CHBE 484 Solvent Recovery Project Group
Department of Chemical and Biological Engineering
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April 18, 2006

ATTN: Mr. Craig Smith
Manager – Occupational Research & Safety
University of British Columbia
Ste. 50-2075 Wesbrook Mall
Vancouver, B.C. Canada
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Dear Mr. Craig Smith:

RE: Solvent Recovery Report for CHBE 484 Green Engineering

The UBC solvent recovery program has been successful in recovering solvents such as acetone, methanol, xylenes and varsol. The availability of these solvent streams has been significantly reduced over the years, reinforcing the need to explore alternative recyclable solvent streams. In this project, Ethyl Acetate will be focused and recovered.

As a group project of CHBE 484 Green Engineering, our 3-member team has performed an analysis for the recovery of ethyl acetate. This report documents the procedure and results involved for the recovery of ethyl acetate.

We are confident that this report will meet your approval. If you have any questions or concerns, please do not hesitate to contact us.

Sincerely,

Yao-Tien (Jim) Chang Margaret Hung Tina Li-Ting Liu

CHBE 484 Solvent Recovery Group

SUMMARY

The objective of this project is to help UBC reduce hazardous waste disposal of ethyl acetate. Waste solvent from the laboratories was collected and distillated. This report includes analysis of experimental results, determination of the feasibility of reusing the recycled solvent, analysis of the environmental impacts associated with waste disposal, and recommendation and possible alternatives to improve waste solvent recovery process.

Out of all the contacted laboratories, eight laboratories which use at least 50 liters each year were identified. Six laboratories participated and only three laboratories were able to accumulate enough ethyl acetate waste solvent within a two-week period. Before distillation, the purities were tested by GC and they are 63.88%, 76.60%, and 87.64%. After distillation, the purities increased to 72.48%, 91.00%, and 92.69%, respectively; however, laboratories required a minimum of 98% purity in order for the distillated solvent to be reused. From the experimental GC results, unknown peaks were reduced after distillation, but were still present. The possible impurities could be hexane or acetone.

For acetone and methanol being the major recovery streams, they were compared in the analysis. Based on last year's survey result, if waste solvents were not properly treated, a release rate of approximately 4020L, 6360L, and 3680L was identified for ethyl acetate, acetone, and methanol, respectively. Ethyl acetate was found to be most harmful to the environment and ecosystem; however, it has the least impact on human health.

Although this stream could be uneconomical and thus unfeasible, it will greatly contribute to reducing environmental and heath impacts if all waste solvents are recycled and re-distributed to the laboratories after distillation. Alternates to acquire a purity of 98% include narrowing the temperature range for distillation, using distillations in series, etc. Waste generators can also separate ethyl acetate waste from other waste stream for a higher purity in the waste and thus improve the quality of recovered ethyl acetate.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

1.0 INTRODUCTION

The Department of Health Safety and Environment in UBC had started the Solvent Recovery Program since 1994. Organic waste solvents are identified, collected and purified for reuse on campus. The volume of recovered solvents distributed back to waste generators increased by 39% in 1997. In 1997, the program was successfully in recovering more than 1400 liters of solvent.

The UBC Solvent Recovery Program has successfully recover Acetone, Methanol, Xylene, and Varsol (part washer solvent). The availability of these solvent streams has been significantly reduced over the years, reinforcing the need to explore alternative recyclable solvent streams; therefore, the objectives of this project are: to help UBC reduce hazardous waste disposal, to collect and distillate ethyl acetate from waste solvent, to determine the feasibility of reusing the recycled solvents, to recommend possible alternatives to improve waste solvent recovery process and to analyze the environmental impacts associated with waste disposal.

The distillation unit, consisting of two spinning band distillation, is used in this recovering process. It has a capacity of distillating up to 60L per day of waste solvent. The distillated solvent is then analyzed using gas chromatography for quality/purity. Recovered solvent is sold at a reduced price to consumers on campus. Other than that, the University also benefits with lower disposal costs.

Waste solvent (ethyl acetate) will be collected in laboratories in Chemistry Department on campus and distillated. The distillated product will be analyzed by Gas Chromatography for purity. The results will be presented to the laboratories (waste generators) for possibility of reusing. Possible improvement of this process will then be made based on the results and feedback from waste generators.

2.0 PREVIOUS PROJECT

Last year, a survey was done by two students (Kosta Sainis and Erin Stevenson) to ascertain kinds of solvents and amounts used on campus. Moreover, how the solvents were used, the grade or quality required, the contaminants present after use, and whether or not the laboratory would use recycled solvent if it were available were also surveyed. From the data obtained, out of a variety of solvents used at UBC, ethyl acetate and petroleum ether/hexanes are good candidates for UBC solvent recovery program. They are used in the largest amounts in which 4020 L/yr of ethyl acetate and 3990 L/yr of petroleum ether/hexanes are used.

In addition, these solvents are primarily utilized for high performance liquid chromatography (HPLC), where HPLC grade (99.6%) is used, and column chromatography, where reagent grade is used. Laboratories using HPLC grade solvent were not interested in purchasing recycled solvent, while laboratories using reagent grade solvent expressed an interest in purchasing recycled solvent if the recycled solvent was of high enough purity. The reason that labs requiring HPLC grade would not buy back recycled solvent because the major cost of research was personnel in which the lab heads would not risk rendering labour time redundant by using untrustworthy solvents, which is how they classified recycled solvents. The labs do not want to risk the integrity of their results by using what they consider to be suspect solvent. However, the market for reagent grade ethyl acetate and petroleum ether/hexanes is promising. It is probable that waste from labs using either grade, could be recycled to reagent grade and sold back to labs utilizing reagent grade solvent.

3.0 ACTION PLAN

Four phases have been proposed and finished by the previous studentsand these are as the following:

Phase 1: Assessment of Alternative Waste Solvent Recovery Streams
Phase 2: Evaluate Advantages and Disadvantages of the Alternative Waste Streams
Phase 3: Detailed Investigation and Research
Phase 4: Recommendation Preparation

In this project of solvent recovery, another four phases will be proposed and this project should be completed. The proposed phases are as the following:

3.1 Phase 1: Solvent Waste Collection

Ten laboratories will be contacted and given empty containers to collect waste solvent. The recovered solvent will be ethyl acetate. 8 laboratories use large volume of ethyl acetate. Each laboratory will collect 2 containers of 4L waste solvent (total 8L) for distillation.

3.2 Phase 2: Solvent Recovery Experiments

Each sample from each lab will be distillated. The experiment is approximately 6 hr/sample for each sample being 4~8 L. This phase will be accomplished with the assistant from Mr. Bang Dang.

3.3 Phase 3: Result Analysis

After the raw data from the distillation is collected, analysis on the data will be done. Meanwhile the recovered samples will be sent back to each laboratory. Data collected from this phase includes:

- Gas chromatography results
- cost analysis
- global impact
- feedback from laboratories

3.4 Phase 4: Recommendation

After the feedback from the laboratories is gathered, recommendation on the solvent recovery will be made. This may include replacement of equipment, change in operating parameters, change in recovering solvent, etc.

4.0 EXPERIMENTAL APPARATUS

4.1 Gas Chromatograph

A gas chromatograph (GC) is a chemical analysis instrument for separating chemicals from a sample. GC was used to identify purity before and after distillation. GC usually contains components including a flowing mobile phase, an injection port, a separation column containing the stationary phase, and a detector. Samples are usually injected into the column using a microsyringe. GC uses a thin capillary fiber known as the column, through which different chemicals progress at different rates depending on various chemical and physical characteristics such as strength of adsorption. As the chemicals pass the detector, they are identified and shown electronically. The time at which each component reaches the outlet and the amount of that component can be determined. A schematic figure of gas chromatograph is shown below.

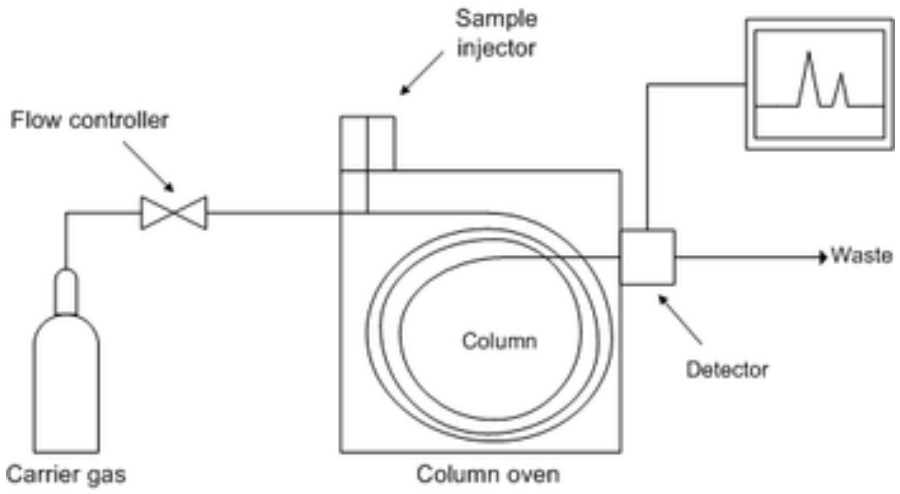

Figure 1. Diagram of a GC machine

Because molecular adsorption and the rate of progression in the column depend on the temperature, the temperature inside the column is carefully controlled. Sometimes temperature is ramped to provide the desired separation.

4.2 Flash Column

Ethyl acetate was used as a liquid solvent (effluent) for the flash column chromatography. Column chromatography is generally used as a purification technique to isolate desired compounds from a mixture. This equipment is used by the laboratories where ethyl acetate waste was generated. The liquid solvent passes through the column by gravity or by the application of air pressure. An equilibrium is established between the solute adsorbed on the adsorbent and the eluting solvent (ethyl acetate) flowing down through the column. Because the different components in the mixture have different interactions with the stationary and mobile phases, they will be carried along with the mobile phase to varying degrees and a separation will be achieved. The individual components, or elutants, are collected as the solvent drips from the bottom of the column.

The polarity of the solvent (ethyl acetate) which is passed through the column affects the relative rates at which compounds move through the column. Polar solvents can more effectively compete with the polar molecules of a mixture for the polar sites on the adsorbent surface and will also better solvate the polar constituents. Consequently, a highly polar solvent will move even highly polar molecules rapidly through the column. If a solvent is too polar, movement becomes too rapid, and little or no separation of the components of a mixture will result. If a solvent is not polar enough, no compounds will elute from the column. A schematic figure is shown below.

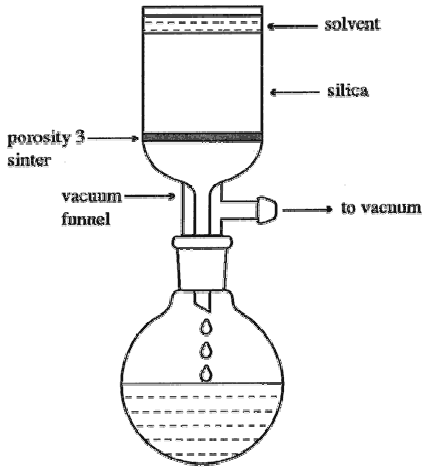

Figure 2. Diagram of a flash column

4.3 Spinning Band Distillation

All distillations attempt to separate a lower boiling material (**A**) from a higher boiling material (**B**). Vapors rise through the column, are condensed by the condenser and fall back down the column. Ascending vapors rise through the column and are forced into intimate contact with the condensate which causes the vapor to become enriched in the lower boiling material.

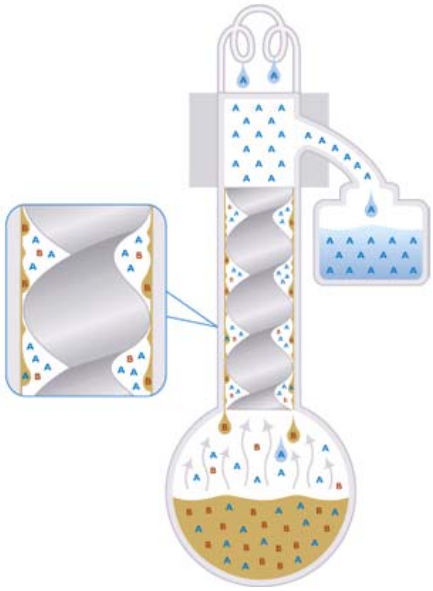

Figure 3. Diagram of a spinning band distillation

Spinning band distillation creates intimate contact between the vapors and the condensate in a dynamic process. Spinning band distillation was used to distillate ethyl acetate waste into purer ethyl acetate. A helix rotating at high speeds is used inside the distillation column. The spinning bands can be made of Teflon or metal. Teflon spinning bands are used for distillations below 225 °C. Metal bands are used for higher temperature distillations where Teflon would become soft. The rotating band forces vapors into intimate contact with the condensate on the wall of the distillation column. This contact takes place in a very thin layer that is refreshed thousands of times per minute. As a result, spinning band distillation gives a very efficient separation in a short distillation column.

5.0 RESULTS AND ANALYSIS

5.1 Laboratories Identified

Out of all the laboratories, eight use large amount of ethyl acetate, 48L to 1065L per year, as shown in table 1 below. Six out of these eight laboratories were two 4L waste solvent containers were dropped off for solvent waste collection.

Table 1: laboratories identified for feasible ethyl acetate recovery

idNumber	*Department*	*Building*	*Annual waste (L)*	*Ethyl acetate (L)*	*Ethyl acetate (%)*
G-0030	**Chemistry**	**Chemistry**	**4528.8**	**1064.6**	**23.5%**
G-0093	Ocenography	Biological Sci	3503	560	16.0%
G-0463	Chemistry	Chemistry	2991	830	27.7%
G-0025	**Chemistry**	**Chem Phys**	**900**	**300**	**33.3%**
G-0420	Chemistry	Chemistry	342	48	14.0%
G-0028	**Chemistry**	**Chemistry**	**1963**	**520**	**26.5%**
G-0061	NeuroMed Technology Inc.	Frederic Lasserre	940	384	40.9%

Waste solvents were collected from three of the laboratories while the other three was not able to aggregate enough waste for distillation. These laboratories that have aggregated enough solvent were G-0030, G-0025, and G-0028 as highlighted in table 1.

The waste solvent was sent to the Solvent Recovery facility and distillated. The waste solvent was analyzed by gas chromatography before and after the distillation for purity.

5.2 Gas Chromatography Results

Pure ethyl acetate was tested for purity using GC. The result is shown as below in figure 4. The purity of pure ethyl acetate should be around 99.9%. Because this bottle of ethyl acetate was open before this sample was taken, only 98.92% purity is shown.

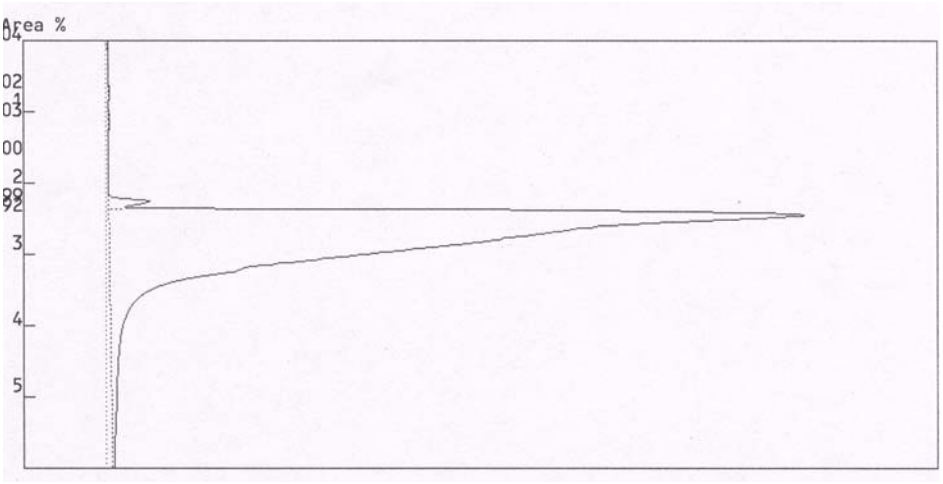

Figure 4. GC result of pure ethyl acetate

The waste solvents collected from the laboratories have 64% to 88% of ethyl acetate. After distillation, the purity was improved and found to be 72% to 93%. The results were summarized in table 2 below

Table 2: purities of solvent before and after distillation

idNumber	Purity before distillation	Purity after distillation
G-0025	76.60 %	92.69 %
G-0028	87.64 %	91.00 %
G-0030	63.88 %	72.48 %

Gas chromatography vaporizes the injected sample onto the head of the chromatographic column. The sample is transported through the column by the flow of inert, gaseous mobile phase. The inert carrier used in this experiment is Helium. The column itself contains a liquid stationary phase which is adsorbed onto the surface of an inert solid.

Different components with different affinity will be separated and hence the concentration of each component can be determined. From GC results, shown below in figure 5, 6 and 7, it can be seen that the peaks of the unknown decreased after distillation and the purity increased. However, it was unsuccessfully separated away from ethyl acetate. According to the feedback from the laboratories, possible impurities were hexane or acetone.

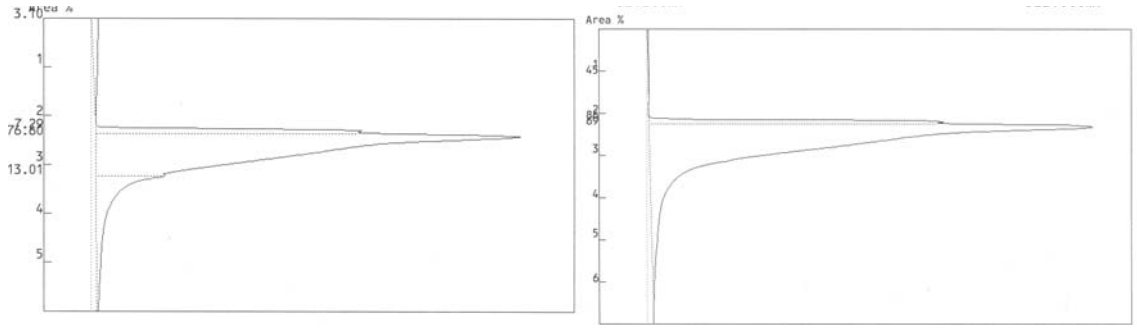

Figure 5. Left GC diagram of solvent G-0025 before distillation
Right GC diagram of solvent G-0025 after distillation

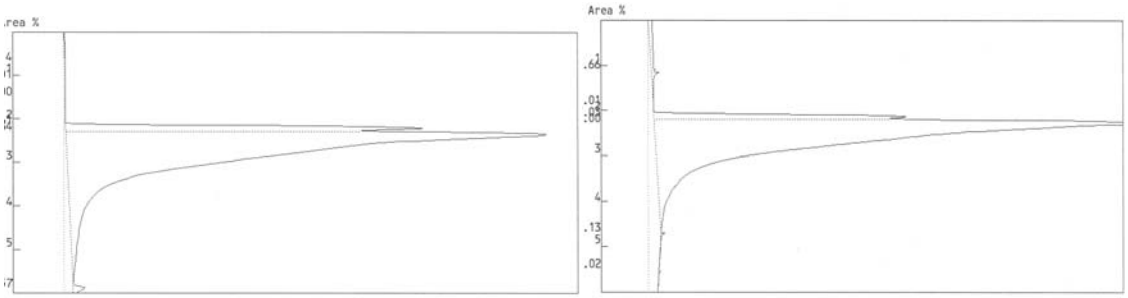

Figure 6. Left GC diagram of solvent G-0028 before distillation
Right GC diagram of solvent G-0028 after distillation

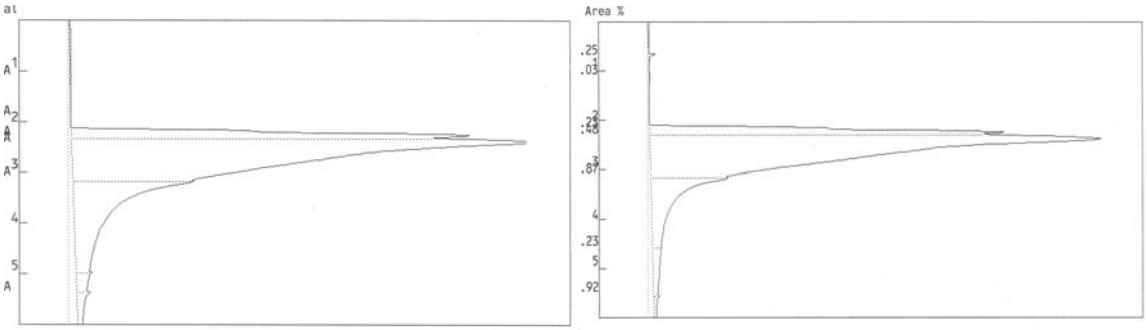

Figure 7. Left GC diagram of solvent G-0030 before distillation
Right GC diagram of solvent G-0030 after distillation

5.3 Environmental Impact and Health Risk Assessment

Since acetone and methanol are currently being recovered by the solvent recovery program, they are included in this assessment as a comparison to ethyl acetate.

From the waste audit done by last year's solvent recovery group, annual waste production of ethyl acetate, acetone and methanol on campus was recorded. Table 3 below shows the result. Using these values, a set of environmental, ecosystem and health impact were considered and calculated.

Table 3: annual release rate of ethyl acetate, acetone and methanol

Pollutants	*Emission rate (L/yr)*	*Density at 20C (kg/L)*	*Emission rate (kg/yr)*
Ethyl Acetate	4019.6	0.905	3637.738
Acetone	6358.7	0.79	5023.373
Methanol	3680.3	0.792	2914.7976
Total	14058.6	0.905	11575.909

5.3.1 Environmental impact assessment

The environmental impact of chemicals can be local, regional and global environmental issues. For these chemicals (acetone, methanol and ethyl acetate), evaluation of the environmental impact of chemical releases based on their impact on global warming and smog formation was done. GWP (global warming potential) and MIR (maximum incremental reactivity) were found from US-EPA website and shown below in table 4.

Table 4: GWP and MIR indexes from US-EPA website

Pollutants	*GWP*	*MIR*
Ethyl Acetate	2	1.1
Acetone	0	0.56
Methanol	1.6	0.56

The calculation of emission is based on maximum which is annual amount of each solvent waste generated on campus (based on survey) as shown in table 3. From the environmental impact shown in table 5, it is found that ethyl acetate is the most harmful

among the three solvents. A total of 11939.2 kg equivalent CO_2 and 2724.8 kg equivalent organic can be reduced if all the solvent are recovered. Out of the total amount, ethyl acetate emits more than half of the emission.

Table 5: annual equivalent CO_2 and ORG release rate

Pollutants	EI_{GW} *(equivalent kg CO_2/yr)*	EI_{SF} *(equivalent kg ORG/yr)*
Ethyl Acetate	7275.48	1290.81
Acetone	0	907.45
Methanol	4663.68	526.54
Total	11939.15	2724.80

5.3.2 Ecosystem impact assessment

Ecosystem impact assessment is based on plants, animal, their physical environment and the dynamic processes that link them. The risk of animal exposure to toxic chemical is characterized by LC50. LC50 is calculated based on Log K_{ow} found in US-EPA website as shown in table 6.

Table 6: Log K_{ow} and half life values from US-EPA website

Pollutants	*Log K_{OW}*	*$\tau_{1/2}$ (days)*
Ethyl Acetate	0.695	8.33
Acetone	-0.24	22
Methanol	-0.77	17.8

With LC50 calculated and the multi-media weighted half life found in the website, EIP (ecotoxicity potential index) can be calculated based on AIChE-CWRT with DDT (***d**ichloro-**d**iphenyl-**t**richloroethane*) as the benchmark. From table 7, it can be seen that again ethyl acetate is the most harmful solvent to the ecosystem. A total of 2.77E-6 kg/year of equivalent DDT is emitted from acetone, methanol and ethyl acetate. Ethyl acetate contributes to more than 85% of the total emission.

Table 7: annual equivalent DDT release rate

Pollutants	*Normalized EIP, day/(μmol/L) DDT equivalent*	*MWt (g/mol)*	*Emission rate (kg/yr)*	*Normalized EIP kg/yr DDT equivalent*
Ethyl Acetate	1.61245E-10	88.11	3637.738	2.35998E-06
Acetone	1.19139E-11	58.08	5023.373	3.65291E-07
Methanol	1.26976E-12	32.04	2914.7976	4.095E-08
Overall			11575.9086	2.76622E-06

5.3.3 Human health risk assessment

There are three pathways for human exposure to the chemicals, ie. inhalation by breathing, ingestion by drinking contaminated water and direct contact through the skin. In our case, inhalation is thought to be the dominant routes of exposure for human contact of the chemicals in the environment due to high volatility of the chemicals.

Human health impact is calculated based on TLV (threshold limit value) found from US-EPA website. The TLV values depend on the length of exposure time, so the TLV found on the website was based on time-weighted average over 8 hours per day and a 40-hour workweek. The health impact index is defined as the inverse of TLV. Health impact is defined as emission divided by TLV and is shown in table 8 below.

Table 8: health impact analysis based on TLV from US-EPA website

Pollutants	*TLV (mg/m^3)*	*Release rate, (kg/yr)*	*Health impact (kg/yr) / (mg/m^3)*
Ethyl Acetate	1440.00	3637.74	2.53
Acetone	1185.31	5023.37	4.24
Methanol	262.00	2914.80	11.13
		Overall	17.89

Based on TLV calculation, methanol has the greatest impact on human while ethyl acetate has the lowest impact.

Currently, it is assumed that none of these three solvent have carcinogenic effect on human because so far no related experiments were done for these solvent.

Another method used for evaluating health risk is using USES-LCA method and assuming all the untreated solvent is dumped onto surface of water. Life cycle assessment (LCA) is a tool for the assessment of the potential environmental impact of a product from its resource extraction to waste disposal. Below is the HTP found in literatures.

Table 9: HTP indexes found in literature on USES-LCA method

Pollutants	NON-Cancer HTP		Exposure route	
	Air	Water	Air	Water
Ethyl Acetate	1.20E-01	4.60E-02	Inh A	Inh W
Acetone	3.60E-01	2.30E-01	Inh A	Inh A
Methanol	1.10E-01	2.90E-02	Inh A	Inh A
DDT	7.30E+04	1.60E+05	Bioaccumulation in aquactic foodchain	

Where Inh A = inhalation through air and Inh W = inhalation through water

Based on HTP (health toxicity potential), health impact can be calculated, again using DDT as benchmark. From Table 10, it is found that methanol has the lowest health impact on human which is the opposite from TLV method. The reason for the opposite result is that TLV method might only based on a product from "gate to grave", not the entire life of the product.

Table 10: health impact result using USES-LCA method

Pollutants	*HTP Impact kg/yr DDT equivalent*
Ethyl Acetate	1.05E-03
Acetone	7.22E-03
Methanol	5.28E-04
Total	8.80E-03

5.3.4 Assessment conclusion

Based on the three impacts, environmental, ecosystem, and health, it is found that by reducing ethyl acetate, the environmental and ecosystem impact would greatly reduce. Human impact is not affected as much as the other two impacts. Based on the solvent recovery program of re-distributing 952L of acetone and 128L of methanol in 2005, table 11 summarize the impact that is currently reduced.

Table 11: summary of environmental impact and health risk asssessment

Pollutants	*Emission rate (L/yr)*	*Emission rate (kg/yr)*	*EI_{GW} (equivalent kg CO_2/yr)*	*EI_{SF} (equivalent kg ORG/yr)*	*Normalized EIP, kg/yr DDT equivalent*	*Health impact,*	
						TVL method kg/yr / (mg/m^3)	*USES-LCA Method kg/yr DDT equivalent*
Acetone	952	752.08	0	171.97	6.92E-08	0.80	1.37E-03
Methanol	128	101.38	204.8	23.12	1.80E-09	0.49	2.32E-05
Total	1080	853.46	204.8	195.10	7.10E-08	1.29	1.39E-03

From table 11, it can be summarized that a total of 204.8 equivalent kg CO_2, 195.1 equivalent ORG, equivalent 7.1E-8 kg DDT of ecosystem impact, and 1.39E-3 kg equivalent DDT are reduced in 2005 by the solvent recovery program.

5.4 Economic Analysis

Typically, estimation of equipment, installation, raw materials, energy, and maintenance costs are involved in the economic evaluation of engineering projects. Environmental costs are often factored into these calculations in determining economic rates of return, but other regulatory and social costs are not. Last year, the program made approximately $1112 out of the two main solvent recovery streams, acetone and methanol; however, costs such as equipment, energy, and maintenance are not included in the calculations. With the amount of money the program is making right now, it is obvious that if the overall costs analysis approach is taken, the program itself is obviously losing a fair amount every year. However the environmental benefit should also be taken into account. Not only does the solvent recovery process improve the environment by reducing emissions but also the laboratories save money on purchasing solvents. If solvents from are acquired from the market and used in the laboratories without recycling, higher prices are paid and disposal costs are not be avoided. On the other hand, although the costs to use the re-distributed solvents from the program could be more expensive than the market price (i.e. methanol), the laboratories are still able to save some money with disposal costs taken into consideration. In 2005, about 952 liter of acetone and 128 liter of methanol were re-distributed to the laboratories and the total amount saved was about $2660. Ethyl acetate is currently in the experimental stages; however, based on the

percentage re-distributed per year of acetone and methanol, that approximately 500 L per year could potentially be distilled and re-distributed was assumed. As a result of the assumption, a total saving could be estimated to be $1365 per year, with a potential buy-back price of $1.50/L, disposal cost of $2.36/L, and current market price of $1.87/L.

Table 12: cost analysis result

Solvent	Amount re-distributed	Price	Disposal Cost	Market Price	Net Savings
	L/year	$/L	$/L	$/L	$/year
Acetone	952	1	2.36	1.25	2484.72
Methanol	128	1.25	2.36	0.27	176.64
Total					2661.36

5.5 Feasibility Analysis

Solvent recyclers frequently handle only certain types of solvents and usually stipulate minimum quantities accepted. Prior to processing, solvent recyclers will test spent solvent to determine its composition. Most solvents used today are blends of different solvents of the same family. When evaluating the logistics of off-site solvent recycling, analyze the economic feasibility of using each available commercial recycling service. When conducting an economic analysis, consider the following factors:

- Quality of spent solvent: Segregate solvents and keep water out to improve recyclability of the spent solvent, and reduce the processing costs.
- Quality of recycled solvent: The tighter the specification for the recycled solvent, the higher the processing costs.
- Quantities: Increasing the batch size of spent solvent lowers unit processing costs.
- Higher recovery or yield of clean solvent is achieved from economy of scale: For example, the set up costs for processing 100 gallons of spent solvent is the same as for processing 1000 gallons. Larger batch sizes also reduce unit transportation costs.

- Disposal costs of the still bottoms or unrecovered portion of the waste stream
- Transportation costs
- Type of solvent: Most chlorinated solvents have higher resale value

In the ethyl acetate solvent recovery project, qualities of both spent and recycled ethyl acetate were quite low, considering that a minimum of 98% is required. The quantities from the laboratories are very low. Thus the processing cost is very high. Moreover, the costs to dispose the waste ethyl acetate solvent is $2.63/L and the transportation of small quantity of solvents is not as efficient as the big quantity. And ethyl acetate is not chlorinated solvents. Based on the evaluation, it is very costly to have the ethyl acetate recover stream constructed on UBC campus.

6.0 CONCLUSION

After finishing the four phases of this project, it was found that the ethyl acetate solvent recovery steam is much weaker comparing to acetone and methanol. The most crucial pull back of this stream is that high enough purity was not achieved after distillation. The highest purity achieved was 93% while the laboratories required a minimum purity of 98%. Since all laboratories will only be willing to reuse ethyl acetate if high purity is achieved, this recovery became unfeasible. Secondly, the amount of waste produced is not large enough for only three out of six laboratories were able to aggregate enough samples for distillation.

From the feasibility analysis, ethyl acetate has poor quality and quantities of recycled solvent and moderate quality of spent solvent which were the first three components for determining feasibility; therefore, the feasibility of recoverying ethyl acetate is low.

Even though this stream could be uneconomical, it will greatly contribute to reducing environmental and health impacts if laboratories use re-distributed ethyl acetate. For a maximum emission rate of 4019.6 L/year, 7275.48 of equivalent CO_2, 1291 kg of equivalent organic and 2.35998E-06 kg of equivalent DDT of environmental impact and 1.05E-3 kg equivalent DDT of health impact can be reduced. This will reduce the global warming and smog formation of the environment.

For ethyl acetate being the most toxic stream among the three solvents compared in this project, further research should be done by chemists to achieve 98% or higher purity after distillation. This will assist UBC much in becoming a sustainable campus.

7.0 RECOMMENDATION

Ethyl acetate and hexane are commonly used for flash chromatography. For laboratories that use flash chromatography, sizable amounts of ethyl acetate – hexane waste are produced. As mentioned above, the feasibility of recycling ethyl acetate with the current facility. Alternatives of recycling or reusing ethyl acetate are recommended. It was found that ethyl acetate – hexanes waste is not easily separated by distillation [1]. An alternative proposed is to recover ethyl acetate – hexane as a mixture from other impurities [2]. As proposed by Wilkinson T.J. 1997, 1,1'-diacetylferrocent was purified using flash column. The composition of the mixture is estimated by developing a TLC plate (Thin Layer Chromotagraphy) of acetylferrocene and/or 1,1'-diacetylferrocene with the mixture, determing the R_f's (retention factor). A figure of R_f versus % ethyl acetate is proposed by Wilkinson and can be used to find percentage composition.

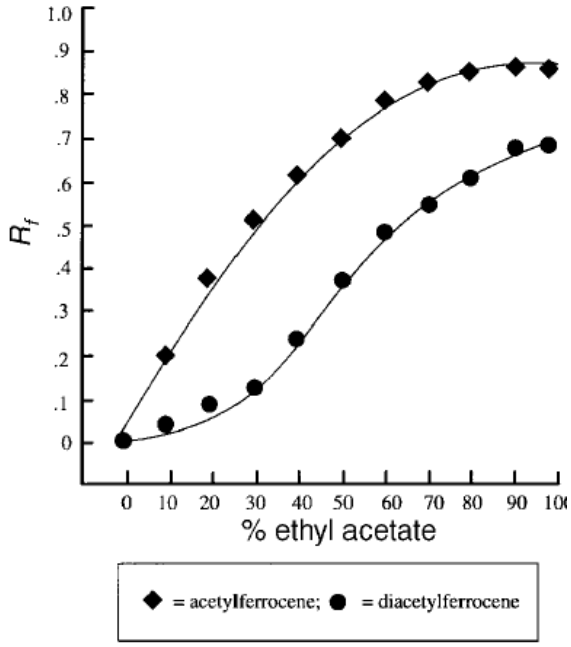

Figure 8. R_f versus % ethyl acetate

In order to reuse the mixture for column or TLC, a calculated amount of additional ethyl acetate is added to a given amount of the mixture to achieve the desired composition as shown below.

$$y = \frac{a(z-n)}{100-z}$$

Where y = volume of ethyl acetate added to achieve the desire composition [mL]

a = volume of ethyl acetate – hexane mixture [mL]

n = percent of ethyl acetate in the mixture [%]

z = desired percent of ethyl acetate

This method applies for laboratories that do not require high purity of ethyl acetate or the ethyl acetate waste with little impurities.

Other alternatives include narrowing the temperature range for distillation, using two distillations in series, etc. Waste generators can also separate ethyl acetate waste from other waste stream for a higher purity in the waste and thus improving the quality of recovered ethyl acetate.

8.0 Acknowledgement

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Appendix A: SAMPLE CALCULATION

Environmental Impact Analysis:

For Ethyl Acetate:

Emission rate = 4019.6 L/yr
GWP (Global Warming Potential) = 2
MIR (Maximum Incremental Reactivity) = 1.1
Density = 0.905 kg/L at STP

Therefore,

$$EI_{GW} = \frac{4019.6L}{yr} \times \frac{0.905kg}{L} \times 2 = 7275.48 \frac{kg}{yr} CO_2 \text{ equivalent}$$

$$EI_{SF} = \frac{\left(\frac{4019.6L}{yr} \times \frac{0.905kg}{L} \times 1.1 \right)}{3.1} = 1290.81 \frac{kg}{yr} ORG \text{ equivalent}$$

Ecosystem Impact Analysis:

For Ethyl Acetate:

Log Kow = 0.695
$\tau_{1/2}$ (multi-media weighted half-life) = 8.33 days
Molecular Weight = 88.11 g/mol

Therefore,

Ecosystem risk index ~ Lethal dose to 50% of the population over a certain exposure period (14 days):

$\log (LC_{50}) = 4.87 - 0.871 \log (Kow)$
$= 4.87 - 0.871 (0.695)$
$= 4.26$
$\rightarrow LC_{50} = 18393.10$ μmol/L

Bioaccumulation factor:

$\log (BCF) = 0.79 \log (Kow) - 0.4$
$= 0.79 (0.695) - 0.4$
$= 0.14905$
$\rightarrow BCF = 1.41$

Ecotoxicity Potential:

$$\text{ETP} = \frac{\tau_{1/2} BCF}{LC_{50}} = \frac{8.33 days \times 1.41}{18393.10\ \mu\text{mol/L}} = 0.00064 \frac{day}{\mu mol / L}$$

Using DDT as the benchmark chemical
For DDT:
$\tau_{1/2}$ (multi-media weighted half-life) = 10 years
LC_{50} = 3.27 µmol/L
BCF = 3548
Molecular Weight = 354.5 g/mol

Therefore,

$$\text{ETP}_{\text{DDT}} = \frac{3650 days \times 3548}{3.27\ \mu\text{mol/L}} = 3960305.81 \frac{day}{\mu mol / L}$$

So, Normalized Ecotoxicity Potential for Ethyl Acetate is,

$$\text{ETP} = \frac{3637.74 kg}{yr} \times \frac{0.00064 \, day / \mu mol / L}{3960305.81 \, day / \mu mol / L} \times \frac{354.5 \, g / mol}{88.11 \, g / mol} = 2.36E-6 \frac{kg}{yr} DDT \text{ equivalent}$$

Emission Rate

Human Health Risk Analysis:

For Ethyl Acetate:
TLV (Threshold Limit Value based on time weighted average) = 1440 mg/m^3
Non-cancer HTP = 4.60E-2 by water pathway

Therefore,
Using TLV value,

$$\text{HTP Impact} = \frac{3637.74 \, kg / yr}{1440 \, mg / m^3 \times kg / 1000000 mg} = 2526207 \frac{m^3}{yr}$$

Using USES-LCA method,

$$\text{HTP Impact} = \frac{3637.74 kg}{yr} \times 4.60E-2 = 1.67E2 \frac{kg}{yr}$$

Using DDT as the benchmark chemical

For DDT:

Non-cancer HTP = 1.60E5 by water pathway

So, Normalized HTP Impact is,

HTP Impact = $\frac{1.67E2kg}{yr} \times \frac{1}{1.60E5} = 1.05E-3 \frac{kg}{yr} DDT$ equivalent

Appendix B: MARKET PRICE

Acetone:	40 cents/lb	= roughly 1.12 U.S. dollars/L = roughly 1.25 Canadian dollar/L
Methanol:	90 cents/Gal	= roughly 23.78 cents U.S. dollars/L = 26.63 cents Canadian dollars/L
Ethyl Acetate:	68 cents/lb	= roughly 1.67 U.S. dollars/L = roughly 1.87 Canadian dollars/L