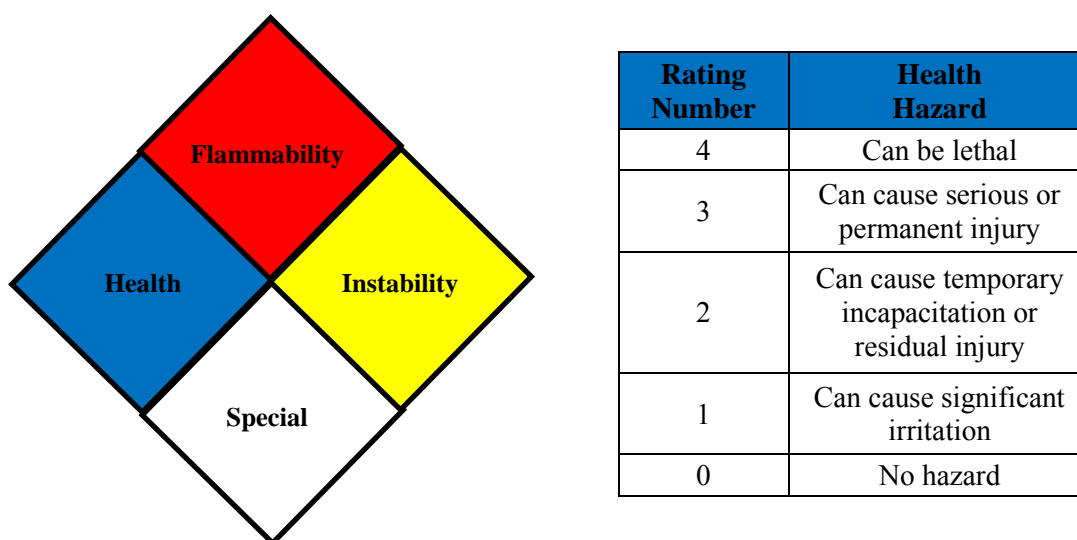


Figure 5-2 NFPA704 Diamond (National Fire Protection Association, 2011)

5.2.4 Solvent Safety Index Calculation

Table 5-2 presents the solvent safety ranking metric. It indicates the hazard level of a solvent associated with the value of LC_{50} , vapor density and NFPA 704. From 1-5, higher priority index values indicate higher toxicity and hazard or risk, while lower priority index values indicate lower toxicity and hazard or risk.

Table 5-2 Solvent Safety Index metric

Priority Index	LC₅₀ rat ppm/4hr	Vapor Density Air = 1	NFPA 704 Health
1	> 100,000	<1	0
2	10,000-100,000	1-1.9	1
3	1000-10,000	2-2.9	2
4	100-1000	3-3.9	3
5	<100	>= 4	4

Furthermore, weighting factors (Pokoo-Aikins et al., 2010) are applied to give greater penalty to solvents that have higher priority index values in each category, as shown in Table 5-3. The SSI value for each solvent is calculated by equation 5-2.

Table 5-3 Weighting Factor (Pokoo-Aikins et al., 2010)

Priority Index	Weighting Factor
(I)	(WF)
1	1
2	2
3	3
4	4
5	5

$$SSI = I_{LC50} \times WF_{LC50} + I_{VD} \times WF_{VD} + I_{NFPA} \times WF_{NFPA}$$

5-2

where

SSI is the Solvent Safety Index value for a solvent

I_{LC50} is the priority index value of LC_{50}

I_{VD} is the priority index value of vapor density

I_{NFPA} is the priority index value of NFPA 704

WF_{LC50} is the weighting factor for the corresponding LC_{50}

WF_{VD} is the weighting factor for the corresponding vapor density

WF_{NFPA} is the weighting factor for the corresponding NFPA 704

After the SSI has been calculated, the Safety Index (SI) is calculated by multiplying the F&EI and the SSI, as shown in equation 5-3. A higher SI value indicates a higher risk or hazard.

$$SI = F\&EI \times SSI \quad 5-3$$

where

SI is the Safety Index

F&EI is the Fire and Explosion Index

SSI is the Solvent Safety Index

The method used to calculate SI from F&EI and SSI is flexible. It can be determined by the weighted average of F&EI and SSI or the product of F&EI and SSI. In addition, it is very important to understand that the process may be inherently safer with respect to one indicator, but unsafe according to another indicator. Therefore, interaction between each sub-index, such as index value range and average weighting, should be considered. In this study, the product of F&EI and SSI is applied to generate SI.

5.3 Potential Loss

In addition to calculating F&EI, SSI and SI for the process, it is necessary to obtain an appropriate dollar value to evaluate the property loss caused by the damage. Dow's F&EI also provides a strategy to estimate the potential loss following the fire or explosion. As shown in Figure 5-3, six factors are developed to determine potential loss:

Damage Factor, Area of Exposure, Replacement Value, Base Maximum Probable Property Damage, Loss Control Credit Factor, and Actual Maximum Probable Property Damage.

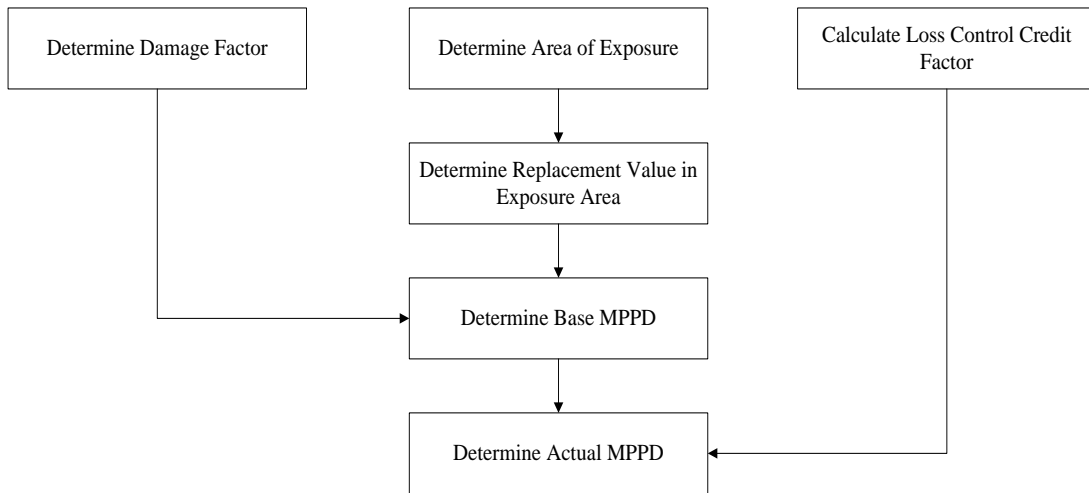


Figure 5-3 Procedure for estimating property loss caused by damage (American Institute of Chemical Engineers., 1994)

5.3.1 Damage Factor

The first step is to determine the Damage Factor for the process unit. It is a function of MF and F3. Figure 5-4 shows the Damage Factor as a function of MF along constant F3 values.

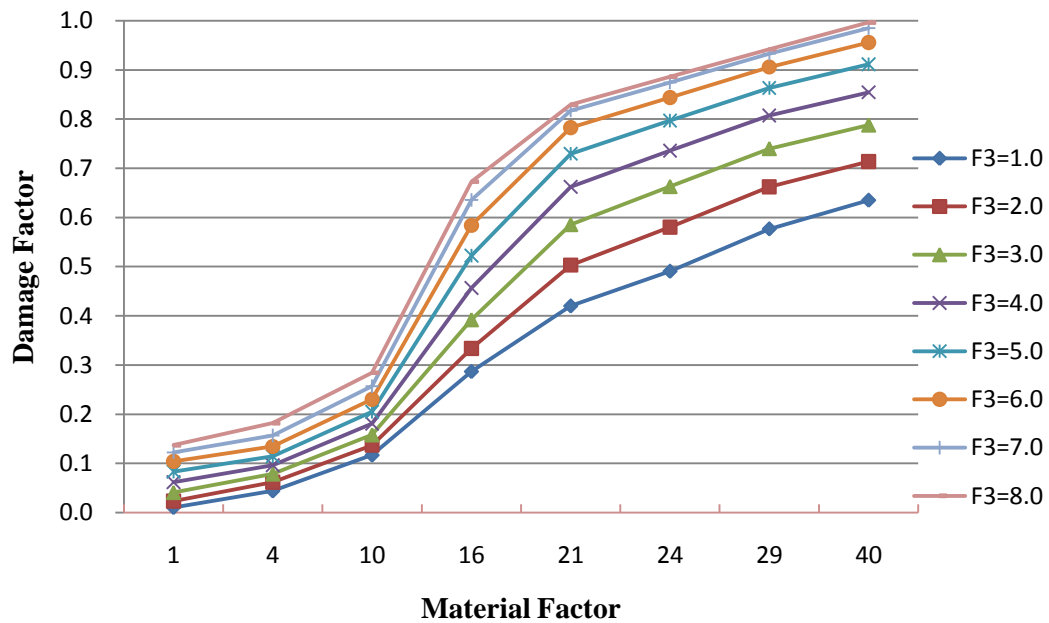


Figure 5-4 Damage Factor (American Institute of Chemical Engineers., 1994)

5.3.2 Area of Exposure

The second step is to calculate the Area of Exposure as shown in Figure 5-5. This represents the damage area affected by a fire or explosion in the process unit. First, the radius of exposure is estimated by multiplying the F&EI by 0.84 (American Institute of Chemical Engineers., 1994). The area of exposure is determined by equation 5-4

$$\text{Area of Exposure} = \pi R^2$$

5-4

where

R is the exposure radius

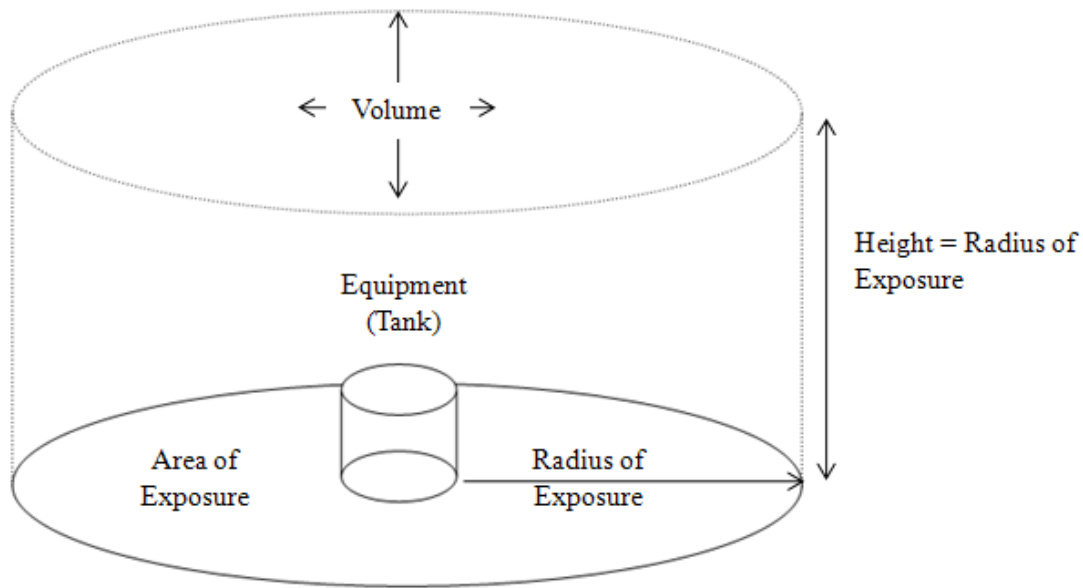


Figure 5-5 Area of exposure (American Institute of Chemical Engineers., 1994)

5.3.3 Replacement Value

The following step is to determine the Replacement Value within area of exposure. It is calculated by equation 5-5 (American Institute of Chemical Engineers., 1994)

$$\text{Replacement Value} = \text{Total Capital Investment} \times 0.82 \quad 5-5$$

5.3.4 Base Maximum Probable Property Damage (Base MPPD)

After Replacement Value and Damage Factor have been determined, the Base Maximum Probable Property Damage is estimated by multiplying the Replacement Value by the Damage Factor. It represents the maximum property damage within the exposure area.

5.3.5 Loss Control Credit Factor

The Loss Control Credit Factors (Table 5-4) allow for the reduction in the potential loss given by the preventive and protective measures incorporated in the design. It is determined by applying the following procedure:

1. Enter the appropriate credit factor to the right of each credit item chosen.
2. A lower credit factor value means a higher loss control protection. If there is no loss control protection, 1.00 is chosen.
3. Each category's Loss Control Credit Factor is the product of all factors used in the category.
4. The overall Loss Control Credit Factor is calculated by $C1 \times C2 \times C3$.

In this study, three scenarios are considered for the sensitivity analysis of loss control credit factor:

1. All loss control features have the highest protection. Therefore, the lowest Loss Control Credit Factor value is chosen for each feature.
2. All loss features have the lowest protection. Therefore, the highest Loss Control Credit Factor value is given for each feature.
3. There is no loss control prevention in the process; thus 1.00 is selected for all loss control features.

Table 5-4 Loss Control Credit Factor (American Institute of Chemical Engineers., 1994)

Loss Control Credit Factors			
1. Process Control Credit Factor (C1)			
	Feature	Credit Factor Range	Credit Factor Used
	a. Emergency Power	0.98	
	b. Cooling	0.97-0.99	
	c. Explosion Control	0.84-0.98	
	d. Emergency Shutdown	0.96-0.99	
	e. Computer Control	0.93-0.99	
	f. Inert Gas	0.94-0.96	
	g. Operation Instructions/Procedures	0.91-0.99	
	h. Reactive Chemical Review	0.91-0.99	
	i. Other Process Hazard Analysis	0.91-0.98	
	C₁ Value	>>>	
2. Material Isolation Credit Factor (C2)			
	Feature	Credit Factor Range	Credit Factor Used
	a. Remote Control Valves	0.96-0.98	
	b. Dump/Blowdown	0.96-0.98	
	c. Drainage	0.91-0.97	
	d. Interlock	0.98	
	C₂ Value	>>>	
3. Fire Protection Credit Factor			
	Feature	Credit Factor Range	Credit Factor Used
	a. Leak Detection	0.94-0.98	
	b. Structural Steel	0.95-0.98	
	c. Fire Water Supply	0.94-0.97	
	d. Special Systems	0.91	
	e. Sprinkler Systems	0.74-0.97	
	f. Water Curtains	0.97-0.98	
	g. Foam	0.92-0.97	
	h. Hand Extinguishers/Monitors	0.93-0.98	
	i. Cable Protection	0.94-0.98	
	C₃ Value	>>>	
	Loss Control Credit Factor		

5.3.6 Actual Maximum Probable Property Damage (Actual MPPD)

Once Loss Control Credit Factors have been determined, the Actual Maximum Probable Property Damage (Actual MPPD) can be calculated by the product of Base MPPD and the Loss Control Credit Factor. The result presents the property loss when the process is equipped with adequate protecting features (Towler and Sinnott, 2008). The value of each factor is entered in Table 5-5, which is used to determine Actual MPPD.

Table 5-5 Table for calculating Potential Loss (American Institute of Chemical Engineers., 1994)

Potential Loss			
1. Fire & Explosion Index (F&EI)			
2. Radius of Exposure		m	
3. Area of Exposure		m ²	
4. Value of Area Exposure		MMS\$	
5. Damage Factor			
6. Base Maximum Probable Property Damage (Base MPPD)		MMS\$	
7. Loss Control Credit Factor	=		
8. Actual Maximum Probable Property Damage (Actual MPPD)		MMS\$	

CHAPTER VI

RESULTS AND DISCUSSION

6.1 Solvent Selection

Seventeen candidates were evaluated for the oil extraction process based on Johnson's suggestions (Johnson and Lusas, 1983), as shown in Table 6-1. Meanwhile, candidates' F&EI values are also presented. Detailed information and calculations are given in Appendix A and B. The greatest value represents the highest process hazard or risk, and the lowest value represents the lowest hazard or risk. Chloroform has the lowest index value, followed by dichloromethane and 1,1,2-trichloroethylene.

Table 6-1 Fire and Explosion Index

	Solvents	Fire and Explosion Index (F&EI)
1	n-Hexane	146.9
2	n-Heptane	147.1
3	Cyclohexane	146.9
4	Benzene	152.3
5	Toluen	152.3
6	Xylene	152.4
7	Dichloromethane	19.3
8	Chloroform	4.5
9	1,2-Dichloroethane	86.4
10	1,1,2-Trichloroethylene	49.1
11	Methanol	153.4
12	Ethanol	143.6
13	Isopropanol	144.5
14	n-Butanol	145.1
15	Acetone	144.1
16	Methyl ethyl ketone	144.7
17	Ethyl acetate	148.6

As shown in Table 6-2, ethanol has the lowest SSI (9) which means it has the best performance in the ranking. In fact, ethanol is the only organic solvent that can be digested by humans, and it exists in natural foods. Furthermore, compared to other candidates, acetone and methyl ethyl ketone present a relatively lower SSI (14) than the remaining solvents. However, though 1,1,2-trichloroethylene, 1,2-dichloroethane, and chloroform have lower F&EI values, their toxicity property increased their SSI subsection. Detailed information including LC₅₀, NFPA and vapor density for each solvent are presented in Appendix C.

Table 6-2 Solvent Safety Index

	Solvents	LC₅₀ ppm/4H rate	NFPA (Health)	Vapor Density (Air = 1)	Solvent Safety Index (SSI) Applied weighting factor
1	n-Hexane	2	2	4	24
2	n-Heptane	2	2	4	24
3	Cyclohexane	3	2	4	29
4	Benzene	3	3	3	27
5	Toluene	2	3	4	29
6	Xylene	2	3	4	29
7	Dichloromethane	3	3	3	27
8	Chloroform	3	3	4	34
9	1,2-Dichloroethan	3	4	4	41
10	1,1,2-Trichloroethylene	3	3	5	43
11	Methanol	2	4	2	24
12	Ethanol	2	2	2	12
13	Isopropanol	3	2	3	22
14	n-Butanol	3	2	3	22
15	Acetone	2	2	3	17
16	Methyl ethyl ketone	2	2	3	17
17	Ethyl acetate	3	3	4	34

Table 6-3 presents the SI for alternative solvents in the *Jatropha* seeds oil extraction process. Moreover, prices for the corresponding solvents were also collected from ICIS.com.

Table 6-3 Safety Index and solvent price

	Solvents	Safety Index (SI)	Price (\$/lb)
1	n-Hexane	3525	0.42
2	n-Heptane	3530	0.365
3	Cyclohexane	4260	0.503
4	Benzene	4112	0.468
5	Toluene	4417	0.387
6	Xylene	4420	0.392
7	Dichloromethane	520	0.41
8	Chloroform	154	0.25
9	1,2-Dichloroethane	3543	0.18
10	1,1,2-Trichloroethylene	2110	0.63
11	Methanol	3681	0.167
12	Ethanol	1723	0.34
13	Isopropanol	3179	0.79
14	n-Butanol	3192	0.94
15	Acetone	2449	0.63
16	Methyl ethyl ketone	2460	0.84
17	Ethyl acetate	5053	0.59

Next, the SI value and price for each candidate is plotted in Figure 6-1. Two criteria are required for selecting solvents. First, both price and SI values are lower than hexane's values. Secondly, solvents that have higher SI values, but their prices are lower than hexane's are also considered.

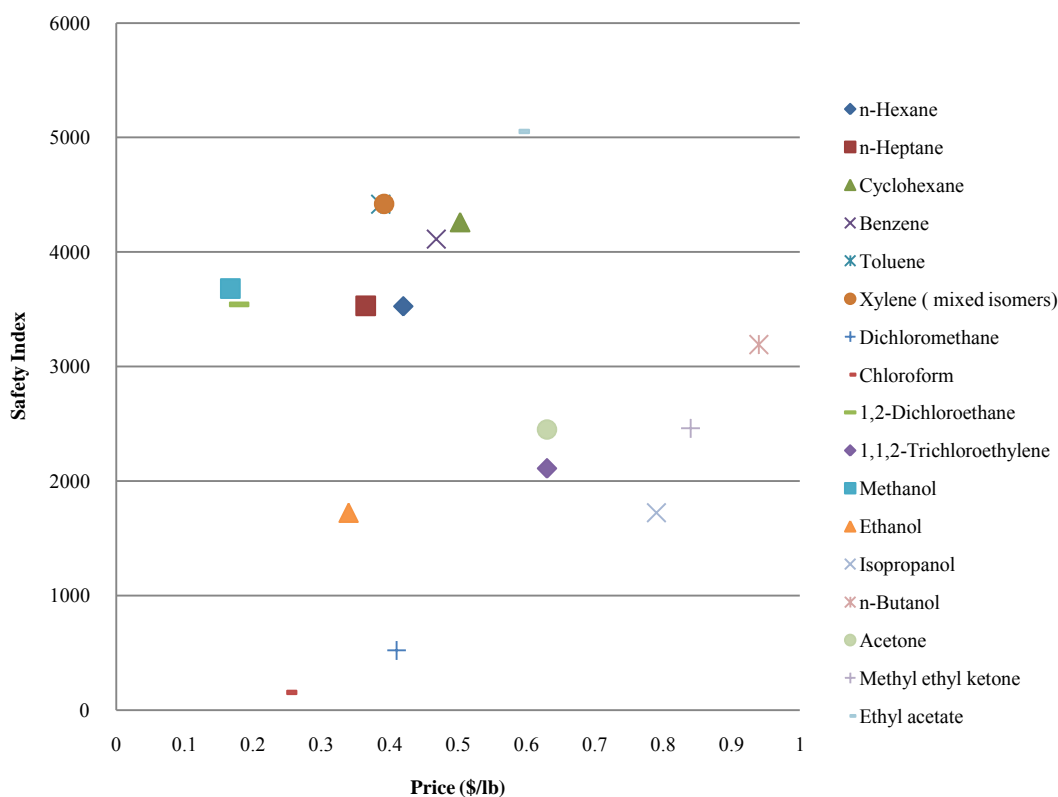


Figure 6-1 Plot of Safety Index (SI) and price

As shown in Figure 6-2, the base point in the plot is n-hexane. One vertical and one horizontal dashed line separate the figure into 4 regions, with n-hexane at the intersection of the two lines. Regions 1–4 consist of areas of lower price and SI, lower price and higher SI, higher price and SI, and higher price and lower SI, respectively. Therefore, solvents located in the regions 1 and 2 satisfy the selection criteria, while solvents located in the regions 3 and 4 will not be considered as viable candidates. Table 6-4 shows the solvents from regions 1 and 2.

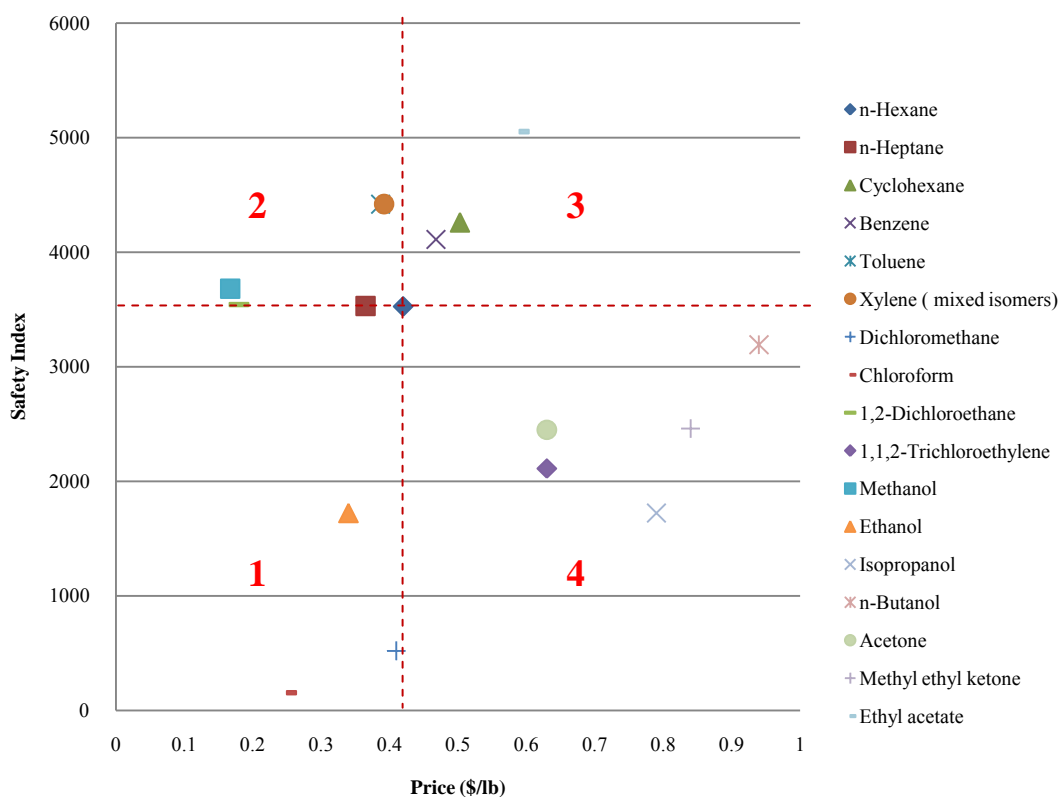


Figure 6-2 Plot of SI value and solvent price with selection regions

Table 6-4 Selected Extraction Solvents

	Solvent
Region 1	Dichloromethane
	Chloroform
	1,2-Dichloroethane
	Methanol
	Ethanol
Region 2	n-Heptane
	Toluene
	Xylene

6.2 Process Analysis and Cost Estimation

6.2.1 Jatropha Oil Yield

The yield from extraction process for each solvent is shown in Table 6-5. The maximum yield of 39.2% is obtained by n-hexane and dichloromethane, and chloroform is next highest. The lowest yield is xylene with 38.6%. Xylene's boiling point (137°C) is higher than other solvents, which decreased oil-solvent separation and resulted in lower yield.

Table 6-5 Product amount and yield

Solvent used	Jatropha Oil Amount (kg/hr)	Yield
n-Hexane	137195	39.2%
n-Heptane	136519	39.0%
Toluene	135329	38.7%
Xylene	134931	38.6%
Dichloromethane	137177	39.2%
Chloroform	136988	39.1%
1,2-Dichloroethane	136491	39.0%
Methanol	135819	38.8%
Ethanol	135811	38.8%

6.2.2 Calculation of Utilities Cost

Energy consumption is known to be one of the largest operating expenses in oil extraction process. Therefore, it is necessary to incorporate heat integration to minimize heating and cooling utilities. Figures 6-3 and 6-4 illustrate energy usage before and after heat integration respectively. The prices for heating (steam), cooling (water), and cooling (refrigerant) utilities are \$7.6, \$5.7, and \$13.3 per million joules (MJ) respectively (Myint and El-Halwagi, 2009). Moreover, the use of refrigerant in the cooling system does not participate in the heat integration process.

Figure 6-5 compares utilities costs before and after heat integration and Table 6-6 presents the percent difference in utilities costs before and after heat integration. They indicate that heat integration plays an important role in reducing external energy usage, especially for n-hexane, n-heptane, toluene, xylene, chloroform, and 1,2-dichloroethane solvents. Methanol and ethanol are the two highest energy consuming solvents whether applying heat integration or not. Less heat is required when considering dichloromethane because of its low boiling point ($^{\circ}\text{C}$). However, refrigerant requirements in the cooling system were greater, requiring more energy consumption.

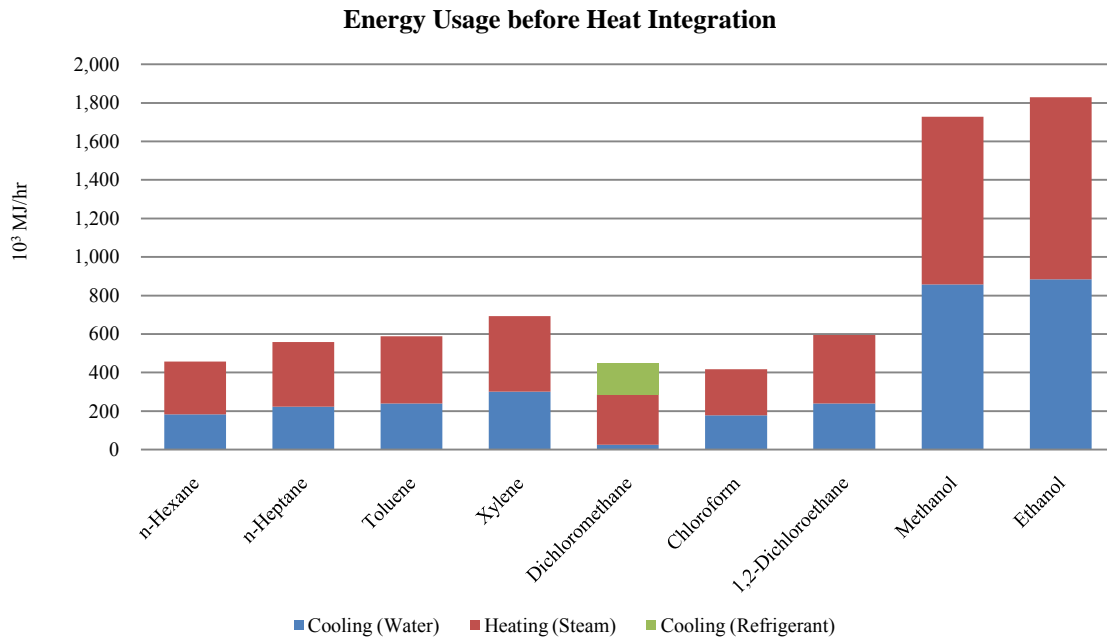


Figure 6-3 Energy usage without heat integration

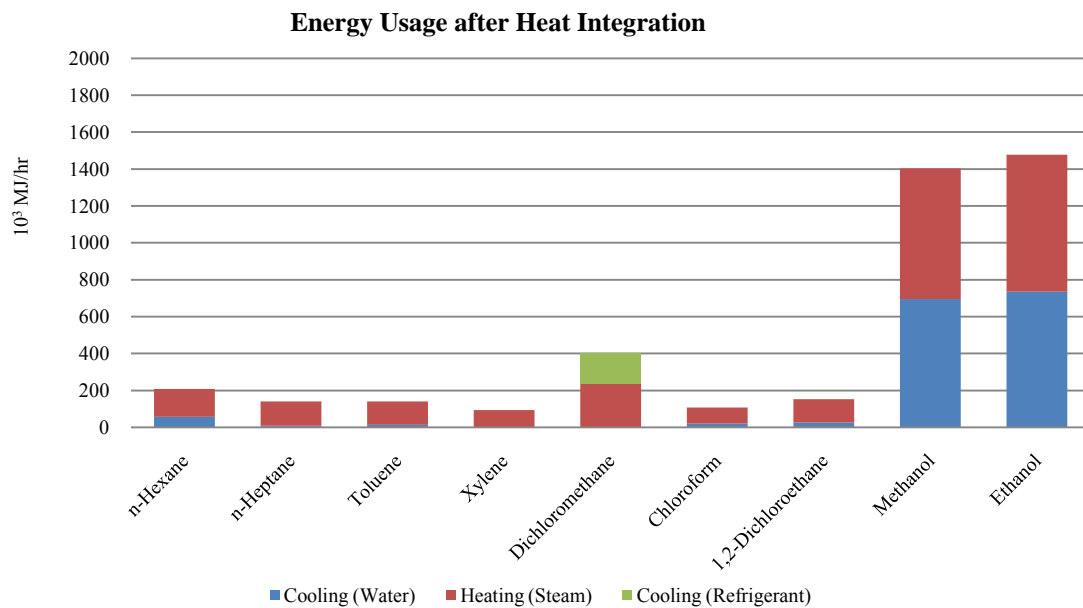


Figure 6-4 Energy usage after heat integration

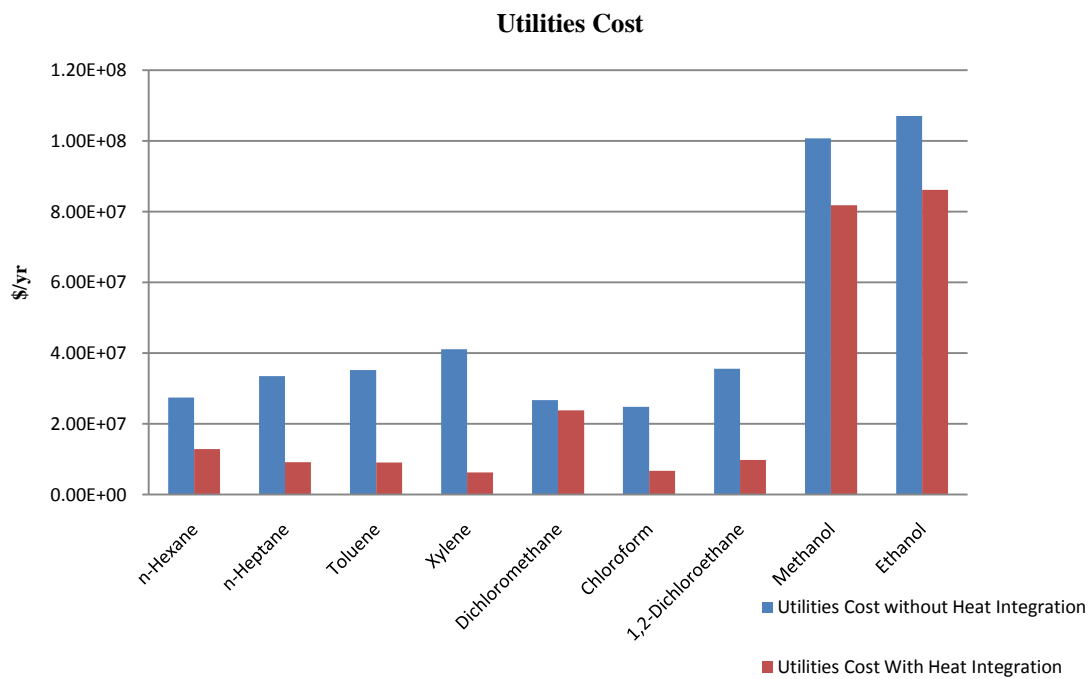


Figure 6-5 Utilities Cost before and after heat integration

Table 6-6 Percentage of utilities cost savings through heat integration

Solvent	Percentage of Utilities Cost Savings
n-Hexane	53.2%
n-Heptane	72.6%
Toluene	74.3%
Xylene	84.9%
Dichloromethane	10.9%
Chloroform	72.8%
1,2-Dichloroethane	72.6%
Methanol	18.7%
Ethanol	19.6%

6.2.3 Solvent Make Up Cost

In the oil extraction process, solvent make up cost is believed to be one of the highest for raw materials costs. Therefore, a cheaper solvent price and lower boiling point can reduce costs greatly. Table 6-7 shows the result of solvent makeup cost. Methanol is found to be the least costly solvent, followed by 1,2-dichloroethane, and xylene has the highest solvent makeup cost.

Table 6-7 Solvent makeup cost

Solvent Name	Recovered Amount (kg/hr)	Solvent Make Up (kg/hr)	Solvent Price (\$/kg)	Solvent Make Up Cost (\$/yr)
n-Hexane	348,931	1,069	0.926	8,673,130
n-Heptane	348,940	1,060	0.805	7,471,765
Toluene	348,936	1,064	0.853	7,953,860
Xylene	347,223	2,777	0.864	21,021,096
Dichloromethane	348,932	1,068	0.904	8,454,227
Chloroform	348,927	1,073	0.551	5,180,977
1,2-Dichloroethane	348,931	1,069	0.397	3,716,924
Methanol	327,996	1,004	0.368	3,236,835
Ethanol	327,987	1,013	0.750	6,648,455

The sum of total utilities cost and solvent make up cost before and after heat integration are illustrated in Figures 6-6 and 6-7. They demonstrated that chloroform has the lowest total cost and ethanol has the highest total cost.

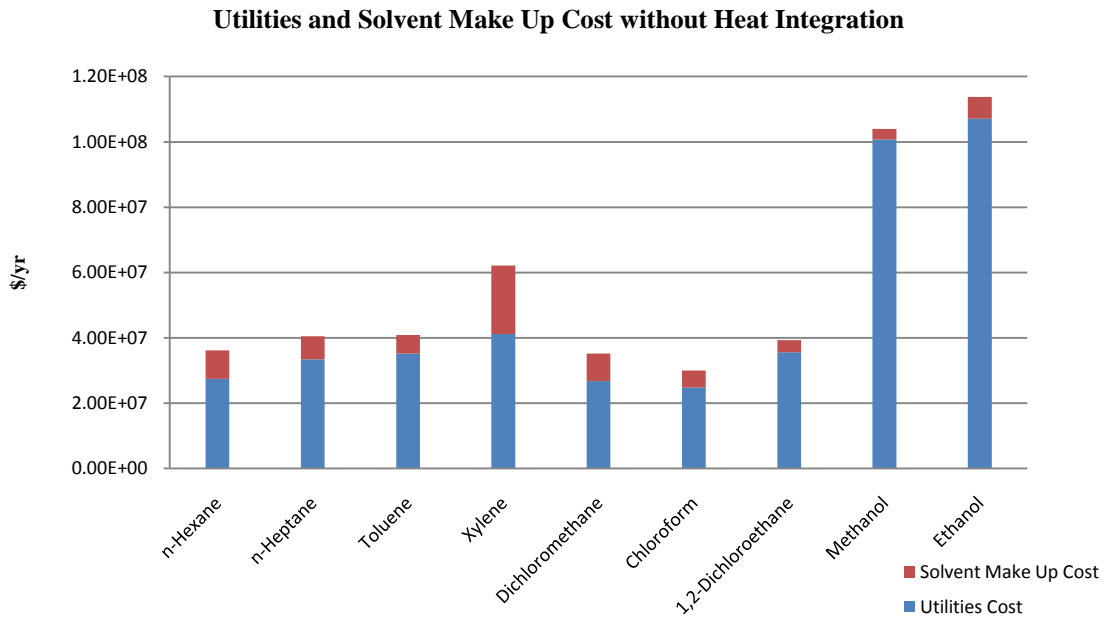


Figure 6-6 Utilities and solvent makeup cost without heat integration

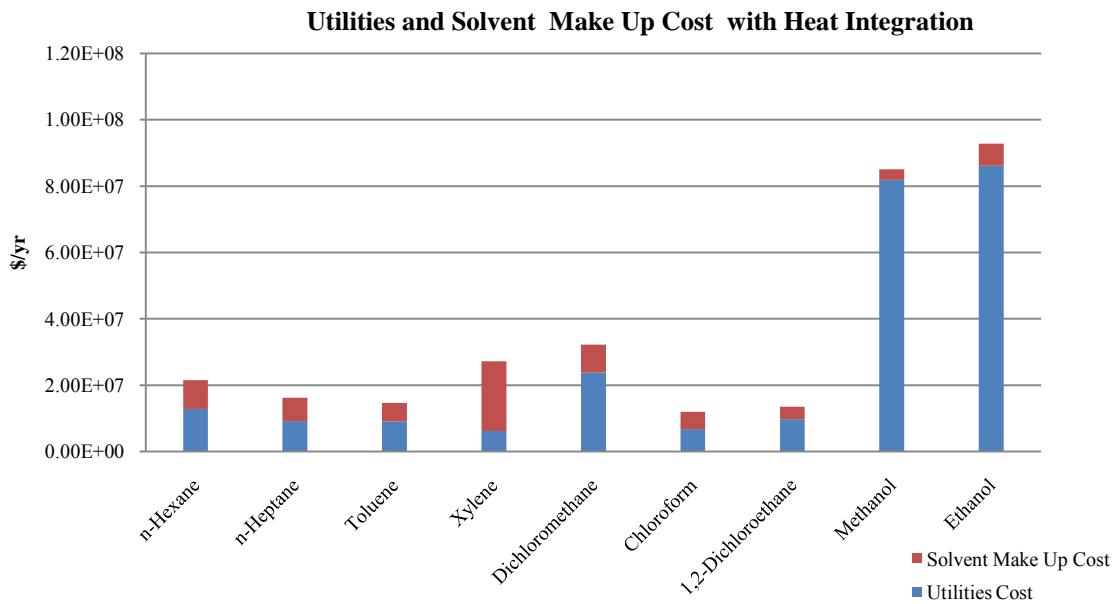


Figure 6-7 Utilities and solvent makeup cost with heat integration

6.2.4 Capital Investment Estimation

Equipment costs for the two cases are estimated by ASPEN ICARUS process evaluator. However, due to its poor ability to model solid materials, equipment costs for desolventizer-toaster and dryer are calculated by the Marshall and Swift equipment cost index (Marshall, 2005; Mujumdar, 2007). Furthermore, direct cost and capital investment are evaluated by Lang factors (Towler and Sinnott, 2008). As shown in Tables 6-8 and 6-9, the total capital investment for cases 1 and 2 are \$35.6 million and \$62.6 million, respectively. Total capital investment will be used to estimate the potential loss in the next section.

Table 6-8 Total capital investment for case 1

Process Unit	Extraction	Evaporation	Desolventizing & Drying	Solvent Recovery
Equipment Cost (MM\$)	4.0	3.2	4.4	0.2
Direct Cost (MM\$)	5.2	5.5	9.7	0.7
Capital Investment (MM\$)	8.6	9.0	16.8	1.2
Total Capital Investment (MM\$)	35.6			

Table 6-9 Total capital investment for case 2

Process Unit	Extraction	Evaporation	Desolventizing & Drying	Solvent Recovery
Equipment Cost (MM\$)	4.8	0.9	4.5	10.2
Direct Cost (MM\$)	6.2	1.9	9.9	19.3
Capital Investment (MM\$)	10.4	3.2	7.2	31.8
Total Capital Investment (MM\$)	62.6			

6.3 Potential Loss

Potential loss is estimated by F&EI, Damage Factor, and total capital investment. In this study, process units are treated as a complete system, including extraction, evaporation, desolventizing-toasting and drying, and solvent recovery. Therefore, each process unit has the same F&EI value associated with a particular solvent. Figures 6-8 through 6-12, show potential property caused by fire or explosion. Lower loss control credit values improved the emergency response and greatly reduced the property loss. Figure 6-8 through 6-12 show that chloroform has the lowest potential loss, while methanol and ethanol are observed to contribute the largest potential loss. Figure 6-12 presents the sum of potential losses for each process unit. It indicates maximum property loss caused by serious damage. Severe damage includes loss from natural disasters, such as earth quakes and hurricanes.

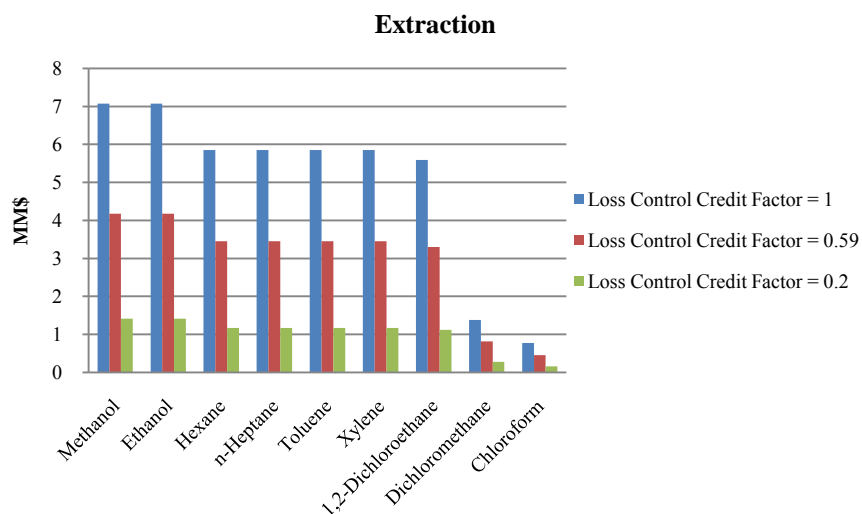


Figure 6-8 Potential loss for extraction unit

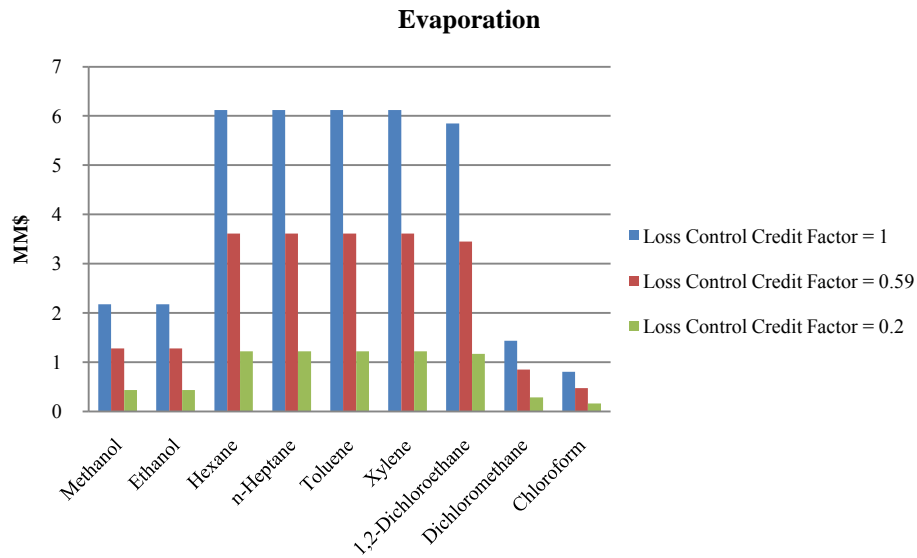


Figure 6-9 Potential loss for evaporation unit

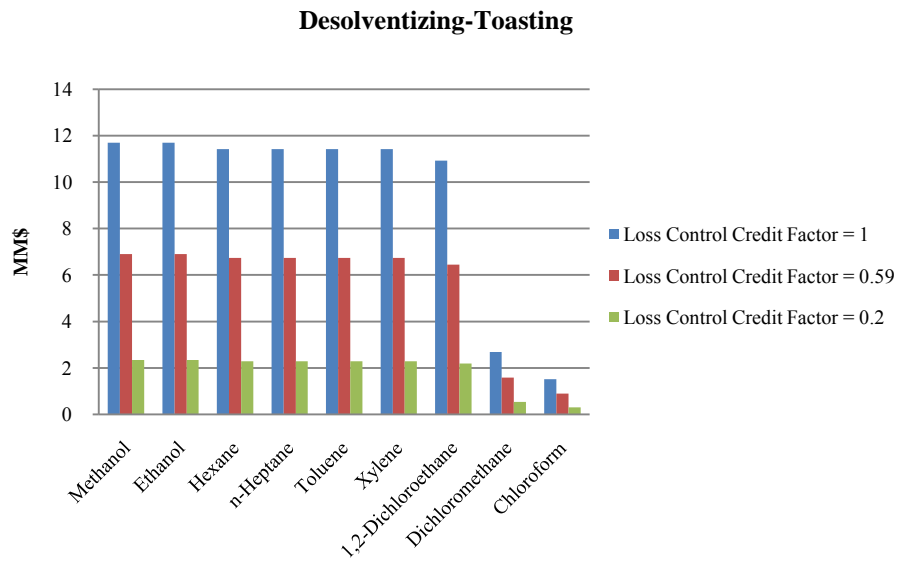


Figure 6-10 Potential loss for desolventizing-toasting unit

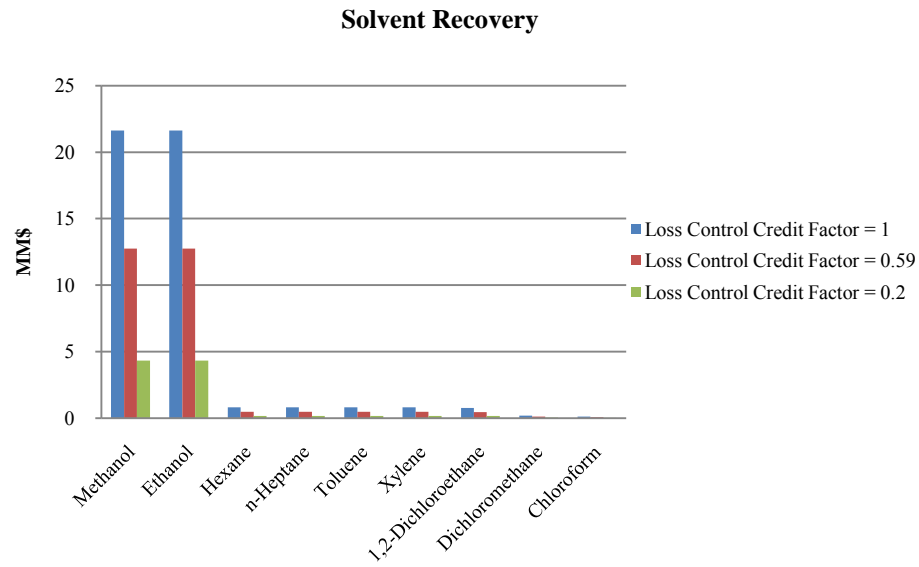


Figure 6-11 Potential loss for solvent recovery

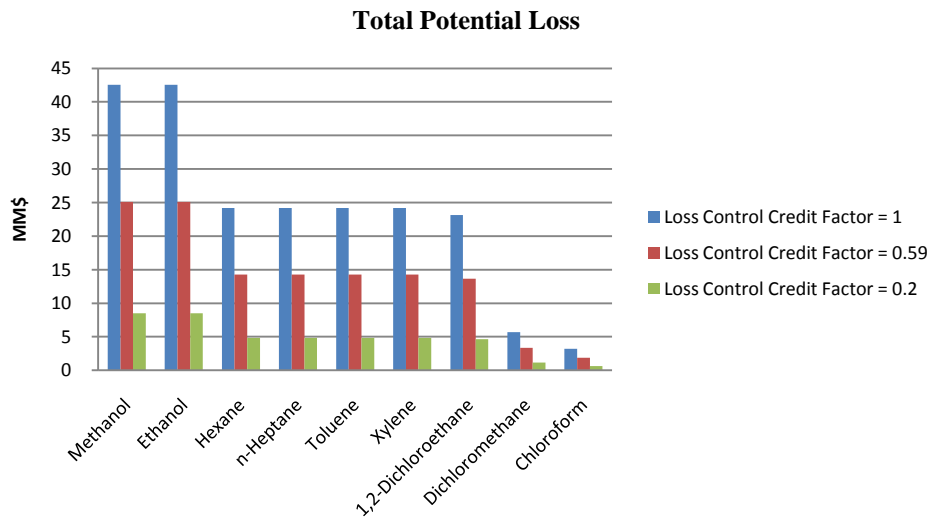


Figure 6-12 Total potential loss

6.4 Multi-Objective Comparison

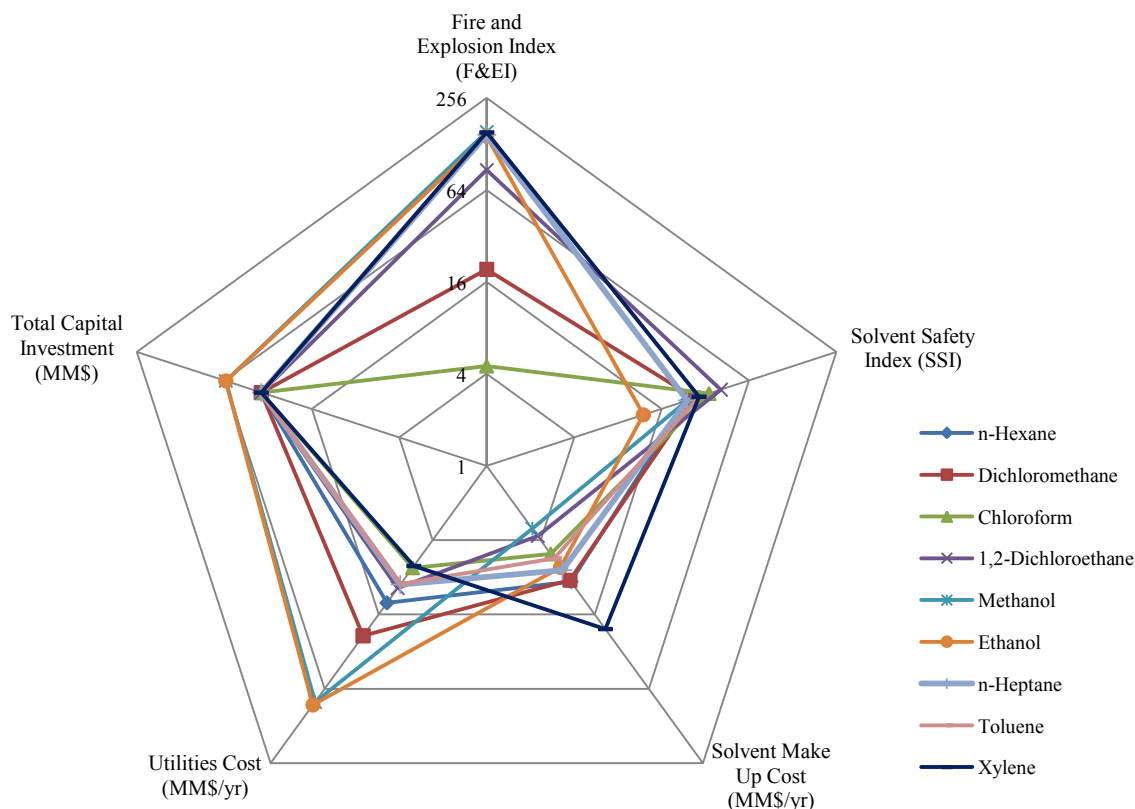


Figure 6-13 Multi-objective comparison of alternative extraction solvents

The main criteria for selection of alternative extraction solvents are F&EI, SSI, solvent makeup cost, utilities cost, and capital investment cost. Figure 6-13 presents the comparison of selected candidate solvents. The axes are scaled by logarithm 4. Lower values correspond to better performance and higher values correspond to worse performance. Consequently, Figure 6-13 suggests that chloroform has the best comparison against the others candidates. In fact, chloroform extraction has been examined and found to be efficient (Johnson and Lusas, 1983). The nonflammability of

chloroform reduces the risk of fire and explosion and its relatively low price also reduces raw material cost. Unfortunately, due to environmental consideration and high toxicity, chloroform has never been used in a commercial edible oil extraction. Since the non-edible *Jatropha* will not be used as food supplement for humans and animals, chloroform is an alternative choice to n-hexane, which is the most commonly used solvent for oil extraction. The second best performance is dichloromethane. Its low flammability and relatively low toxicity produce a reasonably good result. Moreover, dichloromethane is an excellent solvent for extraction. It has been widely used in many commercial extractions such as decaffeination and hops extraction. One disadvantage to using dichloromethane is that refrigerant is required in the cooling system which requires higher utilities expenditures. Ethanol is one of the most popular solvents for extraction. It is non-toxic property, allowing it to be used in food production such as protein extraction. However, intensive energy consumption and high flammability render it a less attractive alternative. Furthermore, since ethanol has also been used as a biofuel, ethanol price volatility should also be considered. Methanol has the lowest solvent makeup cost for its cheap price. The use of methanol as an extraction solvent may have benefit if transesterification is followed by oil extraction, which uses methanol as a catalyst. However, the poor performance in F&EI and utilities cost, and higher toxicity and capital investment caused it to be worst performance in these solvents.

CHAPTER VII

CONCLUSIONS AND RECOMMENDATIONS

This study provided the design, simulation, integration and analysis of Jatropha seed oil extraction. Nine different solvents were considered and screened according to technical, economic, and safety criteria. Two safety indices were used to assess the inherent safety of the process associated with the extraction solvents. The F&EI were used to estimate the hazards and risks of the process based on the material factor and process units hazard factor. The SSI was employed to evaluate the risks and hazards using LC_{50} , vapor density and NFPA 704. Two cases were developed to analyze Jatropha seed oil extraction. Five process units were modeled to conduct the extraction process, including evaporation, desolventizing-toasting, drying, and solvent recovery. The process performance was evaluated using ASPEN Plus. Utilities cost, capital investment, and solvent makeup cost are key factors for process analysis. To evaluate the potential loss caused by fire or explosion, a strategy based on the F&EI was applied. The results demonstrated that improvement of loss control has significant effects, reducing property loss from fire or explosion. Moreover, a multi-objective comparison was carried out to give an assessment based on five significant analysis factors. The results showed that chloroform has the best performance relative to the other solvents and ethanol was found to have the worst performance.

The following are recommendations for future work:

1. Incorporate multiple feedstocks from different indible oil plants and raw material costs analysis
2. Apply mixed or other non-organic solvents for oil extraction
3. Consider supercritical fluid extraction in biodiesel production
4. Study detailed kinetics for extraction time and oil recovery rate of alternative solvents

5. Assess life cycle for Jatropha seed use in oil extraction process.
6. Include economic evaluation of residue handling

REFERENCES

- Abedi, P., Shahriari, M., 2005. Inherent safety evaluation in process plants - a comparison of methodologies. *Central European Journal of Chemistry* 3, 756-779.
- Achten, W.M.J., Verchot, L., Franken, Y.J., Mathijs, E., Singh, V.P., Aerts, R., Muys, B., 2008. *Jatropha* bio-diesel production and use. *Biomass & Bioenergy* 32, 1063-1084.
- Adriaans, T., 2006. Suitability of solvent extraction for *Jatropha curcas*., <http://www.fact-foundation.com/en>
- American Institute of Chemical Engineers (AIChE)., 1994. *Dow's Fire & Explosion Index: Hazard Classification Guide*, 7th ed. Wiley, New York.
- Chen, W.H., Chen, C.H., Chang, C.M.J., Chiu, Y.H., Hsiang, D., 2009. Supercritical carbon dioxide extraction of triglycerides from *Jatropha curcas* L. seeds. *Journal of Supercritical Fluids* 51, 174-180.
- Chhetri, A.B., Tango, M.S., Budge, S.M., Watts, K.C., Islam, M.R., 2008. Non-edible plant oils as new sources for biodiesel production. *International Journal of Molecular Sciences* 9, 169-180.
- Deshpande, S.D., Bal, S., 1999. Specific heat of soybean. *Journal of Food Process Engineering* 22, 469-477.
- Edwards, D.W., Lawrence, D., 1995. Assessing the inherent safety of chemical process routes. *Loss Prevention and Safety Promotion in the Process Industries*, Vols 1 and 2, B473-B482,1474.
- El-Halwagi, M.M., 2006. *Process Integration*, 1st ed. Elsevier Academic Press, Amsterdam.

- Forson, F.K., Oduro, E.K., Hammond-Donkoh, E., 2004. Performance of jatropha oil blends in a diesel engine. *Renewable Energy* 29, 1135-1145.
- Freire, L.M.S., Bicudo, T.C., Rosenhaim, R., Sinfronio, F.S.M., Botelho, J.R., Carvalho, J.R., Santos, I.M.G., Fernandes, V.J., Antoniosi, N.R., Souza, A.G., 2009. Thermal investigation of oil and biodiesel from *Jatropha curcas* L. *Journal of Thermal Analysis and Calorimetry* 96, 1029-1033.
- Garnayak, D.K., Pradhan, R.C., Naik, S.N., Bhatnagar, N., 2008. Moisture-dependent physical properties of jatropha seed (*Jatropha curcas* L.). *Industrial Crops and Products* 27, 123-129.
- Gubitz, G.M., Mittelbach, M., Trabi, M., 1999. Exploitation of the tropical oil seed plant *Jatropha curcas* L. *Bioresource Technology* 67, 73-82.
- Hamm, W., Hamilton, R.J., 2000. *Edible Oil Processing*. CRC Press, Boca Raton, FL.
- Heikkila, A.M., 2000. An index-based approach for the evaluation of inherent safety in process plant design. *Foresight and Precaution*, Vols 1 and 2, 689-695, 1660.
- Henning, R., 2000. The Jatropha booklet- a guide to the Jatropha system and its dissemination. [http:// www.jatropha.de/documents/jcl-booklet-o-b.pdf](http://www.jatropha.de/documents/jcl-booklet-o-b.pdf)
- Hron, R.J., Koltun, S.P., Graci, A.V., 1982. Bio-renewable solvents for vegetable oil extraction. *Journal of the American Oil Chemists Society* 59, 674S-684A.
- Index Mundi, 2011. <http://www.indexmundi.com>
- Johnson, L.A., Lusas, E.W., 1983. Comparison of alternative solvents for oils extraction. *Journal of the American Oil Chemists Society* 60, 229-242.
- Khan, F.I., Amyotte, P.R., 2004. Integrated inherent safety index (I2SI): A tool for inherent safety evaluation. *Process Safety Progress* 23, 136-148.

- King, A.J., He, W., Cuevas, J.A., Freudenberger, M., Ramiamanana, D., Graham, I.A., 2009. Potential of *Jatropha curcas* as a source of renewable oil and animal feed. *Journal of Experimental Botany* 60, 2897-2905.
- Lam, M.K., Lee, K.T., Mohamed, A.R., 2009. Life cycle assessment for the production of biodiesel: A case study in Malaysia for palm oil versus jatropha oil. *Biofuels Bioproducts & Biorefining-Biofr* 3, 601-612.
- Magne, F.C., Skau, E.L., 1953. Phase equilibrium data pertaining to the extraction of cottonseed oil with ethanol and 2-propanol. *Journal of the American Oil Chemists Society* 30, 288-291.
- Makkar, H.R.S., Becker, K., 2009. *Jatropha curcas*, a promising crop for the generation of biodiesel and value-added coproducts. *European Journal of Lipid Science and Technology* 111, 773-787.
- Marshall and Swift equipment cost index., 2005. *Chemical Engineering*. <http://www.che.com/pci/>
- Min, J.A., Li, S.F., Hao, J., Liu, N.H., 2010. Supercritical CO₂ extraction of *Jatropha* oil and solubility correlation. *Journal of Chemical and Engineering Data* 55, 3755-3758.
- Mitchell, D., 2008. A note on rising food prices. *The world bank*. <http://econ.worldbank.org>
- Mujumdar, A.S., 2007. *Handbook of industrial drying*, 3rd ed. CRC, Boca Raton, FL.
- Myint, L.L., El-Halwagi, M.M., 2009. Process analysis and optimization of biodiesel production from soybean oil. *Clean Technologies and Environmental Policy* 11, 263-276.
- National Fire Protection Association, 2011. <http://www.nfpa.org/faq.asp?categoryID=928>.

- Nazir, N., Ramli, N., Mangunwidjaja, D., Hambali, E., Setyaningsih, D., Yuliani, S., Yarmo, M.A., Salimon, J., 2009. Extraction, transesterification and process control in biodiesel production from *Jatropha curcas*. *European Journal of Lipid Science and Technology* 111, 1185-1200.
- Openshaw, K., 2000. A review of *Jatropha curcas*: an oil plant of unfulfilled promise. *Biomass & Bioenergy* 19, 1-15.
- Pokoo-Aikins, G., Heath, A., Mentzer, R.A., Mannan, M.S., Rogers, W.J., El-Halwagi, M.M., 2010. A multi-criteria approach to screening alternatives for converting sewage sludge to biodiesel. *Journal of Loss Prevention in the Process Industries* 23, 412-420.
- Pramanik, K., 2003. Properties and use of *Jatropha curcas* oil and diesel fuel blends in compression ignition engine. *Renewable Energy* 28, 239-248.
- Qian, J.F., Shi, H.X., Yun, Z., 2010. Preparation of biodiesel from *Jatropha curcas* L. oil produced by two-phase solvent extraction. *Bioresource Technology* 101, 7025-7031.
- Rahman, M., Heikkila, A.M., Hurme, M., 2005. Comparison of inherent safety indices in process concept evaluation. *Journal of Loss Prevention in the Process Industries* 18, 327-334.
- Ryan, T.W., Dodge, L.G., Callahan, T.J., 1984. The effects of vegetable oil properties on injection and combustion in 2 different diesel-engines. *Journal of the American Oil Chemists Society* 61, 1610-1619.
- Seider, W.D., 2009. *Product and Process Design Principles : Synthesis, Analysis, and Evaluation*, 3rd ed. Wiley, Hoboken, NJ.
- Shah, S., Sharma, A., Gupta, M.N., 2004. Extraction of oil from *Jatropha curcas* L. seed kernels by enzyme assisted three phase partitioning. *Industrial Crops and Products* 20, 275-279.

- Shah, S., Sharma, A., Gupta, M.N., 2005. Extraction of oil from *Jatropha curcas* L. seed kernels by combination of ultrasonication and aqueous enzymatic oil extraction. *Bioresource Technology* 96, 121-123.
- Sharma, A., Khare, S.K., Gupta, M.N., 2002. Three phase partitioning for extraction of oil from soybean. *Bioresource Technology* 85, 327-329.
- Staubmann, R., Foidl, G., Foidl, N., Gubitz, G.M., Lafferty, R.M., Arbizu, V.M.V., Steiner, W., 1997. Biogas production from *Jatropha curcas* press-cake. *Applied Biochemistry and Biotechnology* 63-5, 457-467.
- Towler, G.P., Sinnott, R.K., 2008. *Chemical Engineering Design : Principles, Practice and Economics of Plant and Process Design*. Elsevier, Boston.
- Tzia, C., Liadakis, G., 2003. *Extraction Optimization in Food Engineering*. Marcel Dekker, Inc., New York.

APPENDIX A
MATERIAL FACTOR

Material	Material Factor MF	Hc kcal/kg×10 ³	NFPA			Flash Point (°C)	Boiling Point (°C)
			Health	Flammability	Instability		
n-Hexane	16	10.7	1	3	0	-22	69
n-Heptane	16	10.7	1	3	0	-4	98
Cyclohexane	16	10.4	1	3	0	-20	82
Benzene	16	9.6	2	3	0	-11	80
Toluene	16	9.7	2	3	0	4	111
Xylene	16	9.8	2	3	0	25	137
Dichloromethane	4	1.3	2	1	0	-	40
Chloroform	1	0.8	2	0	0	-	62
1,2-Dichloroethane	16	2.6	2	3	0	13	83 - 84
1,1,2-Trichloroethylene	10	1.5	2	1	0	-	87
Methanol	16	4.8	3	3	0	11	64
Ethanol	16	6.4	1	3	0	13	78
Isopropanol	16	7.3	1	3	0	12	83
Butanol	16	7.9	1	3	0	29	117
Acetone	16	6.8	1	3	0	-20	56
Methyl Ethyl Ketone	16	7.5	2	3	0	-9	80
Ethyl Acetate	16	5.6	3	3	0	-4	77

Source: Dow's Fire & Explosion Index, 1994

APPENDIX B

CALCULATIONS FOR FIRE AND EXPLOSION INDEX

Fire & Explosion Index					
1. General Process Hazards		Penalty Factor Used			
		n-Hexane	n-Heptane	Cyclohexane	Benzene
Base Factor		1	1	1	1
A. Exothermic Chemical Reactions		0	0	0	0
B. <input type="checkbox"/> Endothermic <input type="checkbox"/> Process		0.4	0.4	0.4	<input type="checkbox"/> 4
C. Material Handling Transfer		0.85	0.85	0.85	0.85
<input type="checkbox"/> Enclosed or Indoor Process Units		0	0	0	0
E. Access		0	0	0	0
F. Drainage and Spill Control (gal or cum)		0	0	0	0
General Process Hazards Factor (F1)		2.25	2.25	2.25	2.25
2. Special Process Hazards					
Base Factor		1	1	1	
A. Toxic Material(s)		0.2	0.2	0.2	0.4
B. Sub-Atmospheric Pressure (<500 mmHg)		0.5	0.5	0.5	0.5
C. Operation In or Near Flammable Range		0	0	0	0
1. Tank Farms Storage Flammable Range		0.5	0.5	0.5	0.5
2. Process Upset or Purge Failure		0	0	0	0
3. Always in Flammable		0	0	0	0
D. Dust Explosion		0	0	0	0
E. Pressure					
Operating Pressure		0	0	0	0
Relief Setting					
F. Low Temperature		0	0	0	0
G. Quantity of Flammable/Unstable Material					
Quantity = 771610 lb					
Hc (BTU/lb)		18700	19200	18700	17300
1. Liquids or Gases in Process		2.46	2.47	2.46	2.44
2. Liquids or Gases in Storage		0	0	0	0
3. Combustible Solids in Storage, Dust in Process					
H. Corrosion and Erosion		0.1	0.1	0.1	0.1
I. Leakage-Joints and Packing		0.1	0.1	0.1	0.1
J. Use of Fired Equipment		0.1	0.1	0.1	0.1
K. Hot Oil Heat Exchange System		0	0	0	0
L. Rotating Equipment		0	0	0	0
Special Process Hazards Factor (F2)		5.0	5.0	5.0	5.1
Process Unit Hazards Factor (F1 x F2) = F3 ¹		9.18	9.19	9.18	9.52
Process Unit Hazards Factor (F1 x F2) = F3 (Maximum = 8) ²		8	8	8	8
Material Factor (MF)		16	16	16	16
Fire and Explosion Index (F3 x MF = F&EI)		146.9	147.1	146.9	152.3

1. Value in this section is applied for selecting extraction solvents

2. Value in this section is applied for calculating Damage Factor

Fire & Explosion Index					
1. General Process Hazards		Penalty Factor Used			
		Toluene	Xylene	Dichloromethane	Chloroform
Base Factor		1	1	1	1
A. Exothermic Chemical Reactions		0	0	0	0
B. Endothermic Process		0	0	0	0
C. Material Handling Transfer		0.85	0.85	0.2	0.2
D. Enclosed or Indoor Process Units		0	0	0	0
E. Access		0	0	0	0
F. Drainage and Spill Control (gal or cum)		0	0	0	0
General Process Hazards Factor (F1)		2.25	2.25	1.6	1.6
2. Special Process Hazards					
Base Factor		1	1	1	1
A. Toxic Material(s)		0.4	0.4	0.4	0.4
B. Sub-Atmospheric Pressure (<50 mmHg)		0.5	0.5	0.5	0.5
C. Operation In or Near Flammable Range		0	0	0	0
1. Tank Farms Storage Flammable Range		0.5	0.5	0	0
2. Process Upset or Purge Failure		0	0	0	0
3. Always in Flammable		0	0	0	0
D. Dust Explosion		0	0	0	0
E. Pressure					
Operating Pressure		0	0	0	0
Relief Setting					
F. Low Temperature		0	0	0	0
G. Quantity of Flammable/Unstable Material					
Quantity = 771610 lb					
Hc (BTU/lb)		17400	17600	2300	1500
1. Liquids or Gases in Process		2.45	2.45	1.81	1.58
2. Liquids or Gases in Storage		0	0	0	0
3. Combustible Solids in Storage, Dust in Process					
H. Corrosion and Erosion		0.1	0.1	0.1	0.1
I. Leakage-Joints and Packing		0.1	0.1	0.1	0.1
J. Use of Fired Equipment		0.1	0.	0.1	0.1
K. Hot Oil Heat Exchange System		0	0	0	0
L. Rotating Equipment		0	0	0	0
Special Process Hazards Factor (F2)		5.1	5.1	4.0	3.8
Process Unit Hazards Factor (F1 x F2) = F3 ¹		9.52	9.53	4.82	4.53
Process Unit Hazards Factor (F1 x F2) = F3 (Maximum = 8) ²		8	8	4.82	4.53
Material Factor (MF)		16	16	4	1
Fire and Explosion Index (F3 x MF = F&EI)		152.3	152.4	19.3	4.5

1. Value in this section is applied for selecting extraction solvents

2. Value in this section is applied for calculating Damage Factor

Fire & Explosion Index		
1. General Process Hazards	Penalty Factor Used	
	1,2-Dichloroethane	1,1,2-Trichloroethylene
Base Factor	1	1
A. Exothermic Chemical Reactions	0	0
B. Endothermic Process	0	0
C. Material Handling Transfer	0.2	0.2
D. Enclosed or Indoor Process Units	0	0
E. Access	0	0
F. Drainage and Spill Control (gal or cum)	0	0
General Process Hazards Factor (F1)	1.6	1.6
2. Special Process Hazards		
Base Factor	1	1
A. Toxic Material(s)	0.6	0.4
B. Sub-Atmospheric Pressure (<500 mmHg)	0.5	0.5
C. Operation In or Near Flammable Range	0	0
<input type="checkbox"/> 1. Tank Farms Storage Flammable Range	0	0
2. Process Upset or Purge Failure	0	0
3. Always in Flammable	0	0
D. Dust Explosion	0	0
E. Pressure		
Operating Pressure	0	0
Relief Setting		
F. Low Temperature	0	0
G. Quantity of Flammable/Unstable Material		
Quantity = 771610 lb		
Hc (BTU/lb)	4600	2700
1. Liquids or Gases in Process	2.10	1.89
2. Liquids or Gases in Storage	0	0
3. Combustible Solids in Storage, Dust in Process		
H. Corrosion and Erosion	0.1	0.1
I. Leakage-Joints and Packing	0.1	0.1
J. Use of Fired Equipment	0.1	0.1
K. Hot Oil Heat Exchange System	0	0
L. Rotating Equipment	0	
Special Process Hazards Factor (F2)	4.5	4.1
Process Unit Hazards Factor (F1 x F2) = F3 ¹	5.4	4.91
Process Unit Hazards Factor (F1 x F2) = F3 (Maximum = 8) ²	5.4	4.91
Material Factor (MF)	16	10
Fire and Explosion Index (F3 x MF = F&EI)	86.4	49.1

1. Value in this section is applied for selecting extraction solvents

2. Value in this section is applied for calculating Damage Factor

Fire & Explosion Index					
1. General Process Hazards		Penalty Factor Used			
		Methanol	Ethanol	Isopropanol	n-Butanol
Base Factor		1	1	1	1
A. Exothermic Chemical Reactions		0	0	0	0
B. Endothermic Process		0	0	0	0
C. Material Handling Transfer		0.85	0.85	0.85	0.85
D. Enclosed or Indoor Process □ Units		0	0	0	0
E. Access		0	0	0	0
F. Drainage and Spill Control (gal or cum)		0	0	0	0
General Process Hazards Factor (F1)		2.25	2.25	2.25	2.25
2. Special Process Hazards					
Base Factor		1	1	1	1
A. Toxic Material(s)		0.6	0.2	0.2	0.2
B. Sub-Atmospheric Pressure (<500 □mmHg)		0.5	0.5	0.5	0.5
C. Operation In or Near Flammable Range		0	0	0	0
1. Tank Farms Storage Flammable Range		0.5	0.5	0.5	0.5
2. Process Upset or Purge Failure		0	0	0	0
3. Always in Flammable		0	0	0	0
D. Dust Explosion		0	0	0	0
E. Pressure					
Operating Pressure		0	0	0	0
Relief Setting					
F. Low Temperature		0	0	0	0
G. Quantity of Flammable/Unstable Material					
Quantity = 771610 lb					
Hc (BTU/lb)		8600	11500	13100	14300
1. Liquids or Gases in Process		2.28	2.35	2.38	2.40
2. Liquids or Gases in Storage		0	0	0	0
3. Combustible Solids in Storage, Dust in Process					
H. Corrosion and Erosion		0.1	0.1	0.1	0.1
I. Leakage-Joints and Packing		0.1	0.1	0.1	0.1
J. Use of Fired Equipment		0.1	0.1	0.1	0.1
K. Hot Oil Heat Exchange System		0	0	0	0
L. Rotating Equipment		0	0	0	0
Special Process Hazards Factor (F2)		5.2	4.9	4.9	4.9
Process Unit Hazards Factor (F1 x F2) = F3 ¹		9.59	8.97	9.03	9.07
Process Unit Hazards Factor (F1 x F2) = F3 (Maximum = 8) ²		8	8	8	8
Material Factor (MF)		16	16	16	16
Fire and Explosion Index (F3 x MF = F&EI)		153.4	143.6	144.5	145.1

1. Value in this section is applied for selecting extraction solvents

2. Value in this section is applied for calculating Damage Factor

Fire & Explosion Index			
1. General Process Hazards	Penalty Factor Used		
	Acetone	Methyl ethyl ketone	Ethyl acetate
Base Factor	1	1	1
A. Exothermic Chemical Reactions	0	0	0
B. Endothermic Process	0	0	0
C. Material Handling Transfer	0.85	0.85	0.85
D. Enclosed or Indoor Process Units	0	0	0
E. Access	0	0	0
F. Drainage and Spill Control (gal or cum)	0	0	0
General Process Hazards Factor (F1)	2.25	2.25	2.25
2. Special Process Hazards			
Base Factor	1	1	1
A. Toxic Material(s)	0.2	0.2	0.4
B. Sub-Atmospheric Pressure (<500 mmHg)	0.5	0.5	0.5
C. Operation In or Near Flammable Range	0	0	0
1. Tank Farms Storage Flammable Range	0.5	0.5	0.5
2. Process Upset or Purge Failure	0	0	0
3. Always in Flammable	0	0	0
D. Dust Explosion	0	0	0
E. Pressure			
Operating Pressure	0	0	0
Relief Setting			
F. Low Temperature	0	0	0
G. Quantity of Flammable/Unstable Material			
Quantity =771610 lb			
Hc (BTU/lb)	12300	13500	10100
1. Liquids or Gases in Process	2.37	2.39	2.32
2. Liquids or Gases in Storage	0	0	0
3. Combustible Solids in Storage, Dust in Process			
H. Corrosion and Erosion	0.1	0.1	0.1
I. Leakage-Joints and Packing	0.1	0.1	0.1
J. Use of Fired Equipment	0.1	0.1	0.1
K. Hot Oil Heat Exchange System	0	0	0
L. Rotating Equipment	0	0	0
Special Process Hazards Factor (F2)	4.9	4.9	5.0
Process Unit Hazards Factor (F1 x F2) = F3 ¹	9.0	9.04	9.29
Process Unit Hazards Factor (F1 x F2) = F3 (Maximum = 8) ²	8	8	8
Material Factor (MF)	16	16	16
Fire and Explosion Index (F3 x MF = F&EI)	144.1	144.7	148.6

1. Value in this section is applied for selecting extraction solvents

2. Value in this section is applied for calculating Damage Factor

APPENDIX C

LC₅₀, NFPA 704 AND VAPOR DENSITY DATA FOR CANDIDATE SOLVENTS

	Solvents	LC ₅₀	NFPA 704	Vapor Density
		(ppm/4hr rate)	(Health)	(Air = 1)
1	n-Hexane	48000	1	3
2	n-Heptane	25000	1	3.5
3	Cyclohexane	4050	1	3
4	Benzene	14380	2	2.7
5	Toluene	4900	2	3.1
6	Xylene	5000	2	3.7
7	Dichloromethane	76000	2	2.9
8	Chloroform	8000	2	4
9	1,2-Dichloroethane	1415	3	3.4
10	1,1,2-Trichloroethylene	8000	2	4.5
11	Methanol	64000	3	1.1
12	Ethanol	20000	1	1.6
13	Isopropanol	2000	1	2.1
14	n-Butanol	8000	1	2.6
15	Acetone	16000	1	2
16	Methyl ethyl ketone	64000	1	2.5
17	Ethyl acetate	22630	2	3

APPENDIX D

LOSS CONTROL CREDIT FACTORS

Loss Control Credit Factors				
1. Process Control Credit Factor (C1)				
Feature	Credit Factor Range	Credit Factor Used		
		Lowest	Highest	Not Applicable
a. Emergency Power	0.98	0.98	0.98	1
b. Cooling	0.97-0.99	0.97	0.99	1
c. Explosion Control	0.84-0.98	0.84	0.98	1
d. Emergency Shutdown	0.96-0.99	0.96	0.99	1
e. Computer Control	0.93-0.99	0.93	0.99	1
f. Inert Gas	0.94-0.96	0.94	0.96	1
g. Operation Instructions/Procedures	0.91-0.99	0.91	0.99	1
h. Reactive Chemical Review	0.91-0.99	0.99	0.99	1
i. Other Process Hazard Analysis	0.91-0.98	0.91	0.98	1
C ₁ Value	>>>	0.55	0.86	1.00
2. Material Isolation Credit Factor (C2)				
Feature	Credit Factor Range	Credit Factor Used		
		Lowest	Highest	Not Applicable
a. Remote Control Valves	0.96-0.98	0.96	0.98	1
b. Dump/Blowdown	0.96-0.98	0.96	0.98	1
c. Drainage	0.91-0.97	0.91	0.97	1
d. Interlock	0.98	0.98	0.98	1
C ₂ Value	>>>	0.82	0.91	1.00
3. Fire Protection Credit Factor (C3)				
Feature	Credit Factor Range	Credit Factor Used		
		Lowest	Highest	Not Applicable
a. Leak Detection	0.94-0.98	0.94	0.98	1
b. Structural Steel	0.95-0.98	0.95	0.98	1
c. Fire Water Supply	0.94-0.97	0.94	0.97	1
d. Special Systems	0.91	0.91	0.91	1
e. Sprinkler Systems	0.74-0.97	0.74	0.97	1
f. Water Curtains	0.97-0.98	0.97	0.98	1
g. Foam	0.92-0.97	0.92	0.97	1
h. Hand Extinguishers/Monitors	0.93-0.98	0.93	0.98	1
i. Cable Protection	0.94-0.98	0.94	0.98	1
C ₃ Value	>>>	0.44	0.75	1
Loss Control Credit Factor		0.20	0.59	1.00

APPENDIX E
POTENTIAL LOSS

Process Unit Risk Analysis Summary			Solvents					
			n-Hexane	n-Heptane	Toluene	Xylene	Dichloromethane	Chloroform
1. Fire & Explosion Index (F&EI)			178.7	178.9	185.3	185.4	25.7	6.0
2. Radius of Exposure	ft		150	150	156	156	22	5
3. Area of Exposure	ft ²		70716	70890	76041	76118	1461	81
4. Value of Area of Exposure (Base on Capital Investment)								
4.1 Extraction	MMS		8.6	8.6	8.6	8.6	8.6	8.6
4.2 Evaporation	MMS		9	9	9	9	9	9
4.3 Desolventizing & Drying	MMS		16.8	16.8	16.8	16.8	16.8	16.8
4.4 Solvent Recovery	MMS		1.2	1.2	1.2	1.2	1.2	1.2
4.5 Total	MMS		35.6	35.6	35.6	35.6	35.6	35.6
5. Damage Factor			0.68	0.68	0.68	0.68	0.16	0.09
6. Base Maximum Probable Property Damage (Base MPPD)								
6.1 Extraction	MMS		5.8	5.8	5.8	5.8	1.4	0.8
6.2 Evaporation	MMS		6.1	6.1	6.1	6.1	1.4	0.8
6.3 Desolventizing & Drying	MMS		11.4	11.4	11.4	11.4	2.7	1.5
6.4 Solvent Recovery	MMS		0.8	0.8	0.8	0.8	0.2	0.1
6.5 Total	MMS		24.2	24.2	24.2	24.2	5.7	3.2
7. Loss Control Credit Factor		Lowest						
		Highest						1
		Not Applicable						0.59
			0.2					
8. Actual Maximum Probable Property Damage (Actual MPPD)								
8.1 Extraction	MMS		5.8	5.8	5.8	5.8	1.4	0.8
8.2 Evaporation	MMS		6.1	6.1	6.1	6.1	1.4	0.8
8.3 Desolventizing & Drying	MMS		11.4	11.4	11.4	11.4	2.7	1.5
8.4 Solvent Recovery	MMS		0.82	0.82	0.82	0.82	0.192	0.108
8.5 Total	MMS		24.2	24.2	24.2	24.2	5.7	3.2

Process Unit Risk Analysis Summary			1,2-Dichloroethane	Methanol	Ethanol
			1. Fire & Explosion Index (F&EI)		115.2
2. Radius of Exposure	ft	97	157	147	
3. Area of Exposure	ft ²	29409	77084	67577	
4. Value of Area of Exposure (Base on Capital Investment)					
4.1 Extraction	MMS	8.6	10.4	10.4	
4.2 Evaporation	MMS	9	3.2	3.2	
4.3 Desolventizing & Drying	MMS	16.8	17.2	17.2	
4.4 Solvent Recovery	MMS	1.2	31.8	31.8	
4.5 Total	MMS	35.6	62.6	62.6	
5. Damage Factor			0.65	0.68	0.68
6. Base Maximum Probable Property Damage (Base MPPD)					
6.1 Extraction	MMS	5.6	7.1	7.1	
6.2 Evaporation	MMS	5.9	2.2	2.2	
6.3 Desolventizing & Drying	MMS	10.9	11.7	11.7	
6.4 Solvent Recovery	MMS	0.8	21.6	21.6	
6.5 Total	MMS	23.1	42.6	42.6	
7. Loss Control Credit Factor	Lowest	1			
	Highest	0.59			
	Not Applicable	0.2			
8. Actual Maximum Probable Property Damage (Actual MPPD)					
8.1 Extraction	MMS	5.6	7.1	7.1	
8.2 Evaporation	MMS	5.9	2.2	2.2	
8.3 Desolventizing & Drying	MMS	10.9	11.7	11.7	
8.4 Solvent Recovery	MMS	0.78	21.6	21.6	
8.5 Total	MMS	23.1	42.6	42.6	

APPENDIX F

PROCESS STREAM DATA: N-HEXANE

	S-101	S-102	S-103	S-104	S-105	S-106	S-107	S-108	S-201	S-202	S-203	S-204	S-205	S-206	S-207	S-208	S-209	S-210	S-211	S-212	S-301	S-302
Temperature K	298.2	298.2	353.2	303.2	303.2	322.2	303.4	322.2	376.2	376.0	376.0	383.2	375.4	375.4	398.4	394.8	394.8	323.2	376.7	341.9	298.2	298.2
Pressure atm	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.5	0.5	0.1	0.1	1.0	0.1	1.0	1.0	1.0
Mass Vapor Fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8	0.0	1.0	0.1	0.0	1.0	0.1	0.0	1.0	0.0	1.0	0.0	0.0	0.0
Total Flow kg/hr	350000	350000	350000	350000	350000	385000	315000	385000	385000	161920	223080	161920	147166	14754	147166	138264	8902	138264	246736	246736	31500	31500
Mass Flow kg/hr																						
n-Hexane	0	0	0	350000	350000	247789	102211	247789	247789	95184	152605	95184	6810	88374	6810	615	6195	615	247174	247174	0	0
Water	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	31500	31500
Palmitic Acid	19964	19964	19964	0	0	19566	398	19566	19566	19566	0	19566	19564	2	19564	19552	12	19552	14	14	0	0
Stearic Acid	8050	8050	8050	0	0	7890	160	7890	7890	7890	0	7890	7889	0	7889	7888	2	7888	2	2	0	0
Oleic Acid	64106	64106	64106	0	0	62829	1277	62829	62829	62829	0	62829	62823	6	62823	62801	22	62801	28	28	0	0
Linoleic Acid	47880	47880	47880	0	0	46926	954	46926	46926	46926	0	46926	46921	5	46921	46900	21	46900	26	26	0	0
Flakes	210000	210000	210000	0	0	0	210000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

	S-303	S-304	S-305	S-306	S-307	S-308	S-309	S-310	S-401	S-402	S-403	S-404	S-405	S-406	S-407	S-408	S-409	S-410	S-411	S-412	S-413	
Temperature K	373.2	346.5	346.5	383.2	373.4	373.4	373.4	313.2	313.2	313.2	329.2	329.2	329.2	353.2	353.2	353.2	319.1	342.0	319.2	329.2	338.3	
Pressure atm	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	
Mass Vapor Fraction	1.0	0.0	1.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	
Total Flow kg/hr	31500	232636	113864	232636	232636	193072	39565	113864	113864	114235	102234	12002	12002	12002	11630	372	372	246736	372	102234	348969	
Mass Flow kg/hr																						
n-Hexane	0	2	102209	2	2	0	2	102209	102209	102449	102209	240	240	240	0	240	240	247174	240	102209	349383	
Water	31500	22597	8903	22597	44026	1712	42314	8903	8903	8947	24	8923	8923	8923	8879	44	44	0	44	24	24	
Palmitic Acid	0	398	0	398	398	398	0	0	0	0	0	0	0	0	0	0	0	14	0	0	14	
Stearic Acid	0	160	0	160	160	160	0	0	0	0	0	0	0	0	0	0	0	2	0	0	2	
Oleic Acid	0	1277	0	1277	1277	1277	0	0	0	0	0	0	0	0	0	0	0	28	0	0	28	
Linoleic Acid	0	954	0	954	954	954	0	0	0	0	0	0	0	0	0	0	0	26	0	0	26	
Flakes	0	210000	0	210000	188571	188571	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	

PROCESS STREAM DATA: N-HEPTANE

	S-101	S-102	S-103	S-104	S-105	S-106	S-107	S-108	S-201	S-202	S-203	S-204	S-205	S-206	S-207	S-208	S-209	S-210	S-211	S-212	S-301	S-302
Temperature K	298.2	298.2	353.2	303.2	303.2	323.4	303.5	323.5	438.2	438.1	438.1	438.2	433.0	433.0	450.2	447.0	447.0	323.2	438.2	371.6	298.2	298.2
Pressure atm	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.5	0.5	0.1	0.1	1.0	0.1	1.0	1.0	1.0
Mass Vapor Fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8	0.0	1.0	0.0	0.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0
Total Flow kg/hr	350000	350000	350000	350000	350000	385000	315000	385000	385000	151916	233084	151916	144541	7375	144541	137578	6963	137578	247422	247422	31500	31500
Mass Flow kg/hr																						
n-Heptane	0	0	0	350000	350000	247789	102211	247789	247789	15118	232671	15118	7764	7354	7764	1059	6706	1059	246730	246730	0	0
Water	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	31500	31500
Palmitic Acid	19964	19964	19964	0	0	19566	398	19566	19566	19478	88	19478	19473	5	19473	19418	56	19418	149	149	0	0
Stearic Acid	8050	8050	8050	0	0	7890	160	7890	7890	7877	12	7877	7877	1	7877	7869	8	7869	21	21	0	0
Oleic Acid	64106	64106	64106	0	0	62829	1277	62829	62829	62674	155	62674	62666	8	62666	62568	98	62568	261	261	0	0
Linoleic Acid	47880	47880	47880	0	0	46926	954	46926	46926	46769	157	46769	46761	8	46761	46665	96	46665	261	261	0	0
Flakes	210000	210000	210000	0	0	0	210000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

	S-303	S-304	S-305	S-306	S-307	S-308	S-309	S-310	S-401	S-402	S-403	S-404	S-405	S-406	S-407	S-408	S-409	S-410	S-411	S-412	S-413
Temperature K	373.2	348.4	348.4	383.2	373.4	373.4	373.4	313.2	313.2	313.2	329.2	329.2	329.2	358.2	358.2	358.2	331.6	371.7	331.6	329.2	359.7
Pressure atm	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Mass Vapor Fraction	1.0	0.0	1.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	31500	232931	113569	232931	232931	193072	39859	113569	113569	113619	102234	11385	11385	11385	11336	50	50	247422	50	102234	349656
Mass Flow kg/hr																					
n-Hexane	0	1	102210	1	1	0	1	102210	102210	102250	102210	40	40	40	0	40	40	246730	40	102210	348940
Water	31500	20140	11360	20140	41569	1712	39857	11360	11360	11369	24	11345	11345	11345	11336	10	10	0	10	24	24
Palmitic Acid	0	398	0	398	398	398	0	0	0	0	0	0	0	0	0	0	0	149	0	0	149
Stearic Acid	0	160	0	160	160	160	0	0	0	0	0	0	0	0	0	0	0	21	0	0	21
Oleic Acid	0	1277	0	1277	1277	1277	0	0	0	0	0	0	0	0	0	0	0	261	0	0	261
Linoleic Acid	0	954	0	954	954	954	0	0	0	0	0	0	0	0	0	0	0	261	0	0	261
Flakes	0	210000	0	210000	188571	188571	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

PROCESS STREAM DATA: TOLUENE

	S-101	S-102	S-103	S-104	S-105	S-106	S-107	S-108	S-201	S-202	S-203	S-204	S-205	S-206	S-207	S-208	S-209	S-210	S-211	S-212	S-301	S-302
Temperature K	298.2	298.2	353.2	303.2	303.2	327.4	303.7	327.5	448.2	448.0	448.0	458.2	452.3	452.3	475.2	471.2	471.2	323.2	449.0	383.9	298.2	298.2
Pressure atm	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.5	0.5	0.1	0.1	1.0	0.1	1.0	1.0	1.0
Mass Vapor Fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8	0.0	1.0	0.1	0.0	1.0	0.1	0.0	1.0	0.0	1.0	0.0	0.0	0.0
Total Flow kg/hr	350000	350000	350000	350000	350000	385000	315000	385000	385000	155041	229959	155041	144055	10986	144055	136271	7784	136271	248729	248729	31500	31500
Mass Flow kg/hr																						
Toluene	0	0	0	350000	350000	247789	102211	247789	247789	18550	229239	18550	7670	10880	7670	942	6728	942	246847	246847	0	0
Water	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	31500	31500
Palmitic Acid	19964	19964	19964	0	0	19566	398	19566	19566	19407	160	19407	19384	23	19384	19157	227	19157	410	410	0	0
Stearic Acid	8050	8050	8050	0	0	7890	160	7890	7890	7867	23	7867	7863	3	7863	7826	38	7826	64	64	0	0
Oleic Acid	64106	64106	64106	0	0	62829	1277	62829	62829	62554	275	62554	62514	40	62514	62111	403	62111	718	718	0	0
Linoleic Acid	47880	47880	47880	0	0	46926	954	46926	46926	46664	262	46664	46625	39	46625	46236	389	46236	690	690	0	0
Flakes	210000	210000	210000	0	0	0	210000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

	S-303	S-304	S-305	S-306	S-307	S-308	S-309	S-310	S-401	S-402	S-403	S-404	S-405	S-406	S-407	S-408	S-409	S-410	S-411	S-412	S-413
Temperature K	373.2	346.1	346.1	383.2	373.4	373.4	373.4	313.2	313.2	313.2	329.2	329.2	329.2	353.2	353.2	353.2	338.9	384.0	339.0	329.2	368.9
Pressure atm	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Mass Vapor Fraction	1.0	0.0	1.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	31500	233748	112752	233748	233748	193056	40692	112752	112752	112840	102166	10674	10674	10674	10586	88	88	248729	88	102166	350895
Mass Flow kg/hr																					
n-Hexane	0	107	102104	107	107	0	107	102104	102104	102179	102089	90	90	90	15	75	75	246847	75	102089	348936
Water	31500	20852	10648	20852	42280	1695	40585	10648	10648	10661	77	10584	10584	10584	10571	13	13	0	13	77	77
Palmitic Acid	0	398	0	398	398	398	0	0	0	0	0	0	0	0	0	0	0	410	0	0	410
Stearic Acid	0	160	0	160	160	160	0	0	0	0	0	0	0	0	0	0	0	64	0	0	64
Oleic Acid	0	1277	0	1277	1277	1277	0	0	0	0	0	0	0	0	0	0	0	718	0	0	718
Linoleic Acid	0	954	0	954	954	954	0	0	0	0	0	0	0	0	0	0	0	690	0	0	690
Flakes	0	210000	0	210000	188571	188571	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

PROCESS STREAM DATA: XYLENE

	S-101	S-102	S-103	S-104	S-105	S-106	S-107	S-108	S-201	S-202	S-203	S-204	S-205	S-206	S-207	S-208	S-209	S-210	S-211	S-212	S-301	S-302
Temperature K	298.2	298.2	353.2	303.2	303.2	327.2	303.7	327.3	443.2	442.9	442.9	473.2	465.4	465.4	476.2	468.9	468.9	323.2	448.9	413.8	298.2	298.2
Pressure atm	1.0	1.0	1.0	1.0	2.0	1.0	1.0	2.0	1.0	1.0	1.0	1.0	0.5	0.5	0.5	0.1	0.1	1.0	0.1	1.0	1.0	2.0
Mass Vapor Fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.6	0.0	1.0	0.3	0.0	1.0	0.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0
Total Flow kg/hr	350000	350000	350000	350000	350000	385000	315000	385000	385000	200101	184899	200101	148761	51341	148761	136919	11841	136919	248081	248081	31500	31500
Mass Flow kg/hr																						
Xylene	0	0	0	350000	350000	247789	102211	247789	247789	63113	184675	63113	12575	50539	12575	1988	10586	1988	245800	245800	0	0
Water	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	31500	31500
Palmitic Acid	19964	19964	19964	0	0	19566	398	19566	19566	19515	51	19515	19339	176	19339	19069	270	19069	497	497	0	0
Stearic Acid	8050	8050	8050	0	0	7890	160	7890	7890	7883	7	7883	7855	28	7855	7810	44	7810	79	79	0	0
Oleic Acid	64106	64106	64106	0	0	62829	1277	62829	62829	62743	86	62743	62437	306	62437	61958	479	61958	871	871	0	0
Linoleic Acid	47880	47880	47880	0	0	46926	954	46926	46926	46847	79	46847	46555	292	46555	46093	462	46093	833	833	0	0
Flakes	210000	210000	210000	0	0	0	210000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

	S-303	S-304	S-305	S-306	S-307	S-308	S-309	S-310	S-401	S-402	S-403	S-404	S-405	S-406	S-407	S-408	S-409	S-410	S-411	S-412	S-413
Temperature K	373.2	410.6	410.6	383.2	373.4	373.4	373.4	348.0	348.0	344.8	329.2	329.2	329.2	373.2	373.2	373.2	337.3	413.9	337.4	329.2	391.1
Pressure atm	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	2.0	1.0	1.0	1.0	2.0	1.0	1.0	1.0	1.0	2.0	2.0	2.0	1.0
Mass Vapor Fraction	1.0	0.0	1.0	1.0	0.9	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3	0.0	1.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	31500	213588	132912	213588	213588	192830	20757	132912	132912	146670	101536	45135	45135	45135	31377	13758	13758	248081	13758	101536	349616
Mass Flow kg/hr																					
n-Hexane	0	788	101423	788	788	4	784	101423	101423	101475	101423	52	52	52	0	52	52	245800	52	101423	347223
Water	31500	51	31449	51	21480	1507	19973	31449	31449	45154	75	45079	45079	45079	31374	13706	13706	0	13706	75	75
Palmitic Acid	0	389	9	389	389	389	0	9	9	9	7	1	1	1	1	0	0	497	0	7	504
Stearic Acid	0	159	1	159	159	159	0	1	1	1	1	0	0	0	0	0	0	79	0	1	80
Oleic Acid	0	1261	16	1261	1261	1261	0	16	16	16	14	2	2	2	2	0	0	871	0	14	885
Linoleic Acid	0	938	16	938	938	938	0	16	16	16	16	0	0	0	0	0	0	833	0	16	849
Flakes	0	210000	0	210000	188571	188571	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

PROCESS STREAM DATA: DICHLOROMETHANE

	S-101	S-102	S-103	S-104	S-105	S-106	S-107	S-108	S-201	S-202	S-203	S-204	S-205	S-206	S-207	S-208	S-209	S-210	S-211	S-212	S-301	S-302
Temperature K	298.2	298.2	353.2	303.2	303.2	331.6	304.0	331.7	365.7	365.5	365.5	378.2	371.2	371.2	410.2	407.6	407.6	323.2	367.4	312.8	298.2	298.2
Pressure atm	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.5	0.5	0.1	0.1	1.0	0.1	1.0	1.0	1.0
Mass Vapor Fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8	0.0	1.0	0.1	0.0	1.0	0.1	0.0	1.0	0.0	1.0	0.0	0.0	0.0
Total Flow kg/hr	350000	350000	350000	350000	350000	385000	315000	385000	385000	162002	222998	162002	147009	14993	147009	138015	8993	138015	246985	246985	31500	31500
Mass Flow kg/hr																						
Dichloromethane	0	0	0	350000	350000	247789	102211	247789	247789	24792	222997	24792	9799	14993	9799	838	8961	838	246951	246951	0	0
Water	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	31500	31500
Palmitic Acid	19964	19964	19964	0	0	19566	398	19566	19566	19566	0	19566	19566	0	19566	19559	7	19559	7	7	0	0
Stearic Acid	8050	8050	8050	0	0	7890	160	7890	7890	7890	0	7890	7890	0	7890	7889	1	7889	1	1	0	0
Oleic Acid	64106	64106	64106	0	0	62829	1277	62829	62829	62828	1	62828	62828	0	62828	62816	12	62816	13	13	0	0
Linoleic Acid	47880	47880	47880	0	0	46926	954	46926	46926	46926	1	46926	46925	0	46925	46913	12	46913	13	13	0	0
Flakes	210000	210000	210000	0	0	0	210000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

	S-303	S-304	S-305	S-306	S-307	S-308	S-309	S-310	S-401	S-402	S-403	S-404	S-405	S-406	S-407	S-408	S-409	S-410	S-411	S-412	S-413
Temperature K	373.2	349.5	349.5	383.2	373.4	373.4	373.4	307.7	307.8	307.8	318.3	318.3	318.4	333.2	333.2	333.2	309.7	312.9	309.7	318.4	312.3
Pressure atm	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Mass Vapor Fraction	1.0	0.0	1.0	1.0	0.9	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	31500	229920	116580	229920	229920	209792	20128	116580	116580	116696	102444	14252	14252	14252	14137	115	115	246985	115	102444	349429
Mass Flow kg/hr																					
n-Hexane	0	133	102078	133	133	0	133	102078	102078	102188	101982	206	206	206	97	110	110	246951	110	101982	348933
Water	31500	16998	14502	16998	21665	1669	19995	14502	14502	14508	462	14045	14045	14045	14040	6	6	0	6	462	462
Palmitic Acid	0	398	0	398	398	398	0	0	0	0	0	0	0	0	0	0	0	7	0	0	7
Stearic Acid	0	160	0	160	160	160	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1
Oleic Acid	0	1277	0	1277	1277	1277	0	0	0	0	0	0	0	0	0	0	0	13	0	0	13
Linoleic Acid	0	954	0	954	954	954	0	0	0	0	0	0	0	0	0	0	0	13	0	0	13
Flakes	0	210000	0	210000	188571	188571	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

PROCESS STREAM DATA: CHLOROFORM

	S-101	S-102	S-103	S-104	S-105	S-106	S-107	S-108	S-201	S-202	S-203	S-204	S-205	S-206	S-207	S-208	S-209	S-210	S-211	S-212	S-301	S-302
Temperature K	298.2	298.2	353.2	298.2	298.2	334.5	299.8	334.5	401.2	401.0	401.0	410.2	404.7	404.7	442.2	440.0	440.0	323.2	402.7	333.2	298.2	298.2
Pressure atm	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.5	0.5	0.1	0.1	1.0	0.1	1.0	1.0	1.0
Mass Vapor Fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.7	0.0	1.0	0.1	0.0	1.0	0.1	0.0	1.0	0.0	1.0	0.0	0.0	0.0
Total Flow kg/hr	350000	350000	350000	350000	350000	385000	315000	385000	385000	160138	224862	160138	147065	13073	147065	137914	9151	137914	247086	247086	31500	31500
Mass Flow kg/hr																						
Chloroform	0	0	0	350000	350000	247789	102211	247789	247789	22952	224837	22952	9884	13068	9884	925	8959	925	246864	246864	0	0
Water	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	31500	31500
Palmitic Acid	19964	19964	19964	0	0	19566	398	19566	19566	19561	5	19561	19560	1	19560	19519	41	19519	48	48	0	0
Stearic Acid	8050	8050	8050	0	0	7890	160	7890	7890	7889	1	7889	7889	0	7889	7883	6	7883	7	7	0	0
Oleic Acid	64106	64106	64106	0	0	62829	1277	62829	62829	62819	10	62819	62817	2	62817	62744	73	62744	85	85	0	0
Linoleic Acid	47880	47880	47880	0	0	46926	954	46926	46926	46916	10	46916	46915	2	46915	46843	72	46843	84	84	0	0
Flakes	210000	210000	210000	0	0	0	210000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

	S-303	S-304	S-305	S-306	S-307	S-308	S-309	S-310	S-401	S-402	S-403	S-404	S-405	S-406	S-407	S-408	S-409	S-410	S-411	S-412	S-413
Temperature K	373.2	356.3	356.3	383.2	373.4	373.4	373.4	318.4	318.4	318.3	329.9	329.9	329.9	363.2	363.2	363.2	308.5	333.2	308.5	329.9	332.2
Pressure atm	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Mass Vapor Fraction	1.0	0.0	1.0	1.0	0.9	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	31500	227208	119292	227208	227208	209803	17405	119292	119292	119504	102204	17299	17299	17299	17088	212	212	247086	212	102204	349290
Mass Flow kg/hr																					
n-Hexane	0	116	102095	116	116	0	116	102095	102095	102253	102063	190	190	190	32	158	158	246864	158	102063	348926
Water	31500	14303	17197	14303	18970	1681	17289	17197	17197	17250	141	17109	17109	17109	17055	54	54	0	54	141	141
Palmitic Acid	0	398	0	398	398	398	0	0	0	0	0	0	0	0	0	0	0	48	0	0	48
Stearic Acid	0	160	0	160	160	160	0	0	0	0	0	0	0	0	0	0	0	7	0	0	7
Oleic Acid	0	1277	0	1277	1277	1277	0	0	0	0	0	0	0	0	0	0	0	85	0	0	85
Linoleic Acid	0	954	0	954	954	954	0	0	0	0	0	0	0	0	0	0	0	84	0	0	84
Flakes	0	210000	0	210000	205333	205333	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

PROCESS STREAM DATA: 1,2-DICHLOROETHANE

	S-101	S-102	S-103	S-104	S-105	S-106	S-107	S-108	S-201	S-202	S-203	S-204	S-205	S-206	S-207	S-208	S-209	S-210	S-211	S-212	S-301	S-302
Temperature K	298.2	298.2	378.2	298.2	298.2	344.6	299.4	344.6	415.2	415.0	415.0	427.2	420.5	420.5	460.2	457.2	457.2	323.2	417.1	353.2	298.2	298.2
Pressure atm	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.5	0.5	0.1	0.1	1.0	0.1	1.0	1.0	1.0
Mass Vapor Fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8	0.0	1.0	0.1	0.0	1.0	0.1	0.0	1.0	0.0	1.0	0.0	0.0	0.0
Total Flow kg/hr	350000	350000	350000	350000	350000	385000	315000	385000	385000	161795	223206	161795	146988	14807	146988	137352	9636	137352	247648	247648	63000	63000
Mass Flow kg/hr																						
1,2-Dichloroethane	0	0	0	350000	350000	247789	102211	247789	247789	24659	223130	24659	9871	14788	9871	861	9010	861	246928	246928	0	0
Water	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	63000	63000
Palmitic Acid	19964	19964	19964	0	0	19566	398	19566	19566	19550	16	19550	19547	4	19547	19411	135	19411	155	155	0	0
Stearic Acid	8050	8050	8050	0	0	7890	160	7890	7890	7888	2	7888	7887	0	7887	7866	21	7866	23	23	0	0
Oleic Acid	64106	64106	64106	0	0	62829	1277	62829	62829	62800	29	62800	62793	7	62793	62556	238	62556	273	273	0	0
Linoleic Acid	47880	47880	47880	0	0	46926	954	46926	46926	46897	30	46897	46890	7	46890	46658	232	46658	268	268	0	0
Flakes	210000	210000	210000	0	0	0	210000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

	S-303	S-304	S-305	S-306	S-307	S-308	S-309	S-310	S-401	S-402	S-403	S-404	S-405	S-406	S-407	S-408	S-409	S-410	S-411	S-412	S-413
Temperature K	373.2	363.6	363.6	383.2	373.4	373.4	373.4	333.2	333.2	332.7	344.6	344.6	344.6	371.2	371.2	371.2	314.1	353.2	314.1	344.7	350.7
Pressure atm	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Mass Vapor Fraction	1.0	0.0	1.0	1.0	0.9	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	63000	232595	145405	232595	232595	209791	22804	145405	145405	147473	102003	45470	45470	45470	43402	2068	2068	247648	2068	102003	349651
Mass Flow kg/hr																					
n-Hexane	0	175	102036	175	175	1	174	102036	102036	102641	102001	640	640	640	35	605	605	246928	605	102001	348928
Water	63000	19631	43369	19631	24298	1669	22629	43369	43369	44832	2	44830	44830	44830	43367	1463	1463	0	1463	2	2
Palmitic Acid	0	398	0	398	398	398	0	0	0	0	0	0	0	0	0	0	0	155	0	0	155
Stearic Acid	0	160	0	160	160	160	0	0	0	0	0	0	0	0	0	0	0	23	0	0	23
Oleic Acid	0	1277	0	1277	1277	1277	0	0	0	0	0	0	0	0	0	0	0	273	0	0	273
Linoleic Acid	0	953	0	953	953	953	0	0	0	0	0	0	0	0	0	0	0	268	0	0	269
Flakes	0	210000	0	210000	205333	205333	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

PROCESS STREAM DATA: METHANE

	S-101	S-102	S-103	S-104	S-105	S-106	S-107	S-108	S-109	S-110	S-201	S-202	S-203	S-204	S-205	S-206	S-207	S-208	S-301
Temperature K	298.2	298.2	343.2	303.2	303.2	333.2	343.6	336.9	343.6	313.2	313.2	313.2	403.2	395.2	395.2	323.2	341.0	341.0	298.2
Pressure atm	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.1	0.1	1.0	1.0	1.0	1.0
Mass Vapor Fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	350000	350000	350000	350000	350000	350000	438000	262000	438000	438000	299164	138836	138836	136544	2292	136544	2292	2292	26200
Mass Flow kg/hr																			
Methanol	0	0	0	329000	329000	329000	255116	73884	255116	255116	252565	2551	2551	572	1979	572	1979	1979	0
Water	29400	29400	29400	21000	21000	21000	45684	4716	45684	45684	45227	457	457	153	304	153	304	304	26200
Palmitic Acid	19964	19964	19964	0	0	0	19565	399	19565	19565	196	19369	19369	19367	2	19367	2	2	0
Stearic Acid	8050	8050	8050	0	0	0	7889	161	7889	7889	79	7810	7810	7810	0	7810	0	0	0
Oleic Acid	64106	64106	64106	0	0	0	62824	1282	62824	62824	628	62196	62196	62192	4	62192	4	4	0
Linoleic Acid	47880	47880	47880	0	0	0	46922	958	46922	46922	469	46453	46453	46450	4	46450	4	4	0
Flakes	180600	180600	180600	0	0	0	0	180600	0	0	0	0	0	0	0	0	0	0	0

	S-302	S-303	S-304	S-305	S-306	S-307	S-308	S-309	S-310	S-311	S-312	S-313	S-401	S-402	S-403	S-404	S-405	S-406
Temperature K	298.2	373.2	353.2	361.1	361.1	383.2	373.4	373.4	373.4	373.1	339.2	339.2	313.2	341.8	373.2	339.2	339.2	339.3
Pressure atm	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Mass Vapor Fraction	0.0	1.0	1.0	0.0	1.0	1.0	0.7	0.0	1.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0
Total Flow kg/hr	26200	26200	262000	184577	103623	184577	184577	181398	3179	25636	77987	77987	299164	299164	30478	268686	268686	348966
Mass Flow kg/hr																		
n-Hexane	0	0	73884	576	73308	576	576	62	513	7	73301	73301	252565	252565	0	252565	252565	327845
Water	26200	26200	4716	602	30314	602	3550	885	2665	25628	4686	4686	45227	45227	29106	16121	16121	21112
Palmitic Acid	0	0	399	399	0	399	399	399	0	0	0	0	196	196	196	0	0	2
Stearic Acid	0	0	161	161	0	161	161	161	0	0	0	0	79	79	79	0	0	0
Oleic Acid	0	0	1282	1282	0	1282	1282	1282	0	0	0	0	628	628	628	0	0	4
Linoleic Acid	0	0	958	958	0	958	958	957	0	0	0	0	469	469	469	0	0	4
Flakes	0	0	180600	180600	0	180600	177651	177651	0	0	0	0	0	0	0	0	0	0

PROCESS STREAM DATA: ETHANOL

	S-101	S-102	S-103	S-104	S-105	S-106	S-107	S-108	S-109	S-110	S-201	S-202	S-203	S-204	S-205	S-206	S-207	S-208	S-301
Temperature K	298.2	298.2	373.2	303.2	303.2	348.2	353.1	353.1	353.1	313.2	313.2	313.2	413.2	406.3	406.3	313.2	348.2	348.2	298.2
Pressure atm	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.1	0.1	1.0	1.0	1.0	1.0
Mass Vapor Fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.9	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	350000	350000	350000	350000	350000	350000	438000	262000	438000	438000	299164	138836	138836	136386	2450	136386	2450	2450	26200
Mass Flow kg/hr																			
Ethanol	0	0	0	329000	329000	329000	255116	73884	255116	255116	252565	2551	2551	435	2116	435	2116	2116	0
Water	29400	29400	29400	21000	21000	21000	45684	4716	45684	45684	45227	457	457	140	317	140	317	317	26200
Palmitic Acid	19964	19964	19964	0	0	0	19565	399	19565	19565	196	19369	19369	19366	3	19366	3	3	0
Stearic Acid	8050	8050	8050	0	0	0	7889	161	7889	7889	79	7810	7810	7810	0	7810	0	0	0
Oleic Acid	64106	64106	64106	0	0	0	62824	1282	62824	62824	628	62196	62196	62189	7	62189	7	7	0
Linoleic Acid	47880	47880	47880	0	0	0	46922	958	46922	46922	469	46453	46453	46447	7	46447	7	7	0
Flakes	180600	180600	180600	0	0	0	0	180600	0	0	0	0	0	0	0	0	0	0	0

	S-302	S-303	S-304	S-305	S-306	S-307	S-308	S-309	S-310	S-311	S-312	S-313	S-401	S-402	S-403	S-404	S-405	S-406
Temperature K	298.2	373.2	359.8	364.6	364.6	383.2	373.4	373.3	373.3	373.2	351.0	351.0	313.2	351.9	373.2	351.3	351.3	351.2
Pressure atm	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Mass Vapor Fraction	0.0	1.0	1.0	0.0	1.0	1.0	0.7	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow kg/hr	26200	26200	262000	184555	103645	184555	184555	181479	3076	25584	78061	78061	299164	299164	30108	269056	269056	349567
Mass Flow kg/hr																		
n-Hexane	0	0	73884	577	73307	577	577	59	519	0	73307	73307	252565	252565	0	252565	252565	327988
Water	26200	26200	4716	578	30338	578	3527	969	2557	25584	4754	4754	45227	45227	28736	16491	16491	21563
Palmitic Acid	0	0	399	399	0	399	399	399	0	0	0	0	196	196	196	0	0	3
Stearic Acid	0	0	161	161	0	161	161	161	0	0	0	0	79	79	79	0	0	0
Oleic Acid	0	0	1282	1282	0	1282	1282	1282	0	0	0	0	628	628	628	0	0	7
Linoleic Acid	0	0	958	957	0	957	957	957	0	0	0	0	469	469	469	0	0	7
Flakes	0	0	180600	180600	0	180600	177651	177651	0	0	0	0	0	0	0	0	0	0

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