ABSTRACT

PONDER, CELIA STEWARD. Life Cycle Inventory Analysis of Medical Textiles and Their Role in Prevention of Nosocomial Infections. (Under the direction of Michael R. Overcash and Christine Grant).

Biocidal finishes grafted onto medical textiles are a potential technology to reduce nosocomial infection transmission. But is the application and use of biocidal finishes worth the environmental cost? Life cycle inventories (LCI) are a tool to show the resources used and emissions generated over the life cycle of a product. In this research, life cycle inventories are utilized in the design of a reusable medical garment with a biocidal finish to: assess options for the biocidal chemical, compare the reusable garment with a disposable garment, and assess the use of a biocidal finish in a hospital setting.

The cradle-to-gate life cycle inventories of two biocidal halamines – 3-allyl-5,5-dimethyl hydantoin (ADMH) and dimethylol-5,5-dimethyl hydantoin (DMDMH) – are compared to allow the manufacturer to select the chemical that consumes less energy and raw materials and generates fewer emissions. The reusable garment is then compared with a disposable gown of similar use to determine, cradle-to-use, which has the better environmental performance.

Life cycle inventory analysis is also used to determine the resources and emissions saved by the hypothetical use of a biocidal patient gown and the subsequent reduction in nosocomial infections. This is a novel area for LCI, as no LCI has been studied for treating an infection previously. When a patient contracts an infection while in the hospital, additional materials are used to test the patient, to provide contact isolation, and to treat the patient. Inventories were analyzed for each phase of this treatment using MRSA

(Methicillin-resistant Staphylococcus aureus) as the nosocomial infection contracted and treated.

Life Cycle Inventory Analysis of Medical Textiles and Their Role in Prevention of Nosocomial Infections

by
Celia Steward Ponder

A dissertation submitted to the Graduate Faculty of
North Carolina State University
in partial fulfillment of the
requirements for the Degree of
Doctor of Philosophy

Chemical Engineering

Raleigh, North Carolina

2009

APPROVED BY:

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DEDICATION

To my husband and my mother-in-law: Your support made this possible

And to Graana: this is your dream as much as it is mine

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Education

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- Ponder C.S., Overcash M.R. Grant, C.S., "Cradle-to-Gate Life Cycle Inventory of Vancomycin Hydrochloride." Submitted to *Science of the Total Environment.*

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- Ponder, C.S. and M.R. Overcash. Life cycle assessment of healthcare garments. International Life Cycle Assessment, Portland, Oregon, October 4, 2007.
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ACKNOWLEDGMENTS

I thank God for this opportunity to grow and develop. I know that all things are possible.

I also wish to thank my advisors Michael Overcash and Christine Grant for their support, guidance, and encouragement during my time at North Carolina State, and Gang Sun for being extremely helpful and responsive in answering my questions on his research on biocidal finishes on protective textiles. Jan Genzer and Marian McCord provided valuable insights during my practice presentations for conferences.

I would like to also thank the American Reusable Textile Association for providing valuable information on laundering and hospital gown use.

Evan Griffing and Yong Li provided knowledge, expertise, and guidance in life cycle inventories that allowed for a smooth the transition into the group.

I would like to give special thanks to my family for their love, support, understanding, and patience, especially when I had to work late.

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Global environmental crises such as global warming and the depletion of fossil fuels have caused a shift to thinking about sustainability. Sustainability is defined as being able to meet our needs to ensure that future generations are able to meet their needs (WCED, 1987). From an engineering perspective, a question often asked is "how can products be designed 'greener' to have less impact on the environment?" Another critical question is, "What raw materials should be used?" The concept and application of sustainability has also entered the healthcare field. In 2000, the first environmental audit was conducted at University Hospital in Germany (Dettenkofer et al., 2000). The US EPA and the American Hospital Association also partnered that year to form Hospitals for a Healthy Environment (H2E) with aims of reducing total solid waste and toxic waste. In 2001, an ecological footprint of Lionsgate Hospital in British Colombia was conducted (Germain, 2000). Each year, hospitals use an average of 2931 MJ of energy per patient per day and generate 11 kg solid waste per patient per day (Hospitals for a Healthy Environment, 2008, Garvin, 1995). Medical gowns and products to treat hospital-acquired infections contribute to this.

The use of a reusable medical gown with a biocidal finish may decrease the amount of raw materials and energy consumed and waste generated by the hospital, if it can be shown that it has (or can be designed to have) a smaller environmental footprint than a disposable gown. As a starting point, one needs to ask, "What has the most impact on the manufacture of a garment?" If the reusable medical patient gown has a biocidal finish that reduces infections, how much of a reduction in infection rate would be necessary to pay back the environmental burden of applying and using the finish? Life cycle assessment is a tool that can be used to answer these questions.

By definition, a life cycle assessment (LCA) is a "methodological framework for estimating and assessing the environmental impacts attributable to the life cycle of a product" (Hendrickson et al., 2006). All raw materials and energy consumption and waste generated during each step in the life of a product, from raw materials extraction, production, transportation, use, and disposal are tabulated and analyzed to show the total cradle-to-grave environmental impact of a product. LCA can allow manufacturers to select more environmentally friendly raw materials. LCA can also be used to improve the environmental performance of a product by highlighting where changes can be made to get the greatest reduction in resource consumption and emissions generated. For instance, LCAs are currently being used to compare alternative feedstocks, such as switchgrass, algae, corn, soybeans, alfalfa, sugar cane, sugar beet, cassava, and coconut to develop environmentally friendly alternatives to gasoline (Adler et al., 2007, Kim and Dale, 2005, Sheehan et al., 1998, von Blottnitz and Curran, 2007, Malça and Freire, 2006).

Prior to the LCA, resource and environmental profile analyses (REPA) were performed by private consulting firms in the 1980s and 1990s. However, there were conflicting results and no commonality, so SETAC (Society of Environmental Toxicology and Chemistry) and ISO (the International Organization for Standardization) worked together to develop the ISO 14040 standards for the life cycle assessment in 1996. According to ISO 14040 (International Standard Organization, 1997), the four phases of an LCA are goal and scope definition, inventory analysis, impact assessment, and interpretation. ISO 14040 provides specific and detailed guidelines for conducting a life cycle assessment, including

- Identifying the goal and scope of the LCA
- Using a functional unit as basis
- Defining the boundary of the system analyzed
- Conducting a peer and/or public review of the study

It is important to note that while some chemical processes have been studied extensively and have LCI data readily available, many chemicals and processes are proprietary. This lack of detailed process information makes the development of a method using unit operations and process engineering design mandatory for acquiring information for an LCI for chemicals and pharmaceuticals. Jimenez-Gonzalez (Jimenez Gonzalez, 2000) used the ISO standards to develop a detailed method for carrying out an LCI for chemicals and products to keep the inventory transparent and consistent, based on Figure 1. Highlights of this method are:

- Gate-to-gate (GTG, within the factory) inventories are summed for the final cradle-to-gate (CTG) inventory
- GTG inventories based on 1000 kg of final product
- A fugitive emissions calculation method

- Potential energy recovery calculations from cooled streams
- The exclusion of non-point source emissions, human labor, and capital (building and decommissioning) emissions
- Heuristics developed for unit operations

The most time-consuming step in creating a life cycle inventory is researching the product to collect the data to generate the detailed process flow diagram to insure an accurate representation. Information must be gathered from several sources. Next, a product chemical tree is generated that shows all chemical inputs for the product. A sample chemical tree (generated in this research) is shown in Figure 2 for dimethyloldimethyl hydantoin, one of the biocidal finishes studied in this work. Mass and energy balances are then used to calculate the inputs, outputs and energy consumption for the GTG inventory. GTG inventories are then created for each chemical used in the manufacture of the product, as shown in the chemical tree. Once all intermediate GTG inventories are completed, the inventories are summed to create the cradle-to-gate inventory of the product.

This LCI approach is refined to complete and analyze life cycle inventories for biocidal halamines, medical patient gowns, and textile coloring processes, and for more complex systems such as the pharmaceutical vancomycin hydrochloride and treating a hospital-acquired infection. Through the use of a common functional unit, the environmental burdens of using a biocidal medical patient gown and treating a nosocomial infection are compared.

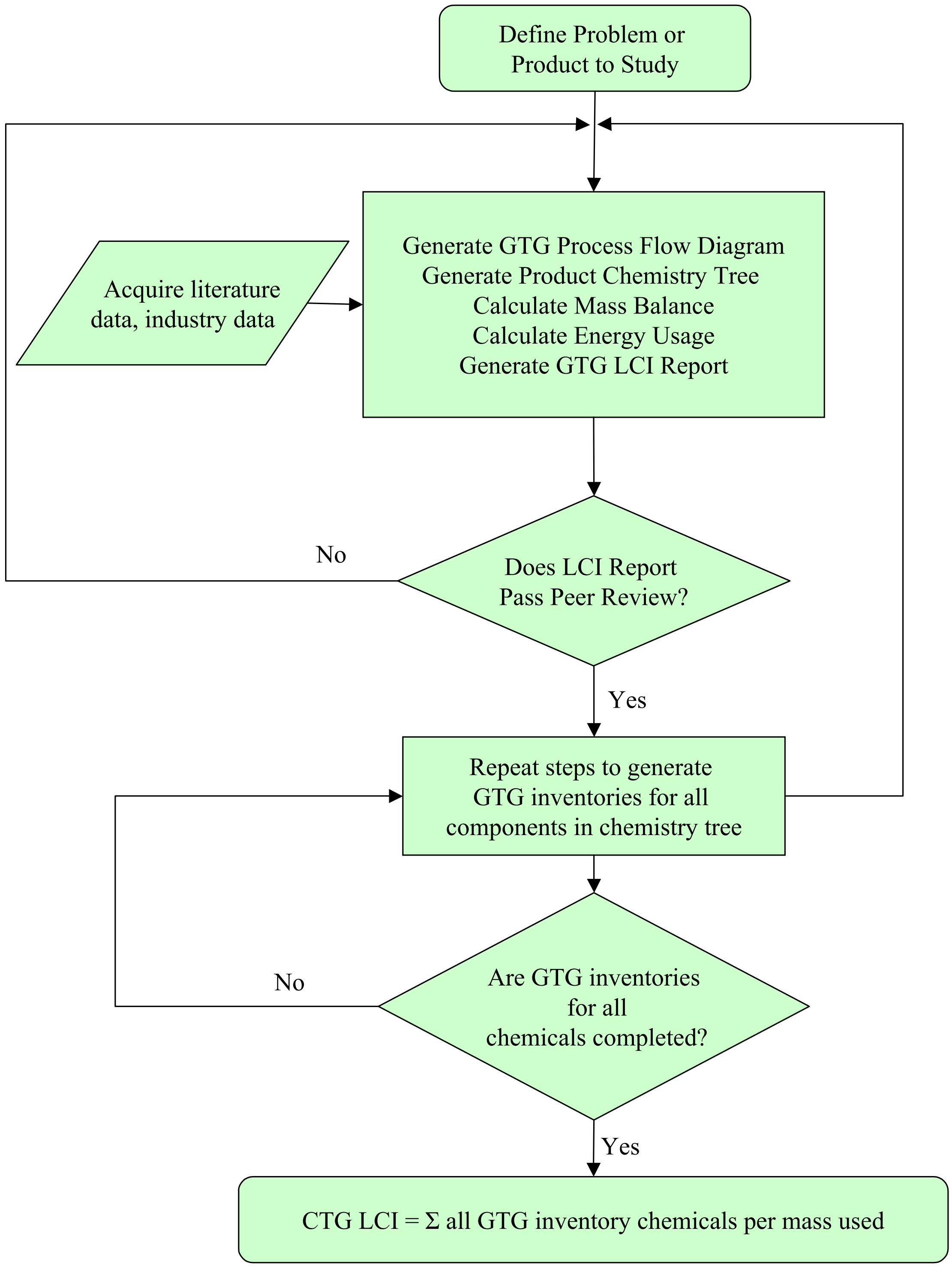

Figure 1.1. Flow Diagram for Generating Cradle-to-Gate Life Cycle Inventory of a Product

Level 1	Level 2	Level 3	Level 4	Level 5	Level 6	Level 7
Dimethyloldimethyl hydantoin	Dimethyl hydantoin	**Acetone**	**Benzene**	**pyrolysis gas**	Naphtha	oil (in ground)
				reformate, from naphtha	Naphtha	oil (in ground)
			Oxygen	Air (untreated)		
			Propylene	Naphtha	oil (in ground)	
		Ammonia	Natural gas	Natural gas (unprocessed)		
			Nitrogen from air	Air (untreated)		
			Oxygen from air	Air (untreated)		
			Water for rxn	Water (untreated)		
		Carbon dioxide	Natural gas	Natural gas (unprocessed)		
			Nitrogen from air	Air (untreated)		
			Oxygen from air	Air (untreated)		
			Water for rxn	Water (untreated)		
		Hydrogen cyanide	**Ammonia**	Natural gas	Natural gas (unprocessed)	
				Nitrogen from air	Air (untreated)	
				Oxygen from air	Air (untreated)	
				Water for rxn	Water (untreated)	
			Natural gas	Natural gas (unprocessed)		
			Oxygen from air	Air (untreated)		
	Formaldehyde	**Methanol**	Natural gas	Natural gas (unprocessed)		
			Water for rxn	Water (untreated)		
		Oxygen from air	Air (untreated)			
	Sodium hydroxide	Sodium chloride	Salt rock			
		Water for rxn	Water (untreated)			

Figure 1.2. Chemical Tree Example (for Dimethyloldimethyl hydantoin biocide used as biocidal finish)

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2. Cradle-to-Gate Life Cycle Inventory of Biocidal Halamine Finishes

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2. Cradle-to-Gate Life Cycle Inventory of Biocidal Halamine Finishes

Abstract

Biocidal finishes on medical textiles are a potential technology to reduce nosocomial infection transmission. The biocidal finishes are chemical structures attached to textile polymers and hence the interest in the environmental life cycle of these compounds. The cradle-to-gate life cycle inventories of two biocidal halamines – 3-allyl-5,5-dimethyl hydantoin (ADMH) and dimethylol-5,5-dimethyl hydantoin (DMDMH) – are compared. Using a life cycle approach, gate-to-gate (within the factory) inventories are created to assess resource and energy consumption and wastes associated with each of the processes. The life cycle inventories are created based on process flow models of product manufacturing to provide transparency. The cradle-to-gate production of DMDMH in solution consumes less energy and raw materials and generates fewer emissions than ADMH. Designers of biocidal medical textiles can use this information to select the more environmentally benign biocidal chemical for application.

Keywords: Life cycle inventory; life cycle analysis; allyl dimethylhydantoin; dimethylol dimethylhydantoin; halamine; energy; emissions

2.1 Introduction

Biocidal heterocyclic N-halamines, such as 3-allyl-5,5-dimethyl hydantoin (ADMH) and dimethylol-5,5-dimethyl hydantoin (DMDMH) (Figure 2.1), can be grafted onto fabrics to create clothing with biocidal properties for use in healthcare and personal protective apparel industry and in the military (Sun, 2001). The biocidal coatings protect the fabric from microbial attack and odor, and reduce microbes that cause illness. The halamine precursors are activated by the addition of a halogen such as chlorine or bromine. Chlorine and bromine halamines are also used in the pool industry to disinfect water (Sun et al., 1995).

(A) 3-Allyl-5,5-dimethylhydantoin (ADMH)

(B) 1,3-dimethylol--5,5-dimethylhydantoin (DMDMH)

Figure 2.1. Chemical structures of allyl dimethyl hydantoin (ADMH) and dimethylol dimethyl hydantoin (DMDMH).

Halamines kill a wide variety of microorganisms, including Escherichia coli and Methicillin resistant Staphylococcus aureus, and can be grafted onto cotton and synthetic fabrics. (See Figure 2.2) Grafted halamines are stable over long-term storage and a wide range of temperatures. In several studies, fabrics with grafted halamines such as dimethylol dimethylhydantoin (DMDMH) and allyl dimethyl hydantoin (ADMH) showed a 6-7 log reduction (99.9999-99.99999% reduction) of bacteria over a contact time of 1-2 hours, although DMDMH needed a shorter contact time than ADMH did. This antimicrobial property is regenerable by bleaching during the laundering cycle (Qian and Sun., 2004, Sun and Worley, 2005).

The halamines kill bacteria by an oxidizing mechanism in the microbial cell that attacks the cell wall and enzymes thus inhibiting enzymatic and metabolic cell processes, causing cell death. Halamine compounds provide the power of chlorine bleach but are non-irritant, non-corrosive, and do not produce HCl or other carcinogenic compounds such as $CHCl_3$ (Sun and Worley, 2005). Figure 2.2 shows DMDMH attached to the fabric by graft polymerization with an initiator. After grafting, a chlorine bleach solution is applied to the fabric, the hydantoin picks up a chlorine atom, and the hydantoin now becomes a chlorine halamine that is now the activated biocide. When bacteria come into contact with the chlorine halamine, the chlorine oxidizes the microbe, effectively killing it. No organisms appear to have developed immunity to this chlorine biocidal action and this offers additional advantage in the hospital setting (Sun and Worley, 2005). After reacting, the halamine structure is reduced to the precursor as shown in Figure 2.2 and can then be regenerated again with the application of bleach.

A life cycle inventory (LCI) study showing the raw materials and energy consumption and waste generated from the cradle-to-gate manufacture of a product is a valuable tool to use during the design phase of a product. It allows for the selection of “greener” raw materials and highlights where to make changes in the manufacturing process to reduce the environmental profile of the product. For the manufacture of medical textiles with a biocidal finish, the two halamine choices for application have similar activity against microbes, but the LCI can be used to select the halamine with the better environmental performance.

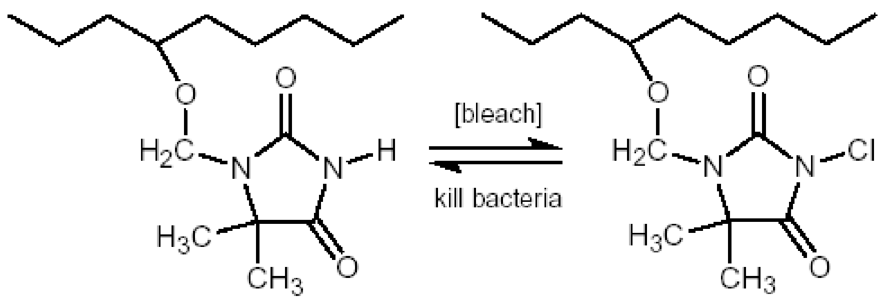


Figure 2.2. Halamine grafted onto fabric showing the reversible reaction of biocide killing bacteria and regenerating.

2.2 Goal and Scope of the Study

The intent of this work is to compare the production of two halamines that will be used in this nosocomial infection reduction strategy – ADMH and DMDMH – using a life cycle approach. Transparent gate-to-gate (GTG, within the factory) inventories are used, and the overall cradle-to-gate (CTG) inventory is the summation of these first level inventories. The halamines will be compared based on raw material and energy requirements and process emissions. The functional unit is 1000 kg halamine, and all processes are compared on that basis.

2.3 Methodology

In spite of more and more interest in LCA, the available life cycle inventory information is still far less than desired. In the chemical industry, companies have considered some information needed in life cycle studies as competitive intelligence. In this study, we use design-based approach methodology (Jimenez Gonzalez, 2000, Overcash, 1994) to obtain most of the life cycle inventory data, in which the life cycle information of each gate-to-gate subsystem is obtained using chemical engineering design techniques. Jimenez-Gonzalez used the ISO 14040 standards (International Standard Organization, 1997) to develop a detailed method for carrying out an LCI to keep the inventory transparent and consistent, based on Figure 2.3. Every life cycle inventory (LCI) follows a similar procedure, like an experiment in a laboratory. Information gathered from articles, books, patents, company websites, and consultations with experts in the field is then used with established process design heuristics to arrive at the LCI results. The gate-to-gate subsystems are linked through a production chain (referred to as the chemical tree), which includes extraction of raw materials and manufacturing processes. Whenever the site-specific information is available, it is applied to the process design in each study. The functional unit is defined as 1000 kg of halamine product. Energy to generate the energy utilities and emissions after waste management are not included.

After researching and selecting a generic process for manufacturing the product, a detailed process flow diagram is created in Microsoft PowerPoint and includes mass flows and process conditions, as shown in Figure 2.4. Using the process flow diagram (PFD), the mass and energy balances are calculated in a Microsoft Excel spreadsheet template created by the Overcash research group. Within the spreadsheet are several worksheets specifically for unit operations, such as heat exchanger, dryer, reactor, pumps, distillation column, evaporator, and mixers. All assumptions for these calculations are referenced in the Overcash group Heuristics for each unit process (Griffing et al., 2009). The process heuristics provide details of the calculations and what assumptions were made. The energy calculated for each unit operation in the PFD is then shown in an energy table, shown in Figure 2.5. The life cycle inventory report presents a written description of the manufacturing process along with the PFD, a summary of all inputs, products, process emissions, and energy used, and detailed calculations. A sample LCI report is shown in Appendix B. Once a gate-to-gate inventory is completed, a technical peer expert in the field reviews the LCI report, and changes are made as needed. This process is completed for the product and each chemical in the chemical tree of the product. The DMDMH chemical tree is shown in Figure 2.6. The product chemical (DMDMH) is on the left, and the natural resources are shown to the right in the shaded blocks. The chemical tree is read from left to right; DMDMH is produced from the raw materials dimethylhydantoin, formaldehyde, and sodium hydroxide. Each block represents a gate-to-gate (GTG), or a chemical factory. The entire tree forms the cradle-to-gate (CTG) for the product.

Transportation of each chemical from the factory is included in each gate-to-gate inventory as transportation consumes energy and resources and generates emissions. Average transportation distances are used, according to Table 2.1 (Research and Innovative Technology Administration (RITA), 1999). Once all GTG inventories for each chemical in the supply chain are completed, the inventories are summed to create the cradle-to-gate inventory of the product.

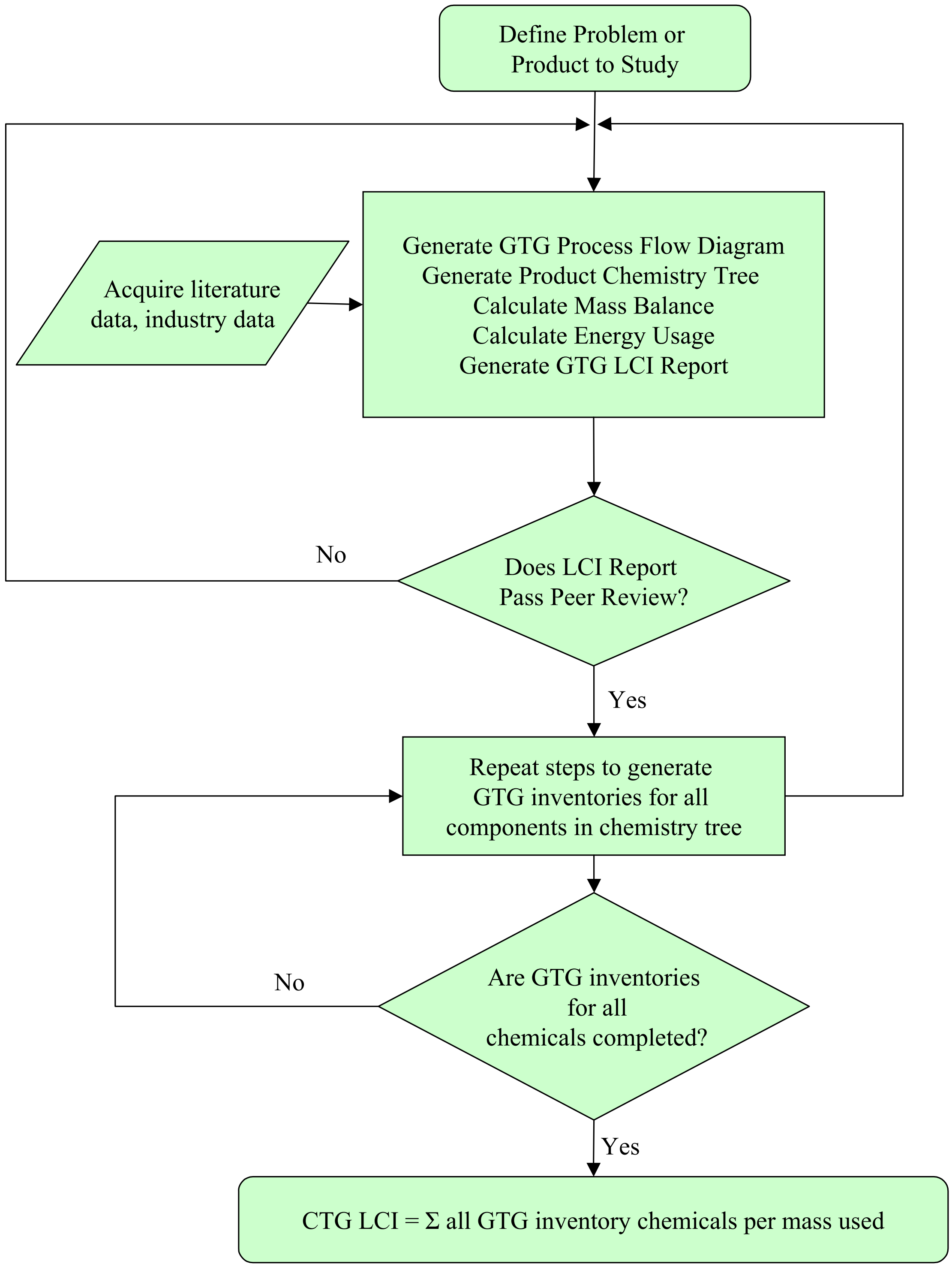


Figure 2.3. Flow Diagram for Generating Cradle-to-Gate Life Cycle Inventory of a Product

1,3-Dimethylol-5,5-Dimethylhydantoin [6440-58-0]

Revised 7-15-05

All cooling water has **20 °C and 50 °C** as input and output temperature respectively.

All steam streams have temperature of **207 °C** but input stream is gas phase and output stream is liquid phase.

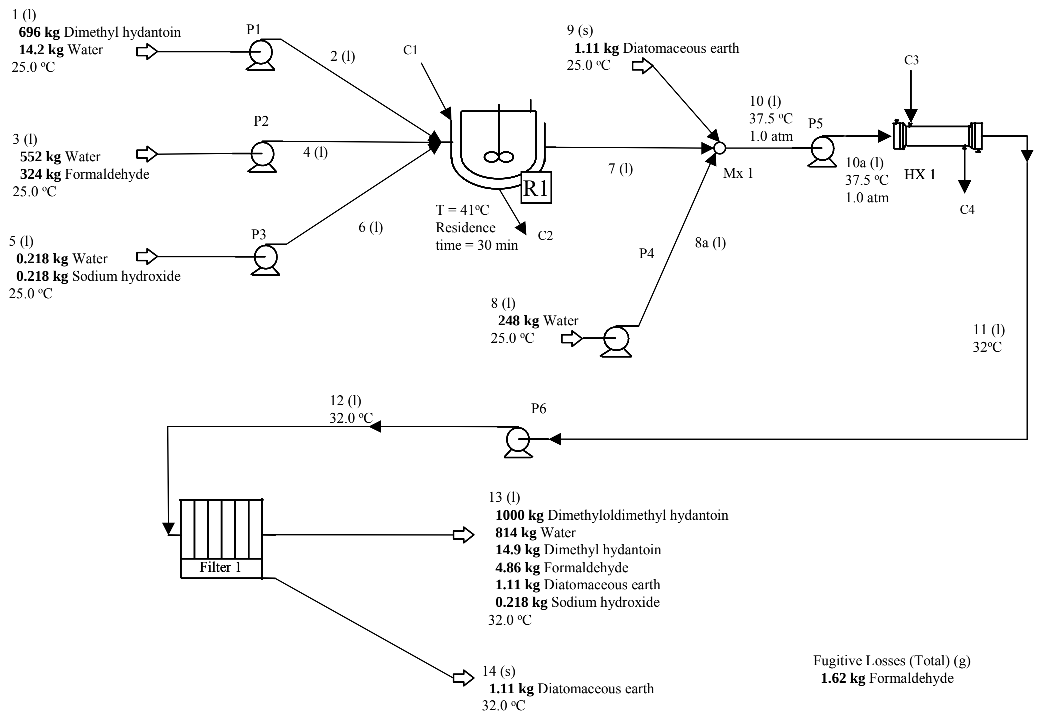


Figure 2.4. DMDMH Process Flow Diagram

Energy Input [MJ / batch]						Cooling Requirements [MJ / batch]							
Process Diagram Label	Unit	Energy input [MJ / 1000 kg Product]	Cumulative energy [MJ / 1000 kg Product]	To [C] (Used to determine energy type)	Energy Type	Process diagram label	Unit	Energy Loss [MJ / 1000 kg Product]	Cumulative cooling water energy [MJ / 1000 kg Product]	Tef [C] (for recovery efficiency)	Recovery Efficiency	Energy Recovered	Cumulative recovered [MJ / 1000 kg Product]
Blw1	Blower 1	0.118	0.118		E	Evp1	Evaporator condenser 1	-630	-630	0	0	0	0
Evp1	Evaporator 1	1139	1139	100	S	Ref1	Refrigerator cooling 1	-73.8	-704	25	0	0	0
P1	Pump 1	4.36E-05	1139		E	R1	Reactor 1	-1772	-2476	65.0	0.250	-443	-443
P2	Pump 2	1.02E-05	1139		E	R2	Crystallizer 1	-73.8	-2550	15.0	0	0	-443
P3	Pump 3	1.87E-04	1139		E	Hx1	Heat exchanger 1	-463	-3013	87.7	0.250	-116	-559
P4	Pump 4	1.15E-05	1139		E								
P5	Pump 5	0.0780	1139		E								
P6	Pump 6	0.102	1139		E								
P7	Pump 7	0.0193	1139		E								
Ref1	Refrigerator elect. 1	6.52	1145		E								
R1	Reactor 1 Agitator	286.58	1432		E								
R2	Crystallizer 1 Agitator	1.00	1433		E								
M1	Mixer 1 Agitator	.05	1433		E								
M2	Mixer 2 Agitator	.3	1433		E								
	Potential recovery	-559	875										
	Net energy		875				Potential recovery:						-559

Electricity	294.8	E	[MJ/1000kg]
DowTherm	0	D	[MJ/1000kg]
Heating steam	1139	S	[MJ/1000kg]
Direct fuel use	0	F	[MJ/1000kg]
Heating natural gas	0	G	[MJ/1000kg]
Energy input requirement	1433		[MJ/1000kg]
Cooling water	-3013		[MJ/1000kg]
Cooling refrigeration	-73.8		[MJ/1000kg]
Potential heat recovery	-559		[MJ/1000kg]
Net energy	875		[MJ/1000kg]

Figure 2.5. Energy Table for DMDMH

Level 1	Level 2	Level 3	Level 4	Level 5	Level 6	Level 7
Dimethyloldimethyl hydantoin 1,000	Dimethyl hydantoin 696	Acetone 324	Benzene 183	pyrolysis gas 53.3	Naphtha 54.3	oil (in ground) 55.0
				reformate, from naphtha 131	Naphtha 133	oil (in ground) 134
			Oxygen 77.3	Air (untreated) 107		
			Propylene 98.4	Naphtha 100	oil (in ground) 102	
		Ammonia 104	Natural gas 21.3	Natural gas (unprocessed) 21.7		
			Nitrogen from air 39.9	Air (untreated) 39.9		
			Oxygen from air 17.7	Air (untreated) 17.7		
			Water for rxn 27.7	Water (untreated) 27.7		
		Carbon dioxide 242	Natural gas 49.6	Natural gas (unprocessed) 50.6		
			Nitrogen from air 93.1	Air (untreated) 93.1		
			Oxygen from air 41.3	Air (untreated) 41.3		
			Water for rxn 64.6	Water (untreated) 64.6		
		Hydrogen cyanide 151	Ammonia 118	Natural gas 24.2	Natural gas (unprocessed) 24.7	
				Nitrogen from air 45.5	Air (untreated) 45.5	
				Oxygen from air 20.2	Air (untreated) 20.2	
				Water for rxn 31.5	Water (untreated) 31.5	
			Natural gas 140	Natural gas (unprocessed) 143		
			Oxygen from air 527	Air (untreated) 527		
	Formaldehyde 326	Methanol 409	Natural gas 253	Natural gas (unprocessed) 258		
			Water for rxn 175	Water (untreated) 175		
		Oxygen from air 230	Air (untreated) 230			
	Sodium hydroxide 0.218	Sodium chloride 0.169	Salt rock 0.215			
		Water for rxn 0.0526	Water (untreated) 0.0526			

Figure 2.6. Chemical Tree of DMDMH

The product chemical is on the left, and natural resources to the right. The amount of each chemical used to make 1000 kg DMDMH is shown.

Table 2.1. Average Transportation Values Used in Each Gate-to-Gate Inventory

	Value to use in GTG modeling					
Mode	**Basic Chemicals**	**Metallic ores and concentrates**	**Non-metallic minerals**	**Cereal grains**	**Coal**	**Fuel Oils**
Average distance/shipment (mi)	330	300	175	125	80	30
Average distance/shipment (km)	530	480	280	200	128	48
Contribution of modes (% of ton-mi)						
Truck	30	5	33	10	2	51
Rail	50	75	44	60	93	2
Water	20	20	23	30	5	12
Air	-	-	-	-	-	-
Pipeline	-	-	-	-	-	35
Multiple modes	-	-	-	-	-	-
Other unknown	-	-	-	-	-	-
Total	100	100	100	100	100	100

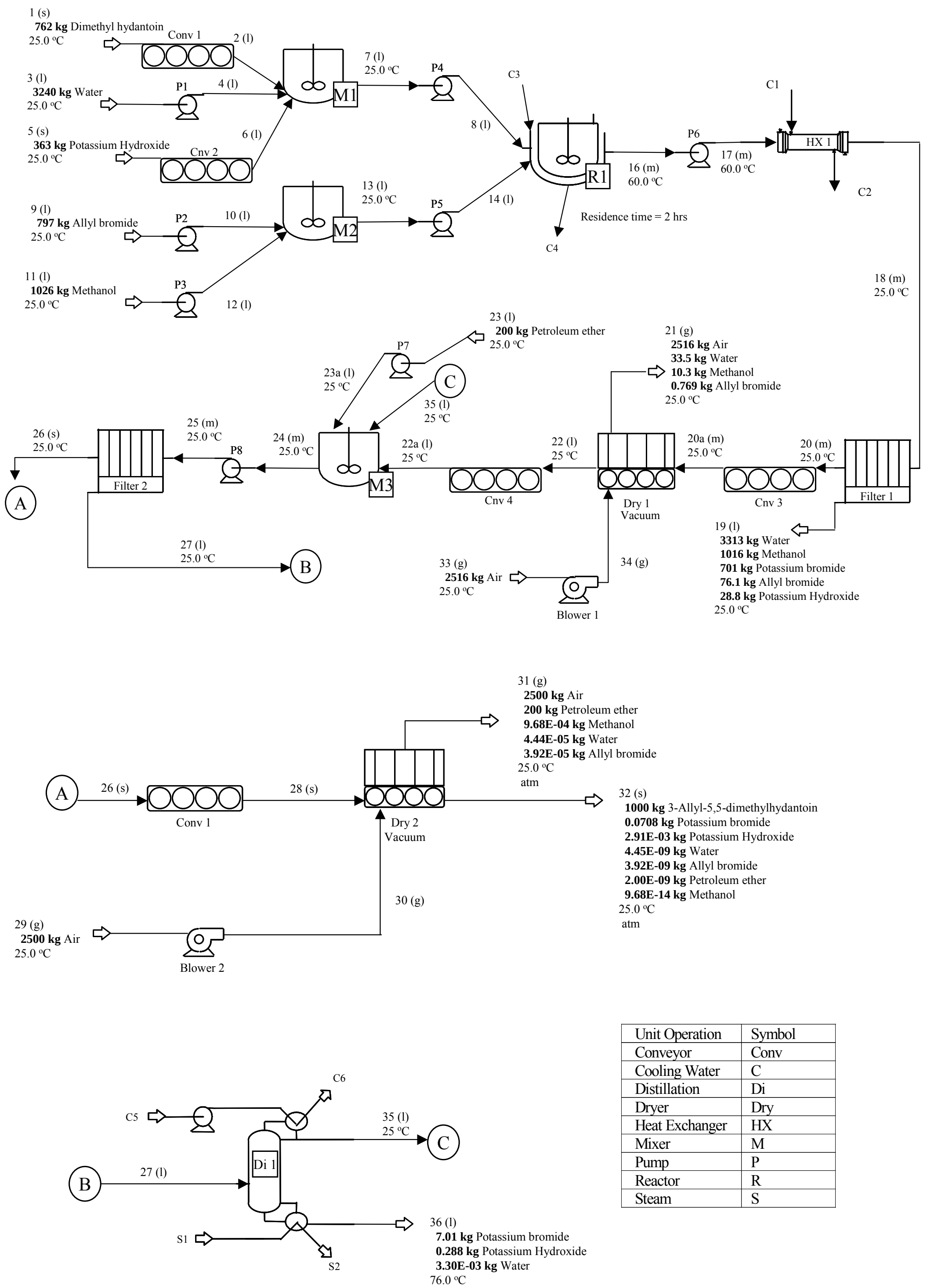
2.4 Halamine Manufacturing

The processes described are the generally used methods for preparing ADMH and DMDMH. As shown in Figure 2.7, 3-Allyl-5,5-Dimethyl hydantoin (ADMH) is produced by mixing a solution of 5,5-dimethyl hydantoin (DMH) and potassium hydroxide (KOH) with a solution of allyl bromide in methanol at 60 °C for 2 hours. The solution is then cooled to 25 °C, filtered and dried. ADMH is then recrystallized using petroleum ether (Sun and Sun, 2001).

The process flow diagram for producing 1,3-Dimethylol-5,5-dimethylhydantoin (DMDMH)is shown in Figure 2.4 (Foelsch, 1976). DMDMH is produced by reacting formaldehyde and dimethyl hydantoin for 30 minutes at 40 °C; the pH is adjusted with sodium hydroxide. Upon exiting the reactor, water is added and the solution is cooled to

32 °C. The solution is filtered with a filter aid, such as diatomaceous earth, and sold as a 55 weight % DMDMH product in water.

Energy for both processes is calculated from the unit operations shown in the process flow diagrams.



Unit Operation	Symbol
Conveyor	Conv
Cooling Water	C
Distillation	Di
Dryer	Dry
Heat Exchanger	HX
Mixer	M
Pump	P
Reactor	R
Steam	S

Figure 2.7. ADMH Process Flow Diagram

2.5 Inventory Results and Discussion

Using the detailed process flow diagrams generated in Figures 2.4 and 2.7, mass and energy balances were calculated. The chemical trees in Figures 2.6 and 2.8 show the mass (in kg) of all chemicals from cradle to gate that went into the production of ADMH and DMDMH starting with the product halamine on the left (Level 1) and the natural resources on the right. The numbers indicate the mass that went into producing ADMH or DMDMH. Gate-to-gate (within the factory) inventories were completed for each chemical shown, and the gate-to-gate inventories were summed to get the complete cradle-to-gate life cycle inventory.

Level 1	Level 2	Level 3	Level 4	Level 5	Level 6	Level 7	Level 8	Level 9
3-Allyl-5,5-dimethylhydantoin 1,000	Allyl bromide 805	Allyl Alcohol 507	Propylene oxide 535	**Ethylene glycol 134**	Ethylene oxide 96.8	**Ethylene 72.7**	Naphtha 74.1	oil (in ground) 75.1
						Oxygen 71.1	Air (untreated) 98.3	
					Water for rxn 37.6	Water (untreated) 37.6		
				Hypochlorous acid 626	**Chlorine 461**	Sodium chloride 358	Salt rock 456	
						Water for rxn 111	Water (untreated) 111	
					Sodium hydroxide 246	Sodium chloride 191	Salt rock 243	
						Water for rxn 59.4	Water (untreated) 59.4	
				Propylene 502	Naphtha 512	oil (in ground) 519		
				Sodium hydroxide 408	Sodium chloride 316	Salt rock 403		
					Water for rxn 98.5	Water (untreated) 98.5		
		Hydrogen bromide 952	Bromine 959	Brine 969	Sea water 969			
				Chlorine 577	Sodium chloride 447	Salt rock 571		
					Water for rxn 139	Water (untreated) 139		
				Sodium hydroxide 137	Sodium chloride 106	Salt rock 136		
					Water for rxn 33.1	Water (untreated) 33.1		
			Hydrogen 13.3	Naphtha 46.5	oil (in ground) 47.1			
				Oxygen 46.4	Air (untreated) 64.2			
				Oxygen from air 30.4	Air (untreated) 30.4			
				Water for rxn 20.2	Water (untreated) 20.2			
	Dimethyl hydantoin 762	**Acetone 355**	**Benzene 201**	**pyrolysis gas 58.3**	Naphtha 59.5	oil (in ground) 60.2		
				reformate, from naphtha 143	Naphtha 145	oil (in ground) 147		
			Oxygen 84.6	Air (untreated) 117				
			Propylene 108	Naphtha 110	oil (in ground) 111			
		Ammonia 114	Natural gas 23.3	Natural gas (unprocessed) 23.8				
			Nitrogen from air 43.7	Air (untreated) 43.7				
			Oxygen from air 19.4	Air (untreated) 19.4				
			Water for rxn 30.3	Water (untreated) 30.3				
		Carbon dioxide 265	Natural gas 54.4	Natural gas (unprocessed) 55.4				
			Nitrogen from air 102	Air (untreated) 102				
			Oxygen from air 45.3	Air (untreated) 45.3				
			Water for rxn 70.7	Water (untreated) 70.7				
		Hydrogen cyanide 166	**Ammonia 129**	Natural gas 26.5	Natural gas (unprocessed) 27.1			
				Nitrogen from air 49.8	Air (untreated) 49.8			
				Oxygen from air 22.1	Air (untreated) 22.1			
				Water for rxn 34.5	Water (untreated) 34.5			
			Natural gas 153	Natural gas (unprocessed) 156				
			Oxygen from air 577	Air (untreated) 577				
	Potassium Hydroxide 363	**KOH in solution (50%) 363**	Potassium chloride 308	Sylvinite ore 902	sylvinite ore (in ground) 902			
			Water for rxn 3.92	Water (untreated) 3.92				

Figure 2.8. Chemical Tree of ADMH.

The product chemical is on the left, and natural resources to the right. The amount of each chemical used to make 1000 kg ADMH is shown.

Table 2.2 indicates that ADMH production uses more raw materials than DMDMH since it is crystallized first while DMDMH remains as a solution. Electrical, steam, and total net energy usage for ADMH production are an order of magnitude higher than that required for DMDMH production. (See Table 2.3)

Table 2.2. Raw materials used in the cradle-to-gate manufacture of 1000 kg biocidal halamine.

Raw material, kg	ADMH				DMDMH			
	Total	Process	Energy-related	Transport	Total	Process	Energy-related	Transport
Air	1,169	1,169	0	0	1,121	1,121	0	0
Coal	771	0	771	0	117	0	117	0
Crude Oil	2,692	960	1,598	135	427	291	96	40
Natural gas	1,971	263	1,708	0	619	498	122	0
Salt rock	1,809	1,809	0	0	0	0	0	0
Sea water	969	969	0	0	0	0	0	0
Sylvinite ore	902	902	0	0	0	0	0	0
Water for reaction	639	639	0	0	298	298	0	0
Total	10,922	6,710	4,077	135	2,583	2,209	335	40

Water added as dilution in product is not shown in the Table. ADMH = allyl dimethyl hydantoin, DMDMH = dimethylol dimethyl hydantoin.

Table 2.3. Cradle-to-Gate Energy Consumption for production of 1000 kg ADMH and DMDMH.

Energy, MJ	ADMH	DMDMH
Electricity	15,696	1,762
Dowtherm	896	108
Heating steam	166,096	12,765
Fuel	20,369	8,509
Total Energy input	203,057	23,144
Cooling water	-201,548	-22,467
Refrigeration	93	51
Potential recovery[A]	-71,742	-10,879
Net energy (Input - Potential recovery)	131,315	12,266

[A] Energy that can be recovered from sources requiring cooling.

Table 2.4 shows the energy consumed by each cradle-to-gate chemical based on the amount of mass that went into ADMH production. In the cradle-to-gate ADMH production, the highest energy consuming chemicals are bromine, ADMH, and propylene. Bromine energy consumption is much higher than all other chemicals since large amounts of steam are required to recover bromine from brine. The lowest energy consuming chemicals are hydrogen cyanide, hydrogen, and ethylene oxide. The manufacture of hydrogen cyanide produces a large amount of heat that can be recovered, giving it a negative net energy consumption.

For the cradle-to-gate analysis of DMDMH production, the highest energy consuming chemicals are methanol, natural gas, and propylene. (See Table 2.5) The lowest energy consuming chemical is hydrogen cyanide. The gate-to-gate energy values of each chemical (MJ) in Tables 2.4 and 2.5 can be obtained by dividing the kJ/kg (MJ/1000 kg) values by the chemical mass/1000 kg halamine.

To compare the natural resource usage and waste generation, mass intensity and E-factor can be used.

$$\text{Mass Intensity} = \frac{\text{Total GTG Raw Materials Mass Used}}{\text{Mass of Final Product}} \quad (2.1)$$

$$\text{E} - \text{Factor} = \frac{\text{Total GTG Waste Mass}}{\text{Mass of Final Product}} \quad (2.2)$$

The mass intensity is the ratio of mass of raw materials used to mass of final product. The E-factor is the ratio of the total waste mass to the final product mass. The mass intensity ideally approaches one when the raw material input equals the product mass; thus, no waste is generated. For a single-product process,

$$\text{E - Factor} = \text{Mass Intensity - 1} \tag{2.3}$$

However, if any by-products are formed, this is not true since by-products are not considered to be waste. The mass intensity is higher for ADMH with a value of 11, compared to DMDMH at 1.023, showing that more raw materials are used in the manufacture of ADMH. ADMH also produces more waste per mass of halamine produced. The E-factor of ADMH is also higher than DMDMH at 10 compared to 0.027. Again, this is due to crystallizing the ADMH and leaving the DMDMH in solution. A lower E-factor is preferable, as a process with zero waste will have an E-factor of zero.

The total cradle-to-gate emissions listed in Table 2.6 come from chemical losses, energy-related emissions, and transportation-related emissions from each GTG inventory. Depending on the physical state, the emissions are listed as air, liquid, or solid. These emissions do not include the effect of waste management processes, and thus are direct process chemical losses. As shown in Table 2.6, ADMH generates more air, water, and solid emissions than DMDMH. Carbon dioxide was the largest contributor to air emissions, primarily due to energy-related emissions.

Table 2.4. ADMH Cradle-to-Gate Energy Consumption per chemical used in the production of ADMH

				CTG Energy, MJ/1000 kg ADMH[a]							
Chemicals, gate-to-gate	Mass, kg[b]	By-products, kg/kg chemical[c]	Allocation factor[d]	Electricity	Dowtherm	Steam	Fuel, Non-transport	Fuel, Transport	Potential recovery[e]	Total net energy	% of Total net energy
3-Allyl-5,5-dimethylhydantoin	1,000		1.000	107	0	1.31E+04	0	440	-2,797	1.08E+04	8.3%
Allyl bromide	805		1.000	15.1	0	492	12.9	354	-91.5	782	0.6%
Allyl Alcohol	507		1.000	75.6	777	1,170	0	223	-665	1,581	1.2%
Propylene oxide	535		1.000	8.03	0	2,032	0	236	-387	1,888	1.4%
Ethylene glycol	134	9.70E-03 kg Ethylene Glycol, Tri; 0.0946 kg Ethylene Glycol,di;	0.906	49.9	0	1,836	0	58.9	-480	1,465	1.1%
Ethylene oxide	96.8		1.000	188	0	3.61	0	42.6	-551	-316	-0.2%
Ethylene	72.7	0.480 kg C4 stream; 0.0881 kg fuel oil; 0.0484 kg Hydrogen; 0.569 kg Methane; 0.634 kg Propylene; 1.03 kg pyrolysis gas;	0.260	103	0	172	841	32.0	-206	943	0.7%

Table 2.4 continued

				CTG Energy, MJ/1000 kg ADMH[a]							
Chemicals, gate-to-gate	Mass, kg[b]	By-products, kg/kg chemical[c]	Allocation factor[d]	Electricity	Dowtherm	Steam	Fuel, Non-transport	Fuel, Transport	Potential recovery[e]	Total net energy	% of Total net energy
Naphtha	947	1.55 kg heavy gas oil, from distillation; 0.644 kg kerosene, from distillation; 0.542 kg light gas oil, from distillation; 0.711 kg residuum, from distillation;	0.225	226	0	106	1,868	0	0	2,201	1.7%
Oxygen	202	0.0690 kg Argon; 3.24 kg Nitrogen;	0.232	225	0	0	0	88.9	0	314	0.2%
Water for reaction	639	0.0000 kg Water;	1.00	0.514	0	0	0	0	0	0.514	0.0%
Hypochlorous acid	626	1.45 kg Sodium chloride;	0.409	392	0	1,778	0	275	0	2,446	1.9%
Chlorine	1,038	0.0295 kg Hydrogen; 1.18 kg Sodium hydroxide;	0.453	5,875	0	0	0	457	-212	6,119	4.7%
Sodium chloride	1,418		1.000	6.41	0	6,903	114	624	0	7,648	5.8%

Table 2.4 continued

				CTG Energy, MJ/1000 kg ADMH[a]							
Chemicals, gate-to-gate	Mass, kg[b]	By-products, kg/kg chemical[c]	Allocation factor[d]	Electricity	Dowtherm	Steam	Fuel, Non-transport	Fuel, Transport	Potential recovery[e]	Total net energy	% of Total net energy
Sodium hydroxide	791	0.848 kg Chlorine; 0.0250 kg Hydrogen;	0.534	4,477	0	0	0	348	-162	4,664	3.6%
Propylene	610	0.756 kg C4 stream; 1.58 kg Ethylene; 0.139 kg fuel oil; 0.0762 kg Hydrogen; 0.898 kg Methane; 1.63 kg pyrolysis gas;	0.165	867	0	1,443	7,061	268	-1,726	7,913	6.0%
Hydrogen bromide	952		1.000	10.1	0	221	0	419	-449	201	0.2%
Bromine	959		1.00	319	0	1.30E+05	0	422	-5.51E+04	7.58E+04	57.7%
Brine	969		1.000	0	0	0	0	0	0	0	0.0%
Hydrogen	13.3		1.000	52.8	0	0	0	5.83	-418	-359	-0.3%
Oxygen from air	694	2.79 kg Nitrogen from air;	0.264	0	0	0	0	0	0	0	0.0%
Dimethyl hydantoin	762		1.000	225	0	1,021	0	335	-426	1,155	0.9%
Acetone	355	1.61 kg Phenol;	0.384	347	0	1,626	0	156	-960	1,170	0.9%

Table 2.4 continued

				CTG Energy, MJ/1000 kg ADMH[a]							
Chemicals, gate-to-gate	Mass, kg[b]	By-products, kg/kg chemical[c]	Allocation factor[d]	Electricity	Dowtherm	Steam	Fuel, Non-transport	Fuel, Transport	Potential recovery[e]	Total net energy	% of Total net energy
Benzene	201	3.40 kg Non-aromatics for gas pool; 1.41 kg Toluene; 1.46 kg Xylenes;	0.138	0.112	0	523	0	88.4	-161	451	0.3%
pyrolysis gas	58.3	0.465 kg C4 stream; 0.970 kg Ethylene; 0.0854 kg fuel oil; 0.0469 kg Hydrogen; 0.552 kg Methane; 0.615 kg Propylene;	0.268	82.9	0	138	675	25.7	-165	757	0.6%
reformate, from naphtha	143	0.0485 kg C5 from reformate; 0.0625 kg H2 rich fuel; 9.67E-04 kg H2S rich stream;	0.899	2.26	119	70.8	539	63.0	-229	565	0.4%
Ammonia	243	1.18 kg Carbon dioxide;	0.459	78.1	0	1,004	1,100	107	-1,021	1,268	1.0%
Natural gas	257		1.000	0	0	0	878	0	0	878	0.7%

Table 2.4 continued

				CTG Energy, MJ/1000 kg ADMH[a]							
Chemicals, gate-to-gate	Mass, kg[b]	By-products, kg/kg chemical[c]	Allocation factor[d]	Electricity	Dowtherm	Steam	Fuel, Non-transport	Fuel, Transport	Potential recovery[e]	Total net energy	% of Total net energy
Nitrogen from air	195	0.358 kg Oxygen from air;	0.736	0	0	0	0	0	0	0	0.0%
Carbon dioxide	265	0.848 kg Ammonia;	0.541	85.2	0	1,095	1,200	117	-1,113	1,383	1.1%
Hydrogen cyanide	166		1.000	76.0	0	697	228	72.9	-4,152	-3,078	-2.3%
Potassium Hydroxide	363		1.000	0.136	0	428	0	160	-152	436	0.3%
KOH in solution (50%)	363	0.634 kg Chlorine; 0.0179 kg Hydrogen;	0.605	1,726	0	20.8	0	160	-122	1,785	1.4%
Potassium chloride	308		1.00	45.5	0	70.3	0	135	-14.9	236	0.2%
Sylvinite ore	902		1.000	29.6	0	0	17.0	120	0	167	0.1%
Total energy				1.57E+04	896	1.66E+05	1.45E+04	5,835	-7.17E+04	1.31E+05	

[a] Amount of energy used cradle-to-gate to produce mass of chemical used in inventory.
[b] Amount used cradle-to-gate to produce 1000 kg product.
[c] By-products generated during the gate-to-gate manufacture of chemical.
[d] Mass allocation is used to distribute the inputs, energy, and emissions to each product formed in that gate-to-gate inventory. Allocation factor will be less than 1.0 when by-products are generated.
[e] Energy that can be recovered from sources requiring cooling.

Table 2.5. DMDMH Cradle-to-Gate Energy Consumption per chemical used in the production of DMDMH.

				CTG Energy, MJ/1000 kg DMDMH[a]							
Chemicals, gate-to-gate	Mass, kg[b]	By-products, kg/kg chemical[c]	Allocation factor	Electricity	Dowtherm	Steam	Fuel, Non-transport	Fuel, Transport	Potential recovery[e]	Total net energy	% of Total net energy
Dimethyloldimethyl hydantoin	1,000	0.0000 kg Dimethyl hydantoin; 0.0000 kg Formaldehyde; 0.0000 kg Sodium hydroxide; 0.0000 kg Water;	1.000	0.282	0	0	0	440	0	440	3.6%
Dimethyl hydantoin	696		1.000	205	0	932	0	306	-389	1,054	8.6%
Acetone	324	1.61 kg Phenol;	0.384	317	0	1,485	0	143	-876	1,068	8.7%
Benzene	183	3.40 kg Non-aromatics for gas pool; 1.41 kg Toluene; 1.46 kg Xylenes;	0.138	0.103	0	478	0	80.7	-147	412	3.4%

Table 2.5 continued

				CTG Energy, MJ/1000 kg DMDMH[a]							
Chemicals, gate-to-gate	Mass, kg[b]	By-products, kg/kg chemical[c]	Allocation factor	Electricity	Dowtherm	Steam	Fuel, Non-transport	Fuel, Transport	Potential recovery[e]	Total net energy	% of Total net energy
pyrolysis gas	53.3	0.465 kg C4 stream; 0.970 kg Ethylene; 0.0854 kg fuel oil; 0.0469 kg Hydrogen; 0.552 kg Methane; 0.615 kg Propylene;	0.268	75.7	0	126	617	23.4	-151	691	5.6%
Naphtha	287	1.55 kg heavy gas oil, from distillation; 0.644 kg kerosene, from distillation; 0.542 kg light gas oil, from distillation; 0.711 kg residuum, from distillation;	0.225	68.7	0	32.2	567	0	0	668	5.4%

Table 2.5 continued

				CTG Energy, MJ/1000 kg DMDMH[a]							
Chemicals, gate-to-gate	Mass, kg[b]	By-products, kg/kg chemical[c]	Allocation factor	Electricity	Dowtherm	Steam	Fuel, Non-transport	Fuel, Transport	Potential recovery[e]	Total net energy	% of Total net energy
reformate, from naphtha	131	0.0485 kg C5 from reformate; 0.0625 kg H2 rich fuel; 9.67E-04 kg H2S rich stream;	0.899	2.06	108	64.7	493	57.5	-209	516	4.2%
Oxygen	77.3	0.0690 kg Argon; 3.24 kg Nitrogen;	0.232	86.0	0	0	0	34.0	0	120	1.0%
Propylene	98.4	0.756 kg C4 stream; 1.58 kg Ethylene; 0.139 kg fuel oil; 0.0762 kg Hydrogen; 0.898 kg Methane; 1.63 kg pyrolysis gas;	0.165	140	0	233	1,139	43.3	-278	1,277	10.4%
Ammonia	222	1.18 kg Carbon dioxide;	0.459	71.3	0	917	1,005	97.7	-932	1,158	9.4%
Natural gas	488		1.000	0	0	0	1,663	0	0	1,663	13.6%
Nitrogen from air	178	0.358 kg Oxygen from air;	0.736	0	0	0	0	0	0	0	0.0%

Table 2.5 continued

				CTG Energy, MJ/1000 kg DMDMH[a]							
Chemicals, gate-to-gate	Mass, kg[b]	By-products, kg/kg chemical[c]	Allocation factor	Electricity	Dowtherm	Steam	Fuel, Non-transport	Fuel, Transport	Potential recovery[e]	Total net energy	% of Total net energy
Oxygen from air	836	2.79 kg Nitrogen from air;	0.264	0	0	0	0	0	0	0	0.0%
Water for reaction	298	0.0000 kg Water;	1.00	0.240	0	0	0	0	0	0.240	0.0%
Carbon dioxide	242	0.848 kg Ammonia;	0.541	77.8	0	1000	1,096	107	-1,017	1,263	10.3%
Hydrogen cyanide	151		1.000	69.4	0	637	208	66.5	-3,792	-2,811	-22.9%
Formaldehyde	326		1.00	251	0	1,809	0	143	-1,458	744	6.1%
Methanol	409	0.0132 kg Dimethyl ether; 0.619 kg Petroleum refinery gas;	0.613	396	0	5,052	0	180	-1,630	3,998	32.6%
Sodium hydroxide	0.218	0.848 kg Chlorine; 0.0250 kg Hydrogen;	0.534	1.23	0	0	0	0.0958	-0.0445	1.28	0.0%
Sodium chloride	0.169		1.000	7.63E-04	0	0.822	0.0136	0.0743	0	0.910	0.0%
Total energy				1,762	108	1.28E+04	6,787	1,722	-1.09E+04	1.23E+04	

[a] Amount of energy used cradle-to-gate to produce mass of chemical used in inventory.
[b] Amount used cradle-to-gate to produce 1000 kg product.
[c] By-products generated during the gate-to-gate manufacture of chemical.
[d] Mass allocation is used to distribute the inputs, energy, and emissions to each product formed in that gate-to-gate inventory. Allocation factor will be less than 1.0 when by-products are generated.
[e] Energy that can be recovered from sources requiring cooling.

Table 2.6. Cradle-to-Gate Air, Water, and Solid Emissions for ADMH and DMDMH production.

	3-Allyl-5,5-dimethylhydantoin				Dimethyloldimethyl hydantoin			
Emissions, kg	Total	Process	Energy-related	Transport	Total	Process	Energy-related	Transport
Air Emissions, kg								
1,3-butadiene	0.147	0.147	0	0	0.0300	0.0300	0	0
1-Pentene	8.03E-03	8.03E-03	0	0	0	0	0	0
Acetone	9.69	9.69	0	0	8.85	8.85	0	0
Acetylene	0.0196	0.0196	0	0	4.02E-03	4.02E-03	0	0
Allyl Alcohol	5.02	5.02	0	0	0	0	0	0
Allyl bromide	16.8	16.8	0	0	0	0	0	0
alpha-Methylstyrene	1.09	1.09	0	0	0.998	0.998	0	0
Ammonia	14.6	14.6	0	0	13.3	13.3	0	0
Argon	3.95	3.95	0	0	2.83	2.83	0	0
Benzene	3.25	3.25	0	0	2.97	2.97	0	0
Bromine	43.1	43.1	0	0	0	0	0	0
Butane	0.0884	0.0884	0	0	0.0196	0.0196	0	0
Butene	0.254	0.254	0	0	0.0520	0.0520	0	0
Carbon dioxide	1.21E+04	351	1.13E+04	444	1,348	205	1,012	131
Carbon monoxide	11.1	2.05	6.56	2.45	104	103	0.395	0.724
Chlorine	102	102	0	0	3.87E-03	3.87E-03	0	0
Cumene	5.90	5.90	0	0	5.39	5.39	0	0
Cumene Hydroperoxide	2.19	2.19	0	0	2.00	2.00	0	0
Cyclohexane	0.544	0.544	0	0	0.497	0.497	0	0
Dichlorine monoxide	22.0	22.0	0	0	0	0	0	0
Dimethyl ether	0	0	0	0	0.0176	0.0176	0	0
Ethane	0.274	0.274	0	0	0.161	0.161	0	0
Ethylene	1.06	1.06	0	0	0.197	0.197	0	0
Ethylene oxide	1.68	1.68	0	0	0	0	0	0
Formaldehyde	0	0	0	0	3.25	3.25	0	0
Heptane	0.0236	0.0236	0	0	7.15E-03	7.15E-03	0	0
Hexene	0.0150	0.0150	0	0	0	0	0	0
Hydrogen	2.60	2.60	0	0	11.8	11.8	0	0
Hydrogen bromide	9.50	9.50	0	0	0	0	0	0
Hydrogen chloride	0.0100	0.0100	0	0	1.18E-06	1.18E-06	0	0
Hydrogen cyanide	3.26	3.26	0	0	2.97	2.97	0	0
Hydrogen sulfide	1.22	1.22	0	0	2.14E-04	2.14E-04	0	0
Hypochlorous acid	4.60	4.60	0	0	3.02E-06	3.02E-06	0	0
Isobutane	8.12E-04	8.12E-04	0	0	2.46E-04	2.46E-04	0	0

Table 2.6 continued

	3-Allyl-5,5-dimethylhydantoin				Dimethyloldimethyl hydantoin			
Emissions, kg	Total	Process	Energy-related	Transport	Total	Process	Energy-related	Transport
Methane	32.2	6.63	25.1	0.438	11.5	9.34	2.07	0.129
Methanol	20.6	20.6	0	0	7.92	7.92	0	0
Naphtha	14.8	14.8	0	0	3.03	3.03	0	0
n-Hexane	0.658	0.658	0	0	0.575	0.575	0	0
Nitrogen dioxide	1.26	1.26	0	0	1.15	1.15	0	0
Nitrogen monoxide	0.821	0.821	0	0	0.750	0.750	0	0
NMVOC	46.7	0.118	43.7	2.86	3.81	0.217	2.75	0.845
NOx	43.1	0.248	34.6	8.31	5.83	0.471	2.91	2.45
n-Pentane	0.0142	0.0142	0	0	3.45E-03	3.45E-03	0	0
Octane	0.0177	0.0177	0	0	5.36E-03	5.36E-03	0	0
Petroleum ether	400	400	0	0	0	0	0	0
Phenol	1.09	1.09	0	0	0.998	0.998	0	0
Propane	0.0570	0.0570	0	0	0.0538	0.0538	0	0
Propylene	5.74	5.74	0	0	0.996	0.996	0	0
Propylene oxide	18.8	18.8	0	0	0	0	0	0
Propyne	0.0176	0.0176	0	0	3.60E-03	3.60E-03	0	0
pyrolysis gas	2.00	2.00	0	0	0.410	0.410	0	0
SOx	43.3	0.286	42.5	0.566	3.70	0.541	3.00	0.167
Toluene	0.398	0.398	0	0	0.363	0.363	0	0
Total Air emissions	1.30E+04	1,081	1.14E+04	459	1,549	390	1,023	135
Water Emissions, kg								
1-Pentene	0.418	0.418	0	0	0	0	0	0
1-Propanol	4.74	4.74	0	0	0	0	0	0
Acetone	6.90	6.90	0	0	1.97	1.97	0	0
Acetophenone	33.0	33.0	0	0	30.1	30.1	0	0
Allyl Alcohol	55.7	55.7	0	0			0	0
Allyl bromide	84.1	84.1	0	0			0	0
Ammonia	0.668	0.668	0	0	0.610	0.610	0	0
Arsenic	7.21E-06	7.21E-06	0	0	2.19E-06	2.19E-06	0	0
barium carbonate	0.440	0.440	0	0			0	0
BaSO4	6.13	6.13	0	0	7.30E-04	7.30E-04	0	0
Benzene	1.69E-04	1.69E-04	0	0	5.14E-05	5.14E-05	0	0
BOD	0.959	3.37E-05	0.934	0.0257	0.0691	6.39E-05	0.0614	7.59E-03
Boron	3.57E-03	3.57E-03	0	0	1.08E-03	1.08E-03	0	0
brine impurities	4.18	4.18	0	0	0	0	0	0

Table 2.6 continued

	3-Allyl-5,5-dimethylhydantoin				Dimethyloldimethyl hydantoin			
Emissions, kg	Total	Process	Energy-related	Transport	Total	Process	Energy-related	Transport
Bromine	9.68	9.68	0	0	0	0	0	0
Calcium carbonate	2.61	2.61	0	0	3.11E-04	3.11E-04	0	0
Carbon dioxide	1.83	1.83	0	0	1.68	1.68	0	0
Chloride	2.63	2.63	0	0	0.798	0.798	0	0
Chlorine	22.2	22.2	0	0	0	0	0	0
COD	10.1	4.66E-04	10.1	0.0545	1.01	8.83E-04	0.990	0.0161
Dimethyl ether	0	0	0	0	0.186	0.186	0	0
Ethylene glycol	134	134	0	0	0	0	0	0
Ethylene Glycol, Tri	0.0108	0.0108	0	0	0	0	0	0
grease / oil	0.0428	0.0428	0	0	0.0130	0.0130	0	0
Hexene	1.38	1.38	0	0	0	0	0	0
Higher Glycols	0.0525	0.0525	0	0	0	0	0	0
Hydrogen bromide	224	224	0	0	0	0	0	0
Hydrogen chloride	1.37E-03	1.37E-03	0	0	0	0	0	0
Hydrogen cyanide	2.45	2.45	0	0	2.24	2.24	0	0
Magnesium hydroxide	0.439	0.439	0	0	5.23E-05	5.23E-05	0	0
Mercury	4.59E-04	4.59E-04	0	0	5.46E-08	5.46E-08	0	0
Methane	0.994	0.994	0	0	0.907	0.907	0	0
Methanol	1,022	1,022	0	0	15.2	15.2	0	0
Mobile ions	8.29	8.29	0	0	2.51	2.51	0	0
n-Hexane	1.38	1.38	0	0	.00	.00	0	0
n-Pentane	0.139	0.139	0	0	.00	.00	0	0
Phenol	2.19	2.19	0	0	2.00	2.00	0	0
Potassium bromide	708	708	0	0	0	0	0	0
Potassium carbonate	2.20	2.20	0	0	0	0	0	0
Potassium chloride	51.8	51.8	0	0	0	0	0	0
Potassium Hydroxide	29.1	29.1	0	0	0	0	0	0
Propanal	4.74	4.74	0	0	0	0	0	0
Propane	1.64	1.64	0	0	0	0	0	0
Propylene	1.57	1.57	0	0	0	0	0	0
Propylene bromide	227	227	0	0	0	0	0	0
Propylene Chlorohydrin	129	129	0	0	0	0	0	0
Propylene oxide	60.3	60.3	0	0	0	0	0	0
pyrolysis gas	0.0159	0.0159	0	0	3.26E-03	3.26E-03	0	0
Sodium	3.39	3.39	0	0	1.03	1.03	0	0

Table 2.6 continued

	3-Allyl-5,5-dimethylhydantoin				Dimethyloldimethyl hydantoin			
Emissions, kg	Total	Process	Energy-related	Transport	Total	Process	Energy-related	Transport
Sodium carbonate	108	108	0	0	0	0	0	0
Sodium chloride	367	367	0	0	0.0152	0.0152	0	0
Sulfur	54.9	54.9	0	0	0	0	0	0
Sulfuric acid	2.09	2.09	0	0	0	0	0	0
TDS	50.8	0.0291	50.6	0.131	2.70	0.0551	2.61	0.0385
Total Water emissions	3,445	3,383	61.6	0.211	63.1	59.4	3.66	0.0622
Solid Emissions, kg								
Calcium dichloride	8.05	8.05	0	0	0	0	0	0
Clay	27.1	27.1	0	0	0	0	0	0
Diatomaceous earth	0	0	0	0	1.11	1.11	0	0
Mud (salt process)	272	272	0	0	0.0324	0.0324	0	0
Potassium chloride	34.9	34.9	0	0	0	0	0	0
Sodium chloride	1,056	1,056	0	0	0	0	0	0
Solid waste	142	1.08	140	0.651	16.8	1.84	14.8	0.192
starch suppressant	1.26	1.26	0	0	.0	.00	.0	0.000
Total Solid emissions	1,541	1,400	140	0.651	18.0	2.98	14.8	0.192

2.6 Conclusions

As summarized in Table 2.7, the cradle-to-gate production of DMDMH in solution used less raw materials and energy than ADMH, which was originally produced as a solid. DMDMH also generated fewer emissions. DMDMH gate-to-gate manufacturing contributed little to the cradle-to-gate energy consumption of DMDMH, whereas ADMH gate-to-gate production was the fourth largest energy consumer in the cradle-to-gate production of ADMH. The energy and raw materials used to make these halamines are to be weighed in future studies against a potential reduction in nosocomial infections. The GTG LCI data presented in this paper can be used by readers in other LCI studies thus increasing the international LCI database.

Table 2.7. Comparison of LCI Results for ADMH and DMDMH

	ADMH	DMDMH
Total CTG Raw Materials, kg	10,922	2,583
Total CTG Energy, MJ	131,315	12,266
Total CTG Emissions, kg	17,947	1,628

2.7 Acknowledgements

The authors would like to thank Drs. Evan Griffing and Yong Li for their foundational contributions in the area of life cycle inventories.

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3. Cradle-to-Use Life Cycle Inventory of a Reusable Medical Gown

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3. Cradle-to-Use Life Cycle Inventory of a Reusable Medical Gown

Abstract

A life cycle inventory is performed on a cotton/polyester blend woven medical patient gown from the cradle through the use phase, including laundering. Manufacturing and using one gown seventy-five times requires 65 MJ of energy, 2.34 kg of raw materials, and generates 6.5 kg of emissions, mostly from carbon dioxide (5.8 kg, 0.28 kg, and 0.42 kg of air, liquid, and solid emissions, respectively). The laundry process step uses the most energy, and reducing water and energy in this process step may have the largest impact on reducing the environmental footprint of the reusable medical gown.

Keywords: Life cycle inventory; life cycle analysis; medical textiles; cotton; laundering; energy; emissions

3.1 Introduction

Medical garments are used in hospitals as barriers to prevent patients and healthcare workers from acquiring infections while in the hospital by preventing bacteria and other microbes from coming into contact with the person's skin. These garments are surgical gowns, surgical drapes (over the surgical site), isolation gowns, patient gowns, and scrubs. The gown of this study is a cotton polyester blend reusable medical patient gown coated with a biocidal finish. The biocidal finish is composed of a halamine precursor grafted onto the fabric and activated with the application of household chlorine bleach (Qian and Sun, 2004, Sun, 2001, Sun and Worley, 2005). To investigate the probability of reducing infection risk to healthcare workers when medical textiles such as bed linens are coated with a biocidal finish, Nicas and Sun used a Markov Chain model and calculated a possible 50% reduction in infection risk, similar to a 45% reduction in respiratory illnesses found in a study on hand washing (Nicas and Sun, 2006, Ryan et al., 2001).

To show the environmental profile for a biocidal medical patient gown, a life cycle inventory is performed. A life cycle assessment (LCA) is a "methodological framework for estimating and assessing the environmental impacts attributable to the life cycle of a product" (Hendrickson et al., 2006). The ISO 14040 series outlines the requirements for conducting life cycle inventory and assessment studies (International Standard Organization, 1997). The backbone of the LCA is the life cycle inventory, or a compilation of all inputs, outputs, and energy use of a product from resource extraction, manufacture, product use, recycling, and disposal (Rebitzer et al., 2004). A life cycle inventory gives the complete environmental picture of a product, and can be used to improve the manufacture of a product by highlighting where changes can be made to get the most impact on reducing the environmental profile. As part of this cradle-to-use life cycle inventory, the life cycle inventory for a healthcare laundry process is also examined. This life cycle inventory is part of a larger study investigating the environmental consequences of biocidal finishes for medical textiles and treating nosocomial infections.

3.2 Goal and Scope of the Study

The intent of this work is to evaluate the cradle-to-use inventory for a reusable medical patient gown composed of a cotton/polyester blend woven fabric and analyze factors affecting the environmental profile of the reusable gown. An additional goal is to increase the amount of life cycle inventory data that can be used by others. Transparent gate-to-gate (within the factory) inventories are used, and the cradle-to-use inventory is the summation of these first level inventories. The LCI scope is from the natural resources through the manufacture of the medical gown and then laundering (use) of the gown, as shown in Figure 3.1. Disposal of the gown is not included in this analysis. The functional unit is 1000 reusable patient gowns used 75 times, or 75,000 patient gown uses.

3.3 Methodology

In this study, we use design-based approach methodology (Jimenez Gonzalez, 2000, Overcash, 1994) to obtain the life cycle inventory data, in which the life cycle information of each gate-to-gate subsystem is obtained using chemical engineering design techniques. Information is gathered from articles, books, patents, company websites, and from consultations with experts in the field, then used with established process design heuristics to arrive at the LCI results. The gate-to-gate subsystems are linked through a production chain (referred to as the chemical tree), which includes extraction of raw materials and manufacturing processes. Whenever site-specific information is available, it is applied to the process design in each study.

After selecting the generic process and creating a detailed flow diagram including mass flows and process conditions, the mass and energy balance is calculated. Next, the LCI report is generated containing all inputs, outputs, and energy consumption. Once a gate-to-gate inventory is completed, a technical peer expert in the field reviews it, and changes are made as needed. This process is repeated for all chemicals in the chemical tree of the product. Once all GTG inventories for each chemical in the supply chain are completed, the inventories are summed to create the cradle-to-gate inventory of the product.

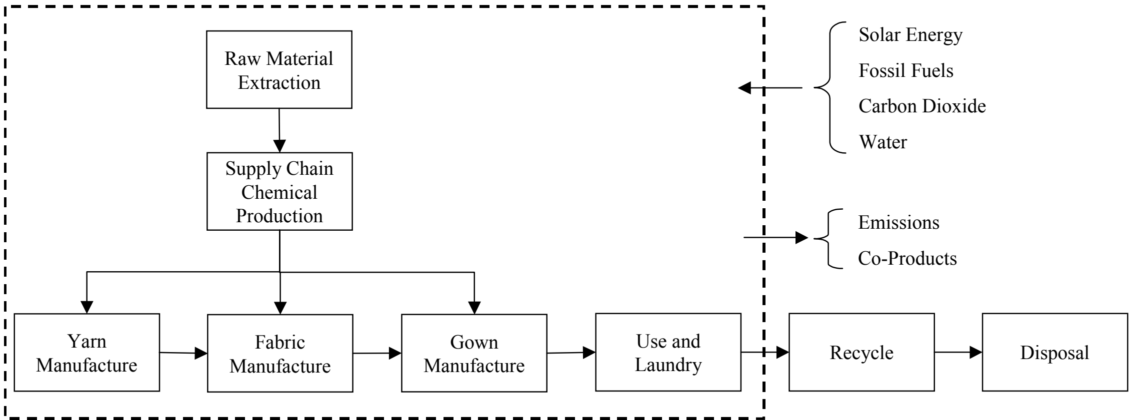


Figure 3.1. Life Cycle of Reusable Gown. Scope of inventory is in dotted line box.

3.4 Gown Manufacturing

The processes and assumptions used in the inventory are described here to insure transparency of the process. Figure 3.1 outlines the general steps to manufacture the reusable (in contrast to disposable) patient gown. Supply chain chemical production includes cotton, polyester, and any other chemicals used to make the product.

3.4.1 Cotton

Cotton is grown, harvested and ginned before it is spun and woven into fabric (See Figure 3.2).

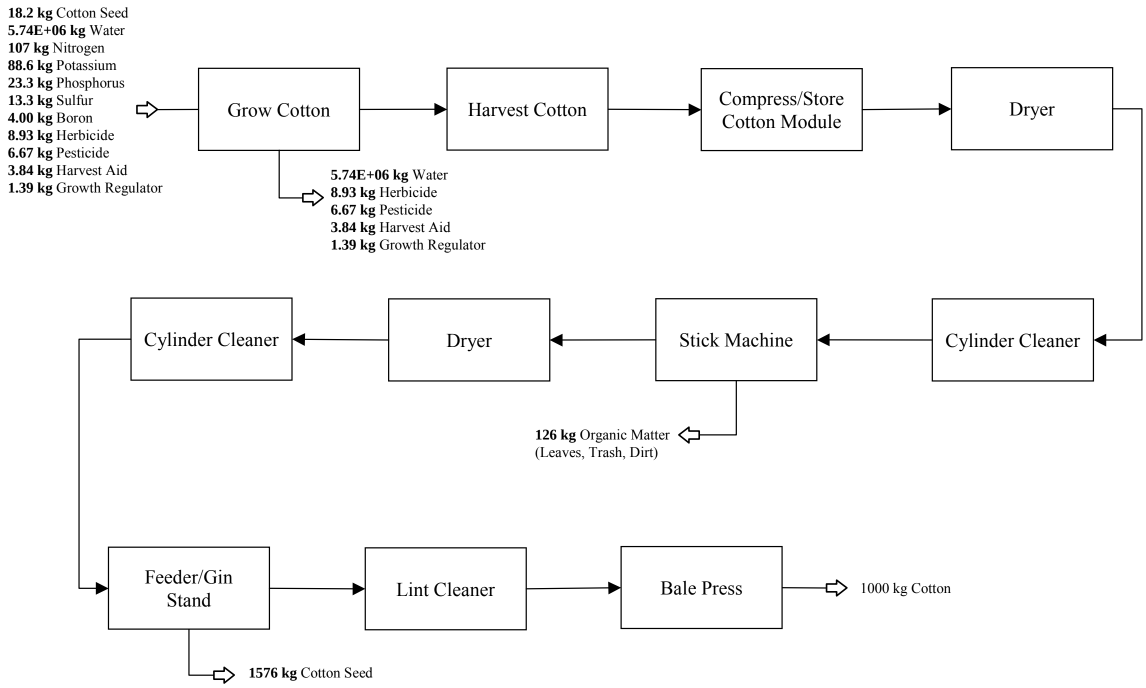


Figure 3.2. Cotton seed production including growing, harvesting, and ginning to produce bales of cotton fibers.

After harvesting, cotton is compressed into a bale for storage. Seed cotton goes through a series of steps to reduce the moisture content and separate the seed and trash from the lint. The seed cotton contains 36% lint cotton, 60% cotton seed, and 4% organic matter (leaves, sticks, dirt, etc.) The stick machine removes larger materials like sticks and burrs before a second stage of drying. The cylinder cleaner breaks up large wads of cotton for downstream processing by scrubbing the cotton over a grid to remove leaves, trash, and dirt. In the feeder/gin stand, cotton is metered into the gin stand where the lint and seed are actually separated. Leaves, dirt, and grass are removed in the lint cleaner before it is pressed into a bale weighing about 227 kg. One acre of land can produce 340.5 kg lint cotton (cotton fibers). Inputs and energy data was obtained from the US Department of Agriculture's Agricultural Research Service and North Carolina State University Agricultural Extension Service (Anthony et al., 1994, Brooks, 2001, Bullen et al., 2008,Wakelyn, 2005).

3.4.2 Cotton/Polyester Yarn

Cotton and polyester (PET) fibers are blended together to create a fabric that has better performance than 100% cotton or 100% polyester. A 100% polyester fabric has static cling, is difficult to dye, but is moisture resistant. Adding cotton improves user comfort (breathability), and reduces static cling. The composite fabric also has increased wear life, crease resistance, and crease recovery than a 100% cotton fabric. A blend of 55% cotton and 45% polyester is used in this life cycle inventory. Data was obtained from several sources (Wakelyn, 2005, El-Mogahzy et al., 2001, Wulfhorst et al., 2005).

Cotton/polyester yarn begins with bales of lint cotton and making bales of polyester staple fibers. To make staple fibers of polyester, thousands of continuous filaments are cut into 38 mm lengths to be similar in morphology to lint cotton. The polyester staple fibers can then be used on the cotton spinning systems to make yarn. As seen in Figure 3.3, polyester is heated and drawn on two sets of rollers at different speeds. The filaments are heat set at 82 ºC and crimped to impart a wavy texture to make it similar to a natural fiber. Heat setting stabilizes the yarn against thermal shrinkage. Crimping also helps in the spinning process by causing the fibers to tangle together. The crimping also gives fabrics greater bulk and softer feel. The crimped filaments are then cut into 38 mm lengths and packaged into 300 kg bales.

To blend the cotton and polyester, polyester bales and cotton bales are opened and blended in the carding process. The carding process opens the fiber tufts to individual fibers and straightens them to produce a continuous fiber strand called a sliver. The fiber mat fed to the carding process may contain two to six million fibers and is reduced to approximately 40,000 fibers by pulling since the speed of the carding machine is faster than the feeding speed (El-Mogahzy et al., 2001). Material wastes account for approximately 1% of the input material.

The drawing (or drafting) process further blends different fiber types (cotton and synthetic) while straightening and reducing the size of the fiber strand. Up to eight slivers fed through a series of rollers are reduced down to one sliver. The front rollers move faster than the back rollers to pull or slide the fibers at different rates into one thinner sliver. After drawing, the sliver is reduced further into a thin fiber strand of 3,000 to 4,000 fibers, and it is twisted and wound onto a bobbin in the roving stage. In the spinning process, the sliver is drawn again to reduce it to the final yarn size and twisted before being wound onto a bobbin.

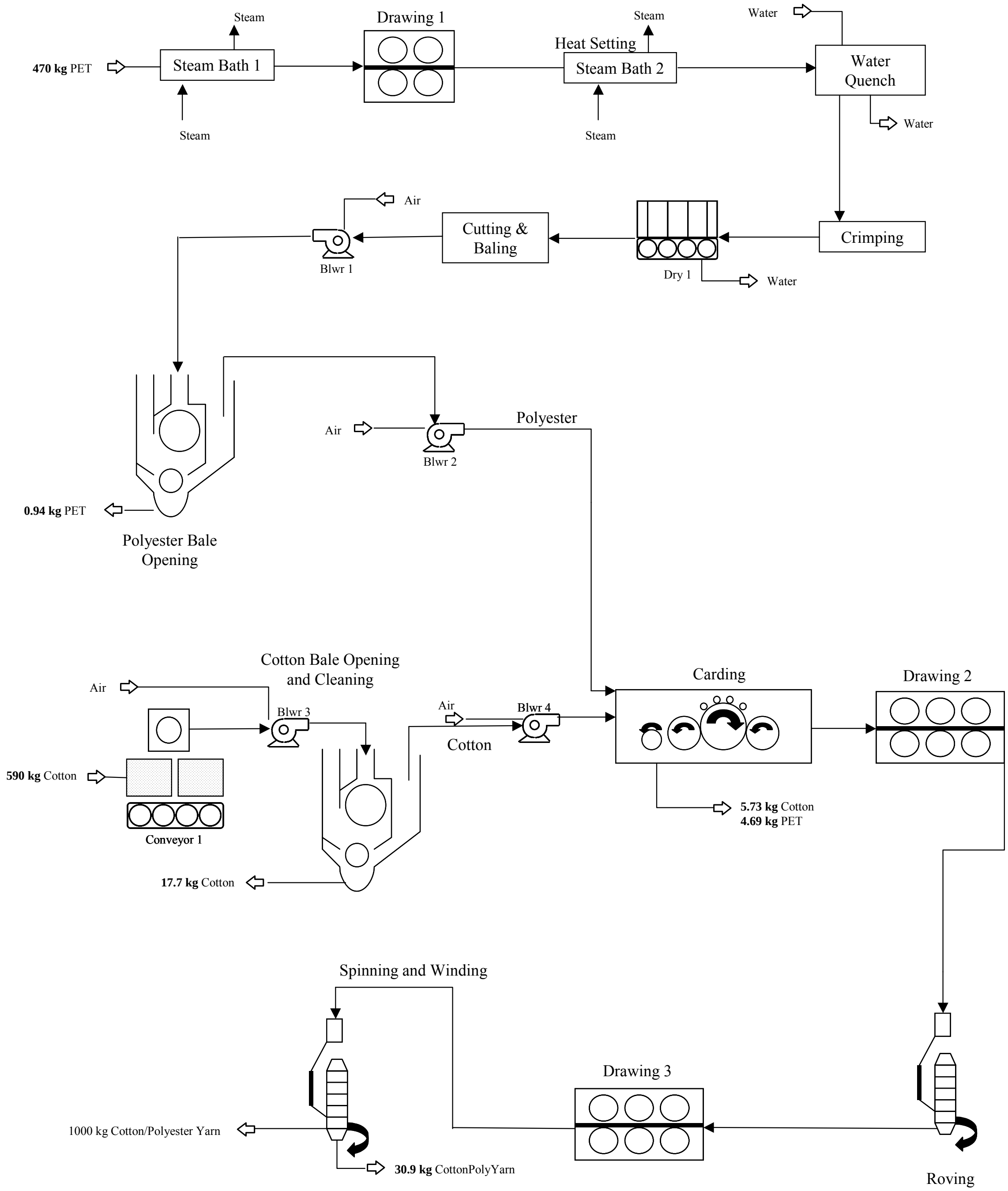


Figure 3.3. Cotton/Polyester Yarn Production

3.4.3 Cotton/Polyester Fabric

Processing yarn into fabric consists of a series of steps as shown in Figure 3.4. Cotton/polyester yarn is first rewound on bobbins and processed into warp beams. Warp is pretreated with starch and polyvinyl alcohol (PVA) sizing to prepare the threads for the mechanical stresses of weaving (Clemson University. College of Commerce and Industry, 1997). Warp threads from the warp beams are dipped in a trough of sizing liquor, excess liquor is squeezed off, and warp threads are dried in a cylinder dryer, followed by weaving into fabric. Sizing must be removed after the weaving process (Karmakar, 1999).

In the singeing process, the surface of the fabric is singed with a gas flame to remove surface fibers and smooth the fabric. Sizing must be removed before dyeing and printing. Starch-based sizes can be removed by enzymatic degradation using amylase to break the starch bonds. PVA is removed in the scouring process. Desizing also removes oils, fats, and waxes, hardening agents and catalysts that are present on the fabric. Not all of the sizing is removed in the desizing process, but after scouring and bleaching is completed, the fabric is completely desized.

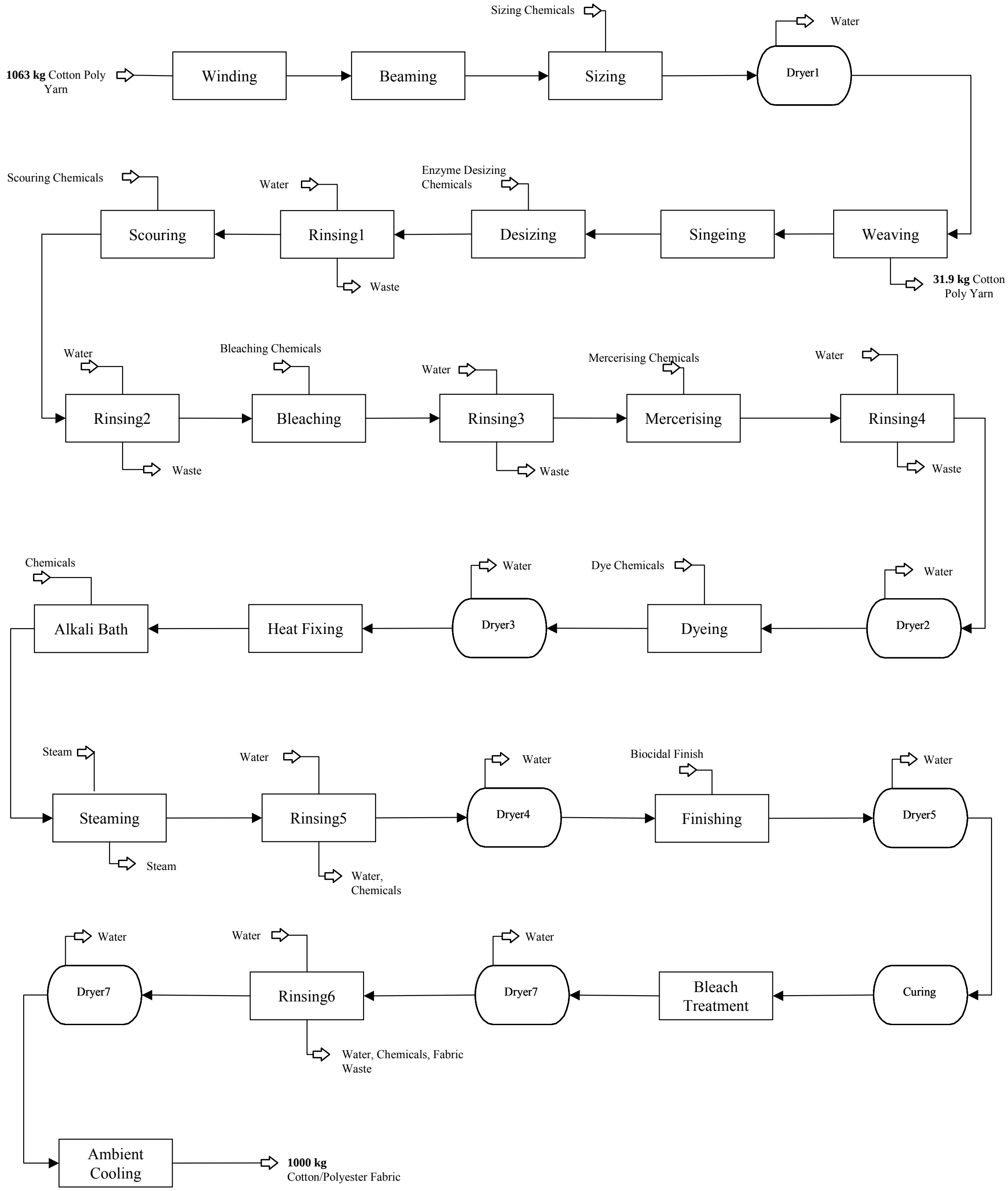


Figure 3.4. Cotton/Polyester Fabric Process Flow Diagram

Scouring is also called alkaline extraction, boiling-off, or kiering. In this step, hydrogen bonds in cellulose are broken and the fiber swells, increasing fiber diameter by 28%. This allows impurities to more easily diffuse out. Alkaline hydrogen peroxide bleaching is used to whiten the fabric before dyeing. Surfactants are also added to keep products from redepositing on the fabric due to the wetting, emulsifying, and dispersion properties. During the bleaching process, seed husks are removed, natural dyes are bleached, residual size and products are removed, and the absorbency of the material becomes uniform. Fabric is treated with caustic solution in the mercerizing process to swell the fibers and to improve dyeability of the cotton, add luster and improve strength of the fabric. Wetting agents are added such as sulfuric half-esters of aliphatic alcohols, alkyl sulfonate, and butylene glycol monoethyl ether. After rinsing and drying, the fabric is now ready for dyeing.

Cotton/polyester blend fabrics are dyed in a two-stage process to completely dye the polyester portion with disperse dyes and the cotton portion with vat dyes. Disperse dyes and vat dyes are combined in a single bath. The fabric is dried at 135ºC and then the disperse dye is set (heat fixed) on the fabric by heating the fabric to 200ºC. The fabric is rinsed in 70ºC water. This is the Thermosol process developed by Du Pont. The fabric is then passed through an alkali bath containing sodium hydrosulfite or sodium dithionite to convert the vat dye to a leuco form to make it soluble.

The fabric is then steamed, rinsed, oxidized by exposure to air, rinsed, and dried. Finishes are also applied to impart properties onto the fiber such as flame-retardancy, wrinkle release, soil release, and water repellency. For the biocidal finish, the fabric is cured and treated with a sodium hypochlorite bleach solution to activate the biocidal finish. Rinsing and drying steps complete the fabric-making process (Sun and Sun, 2000). Fabric production energy data used in this inventory was measured by Balmforth (Balmforth, 1984, Balmforth, 1985a, Balmforth, 1985b).

3.4.4 Garment Assembly

Garment assembly is outlined in the flow diagram in Figure 3.5. Fabric consisting of a blend of 55% cotton and 45% polyester from the bolt is spread in multiple layers to form a stack or ply so that multiple pieces can be cut concurrently. The pattern pieces (markers) are arranged on the fabric so that the least amount of fabric is wasted. Efficiency ranges from 65 to 90% of fabric use depending on consideration of fabric designs, fabric nap, or other constraints (Solinger, 1980). Ninety percent efficiency is used in this LCI. The pieces are then cut and bundled according to sizes and assembled (sewn) into the garment. The garment is finished with a steam press. The finished patient gown weighs 230 grams, or 4347 gowns per metric ton of gowns.

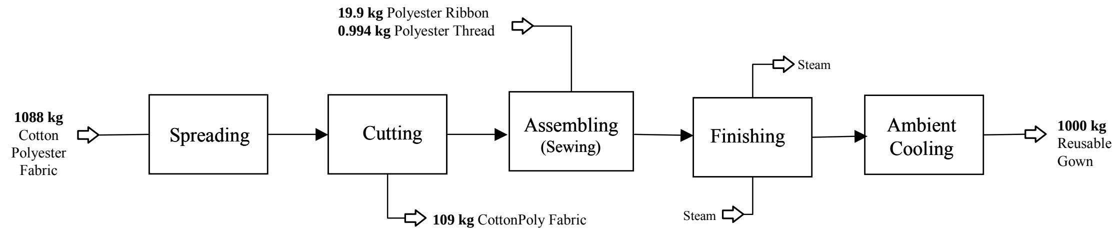
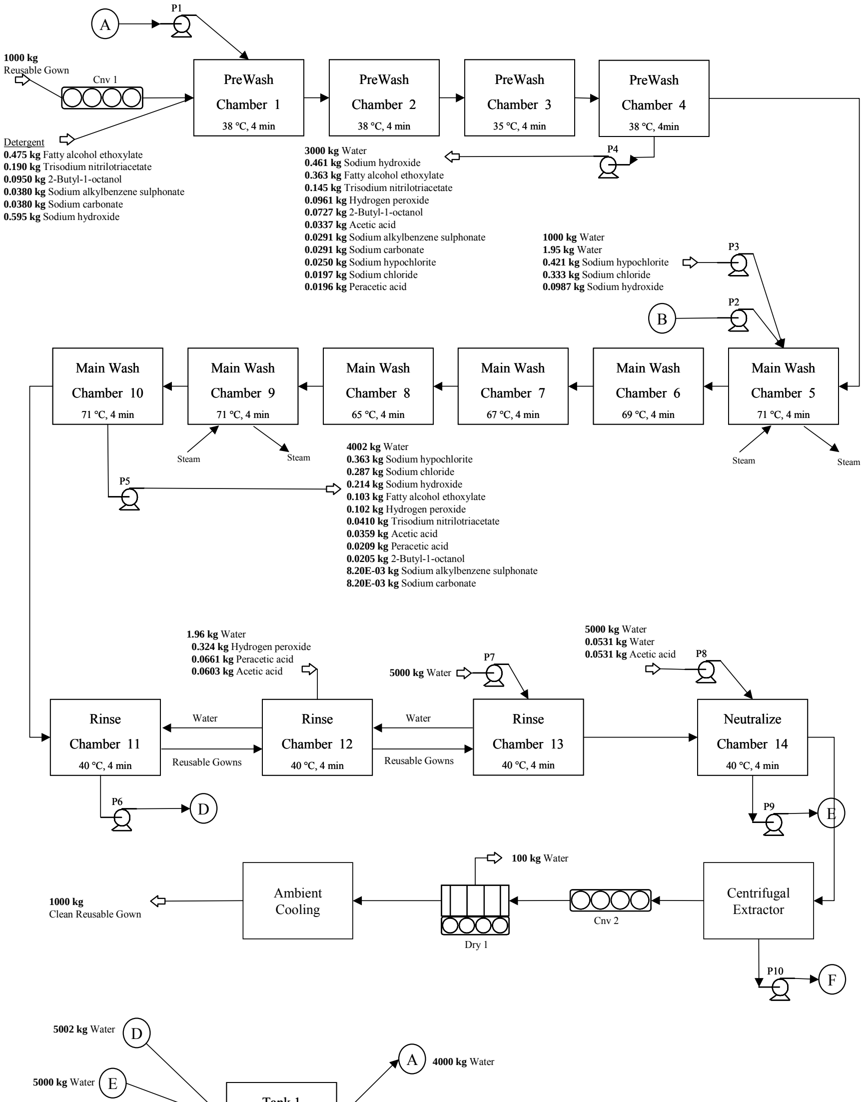


Figure 3.5. Garment Assembly Flow Diagram

3.4.5 Cleaning Process

The cleaning process to remove soil from textiles consists of pre-wash, main wash (including bleach), rinse, and acid sour cycles, followed by drying, as shown in Figure 3.6. Microorganisms on the garments from normal wear and use are killed by agitation and dilution with water, heat from the water and dryer, use of disinfectants, and the shift in pH from an alkaline wash to an acid rinse. The Center for Disease Control recommends washing healthcare textiles at 71ºC for a minimum of 25 minutes for hot water washing or washing at lower temperatures if an anti-microbial agent such as chlorine bleach or oxygen-activated bleach (hydrogen peroxide) is used (Centers for Disease Control and Prevention, 2002).



Unit Operation	Symbol
Conveyor	Cnv
Dryer	Dry
Pump	P

Figure 3.6. Cleaning Process Flow Diagram

Industrially, soiled healthcare gowns can be washed in a multi-chamber tunnel continuous batch washer (Fijan et al., 2008,Leonas, 1998). The inventory for the current study is based on a 14-chamber washer with chambers 1-4 for pre-wash, chambers 5-10 for main wash, chambers 11-13 for rinse, and chamber 14 for neutralization or souring. Water from rinse chamber 11 and neutralization chamber 14 is collected in Tank 1 and re-used in the pre-wash chambers. In the pre-wash, sodium hydroxide is added to the detergent to swell the fibers to help remove soil. Sodium hypochlorite is added in chamber 5 to remove stains. Gowns are washed in co-current flow at 71ºC for 24 minutes (in 6 chambers for 4 minutes each chamber) with 4 liters of water per kg of laundry. Based on Fijan's work, energy loss of 2ºC in temperature for each main washing chamber is assumed. Following the main wash, gowns are rinsed in counter-current flow with fresh water (at 5 L water per kg of laundry) and neutralized to a pH of 6.3 in the final chamber. Excess water is removed in the extractor, and the gowns are dried. A centrifugal extractor removes excess water before the gowns are dried. Dry gowns are then folded manually.

Energy for unit operations in the laundry inventory was calculated based on heuristics written for each unit operation. For example, the heat exchanger energy is calculated from:

$$\text{Heat Exchanger Energy} = \sum_{chemicals} \int_{T_{in}}^{T_{out}} mC_P \, dT + \sum_{chemicals} m\Delta H_v(T) \qquad (3.1)$$

where m = mass of chemicals, C_p = heat capacity, T_{in}, T_{out} = temperature of the chemical going into and coming out of the heat exchanger, and ΔH_v = heat of vaporization of the chemical. The heat exchanger is assumed to be 85% efficient.

3.5 Inventory Results and Discussion

The chemical tree in Figure 3.7 is a modified version of the full medical patient gown chemical tree. It shows the product in the left-most column and the chemicals and solvents in the second column that went into direct production of the gown. The fifth column shows how many chemicals (including duplicates) went into the production of those chemicals traced back to the natural resources from the ground shown in the last column. This life cycle inventory included forty-eight chemicals and the gate-to-gate inventories that were performed for each of these chemicals. Chemicals added in minor amounts, or ancillary inputs, are not shown in this chemical tree and were not included in these studies (Consoli et al., 1993).

<table>
<tr><th>Level 1</th><th>Level 2</th><th>Level 3</th><th colspan="2">Level 4</th><th>Natural Resources</th></tr>
<tr><td rowspan="5">Reusable Gown</td><td rowspan="5">Cotton Polyester Fabric</td><td rowspan="2">Cotton Polyester Yarn</td><td>Cotton</td><td>94 chemicals</td><td rowspan="5">Natural Resources: Air, Coal, Cotton Seed, Crude Oil, Natural gas, Phosphate rock, Salt rock, Sand, Sylvinite ore, Water</td></tr>
<tr><td>PET</td><td>40 chemicals</td></tr>
<tr><td rowspan="3">DMDMH</td><td>Dimethyl hydantoin</td><td>45 chemicals</td></tr>
<tr><td>Formaldehyde</td><td>7 chemicals</td></tr>
<tr><td>Sodium hydroxide</td><td>4 chemicals</td></tr>
</table>

Figure 3.7. Chemical Tree of Patient Gown

The basis for this inventory is 1000 patient gowns, each weighing 0.23 kg, and all raw material and energy consumption and emissions generated shown in this inventory are based on this functional unit. In the cradle-to-gate (CTG) production of the gown, 2336 kg of raw materials, excluding water, were used to produce 1000 gowns. (See Table 3.1) Water for irrigation of cotton was the largest input. Crude oil and natural gas were the next largest inputs. Crude oil is a natural resource for chemicals such as sulfuric acid, acetone, ethylene oxide (for polyester), and p-xylene (for polyester), all used in the production of the gown. Similarly, natural gas is a resource for ammonia, carbon dioxide, hydrogen cyanide, and methanol. To produce the cotton used in the gowns, 0.41 acres of land was used.

The patient gown is re-used seventy-four times and cleaned after each use. Cleaning the gown increases all raw material use as shown in Table 3.1. Water usage is 187,253 kg per 1000 gowns. Crude oil and natural gas are still the next largest inputs.

Table 3.1. Cradle-to-Gate (CTG) and Cradle-to-Use (CTU) Raw Material Consumption for 1000 gowns.

	1000 Reusable Gowns (CTG)			1000 Reusable Gowns, 75 Uses (CTU)		
Raw material, kg	Total	Process	Energy-related	Total	Process	Energy-related
Air	123.13	123.13	0.00	123.13	123.13	0.00
Coal	252.56	0.00	252.56	289.27	0.00	289.27
Cotton Seed	2.53	2.53	0.00	2.53	2.53	0.00
Crude Oil	453.55	97.17	339.84	1,067.54	97.17	970.37
Natural gas	337.86	22.90	314.95	752.38	22.90	729.48
Phosphate rock	27.22	27.22	0.00	27.22	27.22	0.00
Salt rock	0.00	0.00	0.00	0.00	0.00	0.00
Sand	1.13	1.13	0.00	1.13	1.13	0.00
Sylvinite ore	72.31	72.31	0.00	72.31	72.31	0.00
Water for reaction	217.89	217.89	0.00	217.89	217.89	0.00
Water for irrigation	1,183,824.75	1,183,824.75	0.00	1,183,824.75	1,183,824.75	0.00
Water for laundry	0.00	0.00	0.00	187,253.36	187,253.36	0.00
Total	1,185,312.93	1,184,389.04	907.35	1,373,631.52	1,371,642.40	1,989.12

In the ctu analysis, 1000 gowns produced and used seventy-five times used 67,156 MJ of energy. Some energy lost due to cooling can be recovered, and when this is included, the energy consumption is reduced to 65,049 MJ. Cleaning, fabric production, and yarn production account for 92 percent of the total energy consumed, as shown in Table 3.3. The laundry process uses 58 percent of the total energy, most of which comes from the washing process to heat water. This is the highest of the laundry and all other steps shown in Table 3.4. Energy utilized in fabric production is due to heating of liquids for dyeing and to prepare fabric for dyeing, and for drying. Energy from cotton production is due to farm machinery.

The cradle-to-use emissions listed in Table 3.5 come from process chemical losses and energy-related emissions from each GTG inventory, and depending on the physical state, are listed as air, liquid, or solid emissions. These emissions are all process emissions and do not include the effect of waste management processes. No carbon dioxide credit is assumed for growing cotton. Carbon dioxide was the largest contributor to air emissions at 5709 kg per 1000 gowns, primarily due to energy-related emissions. Total water emissions were 276 kg and total solid emissions were 421 kg per 1000 gowns.

Table 3.2. Cradle-to-Use (CTU) Energy Consumption for 75,000 Gown Uses (1000 gowns used and laundered 74 times)

				CTU Energy, MJ/ 75,000 Reusable Gown Uses[a]								
Chemicals, gate-to-gate	**Mass, kg[b]**	**Allocation factor[d]**	**By-products, kg/kg chemical[c]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Total energy**	**Potential recovery[e]**	**Total net energy**	**% of Total**
Laundry, 74 times				764.8	0.0	29,481.4	0.0	7,488.5	37,734.7	0.0	37,734.7	58.0%
Reusable Gown	230.00	1.00		39.8	0.0	74.5	0.0	101.2	215.5	0.0	215.5	0.3%
Cotton Polyester Fabric	250.22	1.00		2,069.2	0.0	15,471.8	1,819.6	110.1	19,470.6	0.0	19,470.6	29.9%
Cotton Polyester Yarn	235.34	1.00		2,156.9	0.0	81.8	0.0	103.6	2,342.2	0.0	2,342.2	3.6%
Cotton	138.62	1.00		216.4	0.0	0.0	1,653.3	61.0	1,930.7	0.0	1,930.7	3.0%
Cotton Seed	2.53	1.00		0.0	0.0	0.0	0.0	1.1	1.1	0.0	1.1	0.0%
K in fertilizer	12.28	1.00		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0%
Potassium chloride	24.66	1.00		3.6	0.0	5.6	0.0	10.9	20.1	-1.2	18.9	0.0%
Sylvinite ore	72.31	1.00		2.4	0.0	0.0	1.4	9.6	13.4	0.0	13.4	0.0%
N in fertilizer	14.79	1.00		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0%
Ammonia	23.07	0.46	Carbon dioxide	7.4	0.0	95.3	104.4	10.2	217.3	-96.9	120.4	0.2%
Natural gas	22.45	1.00		0.0	0.0	0.0	76.6	0.0	76.6	0.0	76.6	0.1%
Nitrogen from air	15.29	0.74	Oxygen from air	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0%
Oxygen from air	78.66	0.26	Nitrogen from air	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0%
Water for reaction	125.89	1.00	Water	0.1	0.0	0.0	0.0	0.0	0.1	0.0	0.1	0.0%

Table 3.2 continued

				CTU Energy, MJ/ 75,000 Reusable Gown Uses[a]								
Chemicals, gate-to-gate	**Mass, kg[b]**	**Allocation factor[d]**	**By-products, kg/kg chemical[c]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Total energy**	**Potential recovery[e]**	**Total net energy**	**% of Total**
N in DAP	1.46	0.48	P in DAP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0%
DAP	10.62	1.00		0.8	0.0	2.3	0.0	4.7	7.8	0.0	7.8	0.0%
Phosphoric acid	10.42	0.92	Fluorosilicic acid	2.5	0.0	32.8	0.0	4.6	39.9	-13.8	26.1	0.0%
Phosphate rock	22.58	0.95	Phosphate rock large	2.8	0.0	0.0	11.8	9.9	24.5	-4.6	20.0	0.0%
Sulfuric acid	19.36	1.00		0.0	0.0	14.0	0.0	8.5	22.5	-6.2	16.3	0.0%
Sulfur trioxide	15.71	0.40	Sulfur dioxide; Sulfuric acid	8.0	0.0	3.0	8.8	6.9	26.7	-64.7	-38.0	-0.1%
Sulfur	6.78	1.00	already allocated	0.0	0.0	0.0	33.2	3.0	36.2	0.0	36.2	0.1%
Urea	11.80	1.00		15.6	0.0	0.0	0.0	5.2	20.8	0.0	20.8	0.0%
Carbon dioxide	16.68	0.54	Ammonia	5.4	0.0	68.9	75.5	7.3	157.1	-70.1	87.0	0.1%
P in fertilizer	3.23	1.00		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0%
P in DAP	3.23	0.52	N in DAP	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0%
PET	110.38	1.00		217.3	137.7	23.8	0.0	48.6	427.4	-18.3	409.1	0.6%
Ethylene glycol	37.06	0.91	Ethylene Glycol, Tri; Ethylene Glycol,di	13.8	0.0	508.5	0.0	16.3	538.6	-133.0	405.7	0.6%
Ethylene oxide	26.82	1.00		52.0	0.0	1.0	0.0	11.8	64.8	-152.5	-87.7	-0.1%

Table 3.2 continued

				CTU Energy, MJ/ 75,000 Reusable Gown Uses[a]								
Chemicals, gate-to-gate	**Mass, kg[b]**	**Allocation factor[d]**	**By-products, kg/kg chemical[c]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Total energy**	**Potential recovery[e]**	**Total net energy**	**% of Total**
Ethylene	20.13	0.26	C4 stream; fuel oil; Hydrogen; Methane; Propylene; pyrolysis gas	28.6	0.0	47.6	233.1	8.9	318.1	-57.0	261.2	0.4%
Naphtha	89.04	0.22	heavy gas oil, from distillation; kerosene, from distillation; light gas oil, from distillation; residuum, from distillation	21.3	0.0	10.0	175.6	0.0	206.8	0.0	206.8	0.3%
Oxygen	21.10	0.23	Argon; Nitrogen	23.5	0.0	0.0	0.0	9.3	32.8	0.0	32.8	0.1%
p-benzenedicarboxylic acid	94.70	1.00		265.7	0.0	391.4	999.5	41.7	1,698.4	-1,018.0	680.4	1.0%
Acetic acid	13.83	1.00		6.4	0.0	59.5	0.0	6.1	72.0	-30.4	41.6	0.1%
Carbon monoxide	7.27	0.89	Hydrogen	7.2	0.0	21.8	47.0	3.2	79.3	-18.0	61.3	0.1%

Table 3.2 continued

				CTU Energy, MJ/ 75,000 Reusable Gown Uses[a]								
Chemicals, gate-to-gate	**Mass, kg[b]**	**Allocation factor[d]**	**By-products, kg/kg chemical[c]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Total energy**	**Potential recovery[e]**	**Total net energy**	**% of Total**
Methanol	15.06	0.61	Dimethyl ether; Petroleum refinery gas	14.6	0.0	185.9	0.0	6.6	207.1	-60.0	147.1	0.2%
p-Xylene	60.94	0.58	Benzene	2.5	0.0	44.2	165.3	26.8	238.8	-58.1	180.7	0.3%
Toluene	62.07	0.19	Benzene; Non-aromatics for gas pool; Xylenes	0.0	0.0	161.7	0.0	27.3	189.1	-49.6	139.5	0.2%
pyrolysis gas	18.99	0.27	C4 stream; Ethylene; fuel oil; Hydrogen; Methane; Propylene	27.0	0.0	44.9	219.8	8.4	300.1	-53.7	246.4	0.4%
reformate, from naphtha	46.61	0.90	C5 from reformate; H2 rich fuel; H2S rich stream	0.7	38.6	23.1	175.6	20.5	258.6	-74.5	184.1	0.3%

Table 3.2 continued

				CTU Energy, MJ/ 75,000 Reusable Gown Uses[a]								
Chemicals, gate-to-gate	**Mass, kg[b]**	**Allocation factor[d]**	**By-products, kg/kg chemical[c]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Total energy**	**Potential recovery[e]**	**Total net energy**	**% of Total**
Dimethyloldimethyl hydantoin	18.25	1.00	Dimethyl hydantoin; Formaldehyde; Sodium hydroxide; Water	0.0	0.0	0.0	0.0	8.0	8.0	0.0	8.0	0.0%
Dimethyl hydantoin	12.69	1.00		3.7	0.0	17.0	0.0	5.6	26.3	-7.1	19.2	0.0%
Acetone	5.91	0.38	Phenol	5.8	0.0	27.1	0.0	2.6	35.5	-16.0	19.5	0.0%
Benzene	3.35	0.14	Non-aromatics for gas pool; Toluene; Xylenes	0.0	0.0	8.7	0.0	1.5	10.2	-2.7	7.5	0.0%
Propylene	1.80	0.16	C4 stream; Ethylene; fuel oil; Hydrogen; Methane; pyrolysis gas	2.6	0.0	4.2	20.8	0.8	28.4	-5.1	23.3	0.0%
Hydrogen cyanide	2.76	1.00		1.3	0.0	11.6	3.8	1.2	17.9	-69.2	-51.3	-0.1%
Formaldehyde	5.94	1.00		4.6	0.0	33.0	0.0	2.6	40.2	-26.6	13.6	0.0%
Sodium hydroxide	.004	0.53	Chlorine; Hydrogen	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0%

Table 3.2 continued

				CTU Energy, MJ/ 75,000 Reusable Gown Uses[a]									
Chemicals, gate-to-gate	**Mass, kg[b]**	**Allocation factor[d]**	**By-products, kg/kg chemical[c]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Total energy**	**Potential recovery[e]**	**Total net energy**	**% of Total**
Sodium chloride	.003	1.00										0.0%
Total energy				5994	176	46956	5825	8204	67156	-2107	65049	100.0%

[a] Amount of energy used cradle-to-gate to produce mass of chemical used in inventory.
[b] Amount used cradle-to-gate to produce 1000 kg product.
[c] Mass allocation is used to distribute the inputs, energy, and emissions to each product formed in that gate-to-gate inventory. Allocation factor will be less than 1.0 when by-products are generated.
[d] By-products generated during the gate-to-gate manufacture of chemical.
[e] Energy that can be recovered from sources requiring cooling.

Table 3.3. Energy Consumption of Steps for Largest Consuming Processes in Gown Inventory

	Steps	MJ/1000 kg Gown	MJ/1000 Gowns
Laundry (74 times)	Wash/Rinse/Neutralize	110,843.3	25,154.0
	Extract	1,005.1	228.1
	Dry	21,438.9	4865.2
Fabric	Weaving	10,837.5	2,709.4
	Dye Prep	20,290.6	5,072.6
	Dyeing	34,253.5	8,563.4
	Finishing	5,734.4	1,433.6
	Biocide App	6,258.8	1,564.7
Yarn	Steam Bath 1	47.7	11.0
	Drawing 1	1,067.4	245.2
	Steam Bath 2	116.7	26.8
	Crimping	243.6	56.0
	Dryer 1	191.1	43.9
	Cutting & Baling	394.5	90.6
	Opening (PET Fiber)	97.2	22.3
	Opening (Cotton Fiber)	269.6	61.9
	Carding	399.0	91.7
	Drawing 2	644.5	148.1
	Roving	368.3	84.6
	Spinning	5,739.0	1,318.4
	Winding	152.4	35.0
Cotton	Cotton Growing	6,691.5	1,542.5
	Seed Handling	206.8	47.7
	Ginning	993.1	228.9
	Lint Handling	97.7	22.5
	Trash Handling	47.6	11.0
	Packaging	83.2	19.2
	Miscellaneous	13.3	3.1
	Total	228,526.4	54,110.0

Table 3.4. Cradle-to-Use Emissions for 75,000 gown uses, prior to any waste management.

Cradle-to-Use Gown Emissions per 1000 Reusable Gowns	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Process Emissions
Air emissions [kg]			
1,3-butadiene	8.10E-03	8.10E-03	3.56E-04kg from Propylene, 3.76E-03kg from pyrolysis gas, 3.99E-03kg from Ethylene,
Acetaldehyde	1.76E-01	1.76E-01	1.42E-05kg from Acetic acid, 1.76E-01kg from PET,
Acetic acid	1.58E+00	1.58E+00	1.42E-01kg from Acetic acid, 1.42E+00kg from p-benzenedicarboxylic acid, 2.61E-04kg from Reusable Gown, Cleaned,
Acetic Peroxide	1.14E-02	1.14E-02	1.52E-04kg from Reusable Gown, Cleaned,
Acetone	1.61E-01	1.61E-01	4.55E-02kg from Acetone, 1.16E-01kg from Dimethyl hydantoin,
Acetylene	1.08E-03	1.08E-03	4.76E-05kg from Propylene, 5.04E-04kg from pyrolysis gas, 5.34E-04kg from Ethylene,
alpha-Methylstyrene	1.82E-02	1.82E-02	1.82E-02kg from Acetone,
Ammonia	4.38E-01	4.38E-01	1.35E-02kg from Hydrogen cyanide, 2.04E-01kg from Dimethyl hydantoin, 1.70E-05kg from reformate, from naphtha, 1.93E-02kg from Carbon monoxide, 4.92E-02kg from Carbon dioxide, 7.55E-02kg from Urea, 8.50E-03kg from DAP, 6.80E-02kg from Ammonia,
Argon	4.78E-01	4.78E-01	2.36E-01kg from Ethylene oxide, 1.02E-01kg from Carbon dioxide, 1.41E-01kg from Ammonia,
Benzene	7.10E-01	7.10E-01	4.71E-03kg from Benzene, 3.28E-02kg from Acetone, 3.27E-01kg from reformate, from naphtha, 8.73E-02kg from Toluene, 2.58E-01kg from p-Xylene, 1.91E-05kg from Naphtha,
Butane	5.46E-03	5.46E-03	1.78E-04kg from Propylene, 1.88E-03kg from pyrolysis gas, 1.41E-03kg from Naphtha, 1.99E-03kg from Ethylene,
Butene	1.40E-02	1.40E-02	6.16E-04kg from Propylene, 6.51E-03kg from pyrolysis gas, 6.90E-03kg from Ethylene,
Carbon dioxide	5.71E+03	2.03E+01	9.63E-01kg from Formaldehyde, 2.44E+00kg from Hydrogen cyanide, 2.20E-02kg from Dimethyl hydantoin, 2.13E-02kg from Carbon monoxide, 1.02E+00kg from Acetic acid, 1.46E-02kg from Oxygen, 2.69E+00kg from Naphtha, 9.13E+00kg from Ethylene oxide, 4.02E-01kg from Carbon dioxide, 4.37E-02kg from Urea, 1.98E+00kg from Sulfur, 9.73E-01kg from Phosphoric acid, 5.95E-03kg from Natural gas, 5.56E-01kg from Ammonia,

Table 3.4 continued

Cradle-to-Use Gown Emissions per 1000 Reusable Gowns	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Process Emissions
Air emissions [kg]			
Carbon monoxide	8.39E+00	2.01E+00	1.77E+00kg from Formaldehyde, 1.50E-02kg from Hydrogen cyanide, 2.69E-06kg from Propylene, 2.85E-05kg from pyrolysis gas, 5.00E-02kg from Methanol, 3.22E-02kg from Carbon monoxide, 8.87E-02kg from Acetic acid, 3.02E-05kg from Ethylene, 2.22E-02kg from Carbon dioxide, 5.58E-04kg from Sulfur, 6.20E-03kg from Natural gas, 3.07E-02kg from Ammonia,
Chlorine	7.06E-05	7.06E-05	4.62E-08kg from Sodium chloride, 7.05E-05kg from Sodium hydroxide,
Cumene	9.83E-02	9.84E-02	9.84E-02kg from Acetone,
Cumene Hydroperoxide	3.64E-02	3.64E-02	3.64E-02kg from Acetone,
Cyclohexane	1.77E-01	1.77E-01	1.77E-01kg from reformate, from naphtha,
Dimethyl ether	6.46E-04	6.46E-04	6.46E-04kg from Methanol,
Ethane	1.91E-02	1.91E-02	5.50E-04kg from Propylene, 5.81E-03kg from pyrolysis gas, 4.06E-03kg from Methanol, 1.29E-03kg from Carbon monoxide, 1.22E-03kg from Naphtha, 6.16E-03kg from Ethylene,
Ethanol	9.67E-05	9.67E-05	9.67E-05kg from Acetic acid,
Ethylene	8.08E-02	8.08E-02	2.33E-03kg from Propylene, 2.46E-02kg from pyrolysis gas, 2.61E-02kg from Ethylene, 2.78E-02kg from Ethylene oxide,
Ethylene carbonate	4.26E-01	4.26E-01	4.26E-01kg from Carbon monoxide,
Ethylene glycol	2.55E-02	2.55E-02	2.55E-02kg from PET,
Ethylene Glycol,di	4.23E-05	4.23E-05	4.23E-05kg from PET,
Ethylene oxide	4.65E-01	4.65E-01	3.32E-01kg from Ethylene oxide, 1.33E-01kg from Ethylene glycol,
Formaldehyde	7.77E-02	7.77E-02	4.82E-02kg from Formaldehyde, 2.96E-02kg from Dimethyloldimethyl hydantoin,
Heptane	2.21E-03	2.21E-03	2.21E-03kg from Naphtha,
High alkanes	6.45E-04	6.45E-04	6.45E-04kg from Carbon monoxide,

Table 3.4 continued

Cradle-to-Use Gown Emissions per 1000 Reusable Gowns	**Total Emissions, kg**	**Process Emissions, kg**	**Chemicals Contributing to Process Emissions**
Air emissions [kg]			
Hydrogen	7.00E-01	7.00E-01	3.98E-07kg from Sodium hydroxide, 1.61E-01kg from Formaldehyde, 1.50E-03kg from Hydrogen cyanide, 1.10E-04kg from Propylene, 2.27E-02kg from reformate, from naphtha, 1.16E-03kg from pyrolysis gas, 3.80E-01kg from p-Xylene, 1.49E-02kg from Methanol, 3.87E-03kg from Carbon monoxide, 4.64E-02kg from Acetic acid, 1.16E-02kg from p-benzenedicarboxylic acid, 1.23E-03kg from Ethylene, 2.35E-02kg from Carbon dioxide, 3.25E-02kg from Ammonia,
Hydrogen chloride	2.15E-08	2.15E-08	2.15E-08kg from Sodium hydroxide,
Hydrogen cyanide	5.42E-02	5.42E-02	1.39E-04kg from Hydrogen cyanide, 5.41E-02kg from Dimethyl hydantoin,
Hydrogen fluoride	1.23E-06	1.23E-06	1.23E-06kg from Phosphoric acid,
Hydrogen sulfide	3.92E-05	3.92E-05	2.01E-06kg from Sodium chloride, 3.71E-05kg from reformate, from naphtha,
Hypochlorous acid	5.52E-08	5.52E-08	5.52E-08kg from Sodium hydroxide,
Isobutane	7.64E-05	7.64E-05	7.64E-05kg from Naphtha,
Methane	1.19E+01	6.37E-01	1.29E-02kg from Hydrogen cyanide, 1.28E-03kg from Propylene, 1.36E-02kg from pyrolysis gas, 3.81E-02kg from Methanol, 9.67E-03kg from Carbon monoxide, 5.81E-02kg from Naphtha, 1.44E-02kg from Ethylene, 1.12E-01kg from Ethylene oxide, 1.71E-02kg from Carbon dioxide, 2.18E-02kg from Sulfur, 3.14E-01kg from Natural gas, 2.36E-02kg from Ammonia,
Methanol	2.98E-01	2.98E-01	3.21E-02kg from Formaldehyde, 1.90E-01kg from Methanol, 7.57E-02kg from Acetic acid,
Methyl acetate	6.27E-02	6.27E-02	6.27E-02kg from Acetic acid,
Naphtha	8.18E-01	8.18E-01	3.59E-02kg from Propylene, 3.80E-01kg from pyrolysis gas, 4.02E-01kg from Ethylene,
n-Hexane	2.05E-01	2.05E-01	2.03E-01kg from reformate, from naphtha, 1.89E-03kg from Naphtha,
Nitrogen dioxide	9.83E-02	9.83E-02	4.13E-02kg from Carbon dioxide, 5.71E-02kg from Ammonia,
Nitrogen monoxide	6.42E-02	6.42E-02	2.70E-02kg from Carbon dioxide, 3.73E-02kg from Ammonia,
NMVOC	2.42E+01	6.86E-02	4.20E-04kg from Naphtha, 5.83E-02kg from Sulfur, 9.92E-03kg from Natural gas,

Table 3.4 continued

Cradle-to-Use Gown Emissions per 1000 Reusable Gowns	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Process Emissions
Air emissions [kg]			
NOx	2.70E+01	4.14E-02	1.98E-02kg from Sulfur, 2.17E-02kg from Natural gas,
n-Pentane	1.07E-03	1.07E-03	1.07E-03kg from Naphtha,
Octane	1.66E-03	1.66E-03	1.66E-03kg from Naphtha,
Particulate matter	2.70E-01	2.70E-01	2.70E-01kg from Phosphate rock,
Phenol	1.82E-02	1.82E-02	1.82E-02kg from Acetone,
Propane	4.32E-03	4.32E-03	4.63E-07kg from Propylene, 4.89E-06kg from pyrolysis gas, 1.75E-03kg from Methanol, 6.45E-04kg from Carbon monoxide, 1.91E-03kg from Naphtha, 5.19E-06kg from Ethylene,
Propylene	1.43E-01	1.43E-01	5.89E-03kg from Propylene, 9.11E-03kg from Acetone, 6.22E-02kg from pyrolysis gas, 6.60E-02kg from Ethylene,
Propyne	9.72E-04	9.72E-04	4.26E-05kg from Propylene, 4.51E-04kg from pyrolysis gas, 4.78E-04kg from Ethylene,
p-Xylene	4.36E-02	4.36E-02	4.36E-02kg from p-benzenedicarboxylic acid,
pyrolysis gas	1.10E-01	1.10E-01	4.85E-03kg from Propylene, 5.13E-02kg from pyrolysis gas, 5.44E-02kg from Ethylene,
Sodium hypochlorite	1.49E+01	1.49E+01	9.67E-04kg from Reusable Gown, Cleaned, 1.49E+01kg from CotPoly Fabric Biocide,
SOx	2.11E+01	3.28E-01	1.24E-02kg from Sulfur, 2.90E-01kg from Sulfur trioxide, 2.49E-02kg from Natural gas,
Sulfur	3.23E-02	3.23E-02	3.23E-02kg from Sulfur trioxide,
Sulfur trioxide	9.41E-02	9.41E-02	9.41E-02kg from Sulfuric acid,
Toluene	1.26E+00	1.26E+00	6.63E-03kg from Benzene, 1.23E-01kg from Toluene, 1.13E+00kg from p-Xylene,
Urea	1.64E-02	1.64E-02	1.64E-02kg from Urea,

Table 3.4 continued

Cradle-to-Use Gown Emissions per 1000 Reusable Gowns	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Process Emissions
Air emissions [kg]			
Total Air emissions	5.83E+03	4.76E+01	2.06E-06kg from Sodium chloride, 7.10E-05kg from Sodium hydroxide, 2.97E+00kg from Formaldehyde, 2.49E+00kg from Hydrogen cyanide, 5.22E-02kg from Propylene, 1.13E-02kg from Benzene, 2.59E-01kg from Acetone, 3.96E-01kg from Dimethyl hydantoin, 2.96E-02kg from Dimethyloldimethyl hydantoin, 7.30E-01kg from reformate, from naphtha, 5.52E-01kg from pyrolysis gas, 2.10E-01kg from Toluene, 1.77E+00kg from p-Xylene, 3.00E-01kg from Methanol, 5.15E-01kg from Carbon monoxide, 1.44E+00kg from Acetic acid, 1.48E+00kg from p-benzenedicarboxylic acid, 1.46E-02kg from Oxygen, 2.76E+00kg from Naphtha, 5.85E-01kg from Ethylene, 9.83E+00kg from Ethylene oxide, 1.33E-01kg from Ethylene glycol, 2.02E-01kg from PET, 6.84E-01kg from Carbon dioxide, 1.36E-01kg from Urea, 2.09E+00kg from Sulfur, 3.23E-01kg from Sulfur trioxide, 9.41E-02kg from Sulfuric acid, 2.70E-01kg from Phosphate rock, 9.73E-01kg from Phosphoric acid, 8.50E-03kg from DAP, 3.83E-01kg from Natural gas, 9.46E-01kg from Ammonia, 1.38E-03kg from Reusable Gown, Cleaned, 1.49E+01kg from CotPoly Fabric Biocide,
Water emissions [kg]			
Acetaldehyde	1.38E-05	1.38E-05	1.38E-05kg from Acetic acid,
Acetic acid	1.45E+01	1.45E+01	1.39E-01kg from Acetic acid, 1.24E+01kg from p-benzenedicarboxylic acid, 2.61E-02kg from Reusable Gown, Cleaned,
Acetic Peroxide	1.14E+00	1.14E+00	1.52E-02kg from Reusable Gown, Cleaned,
Acetone	3.59E-02	3.59E-02	3.59E-02kg from Dimethyl hydantoin,
Acetophenone	5.50E-01	5.50E-01	5.50E-01kg from Acetone,
Ammonia	1.11E-02	1.11E-02	1.11E-02kg from Hydrogen cyanide,
Arsenic	6.77E-07	6.77E-07	6.77E-07kg from Naphtha,
BaSO4	1.33E-05	1.33E-05	1.33E-05kg from Sodium hydroxide,
Benzene	1.59E-05	1.59E-05	1.59E-05kg from Naphtha,
BOD	4.56E-01	2.94E-06	2.94E-06kg from Natural gas,

Table 3.4 continued

Cradle-to-Use Gown Emissions per 1000 Reusable Gowns	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Process Emissions
Water emissions [kg]			
BOD5	1.36E-03	1.36E-03	1.36E-03kg from Sulfur,
Boron	3.35E-04	3.35E-04	3.35E-04kg from Naphtha,
Calcium carbonate	5.67E-06	5.67E-06	5.67E-06kg from Sodium hydroxide,
Carbon dioxide	3.06E-02	3.06E-02	3.06E-02kg from Dimethyl hydantoin, 1.11E-06kg from Acetic acid,
Carbon monoxide	5.83E-08	5.83E-08	5.83E-08kg from Acetic acid,
Chloride	2.47E-01	2.47E-01	2.47E-01kg from Naphtha,
COD	4.00E+00	2.92E-03	2.88E-03kg from Sulfur, 4.06E-05kg from Natural gas,
Cotton Polyester Yarn	6.85E+00	6.85E+00	6.85E+00kg from CotPoly Fabric Biocide,
DAP	7.01E-02	7.01E-02	7.01E-02kg from DAP,
Diastase	1.14E+00	1.14E+00	1.14E+00kg from CotPoly Fabric Biocide,
Dimethyl ether	6.83E-03	6.83E-03	6.83E-03kg from Methanol,
Ethanecarboxylic acid	8.45E-02	8.45E-02	8.45E-02kg from Acetic acid,
Ethanol	9.48E-04	9.48E-04	9.48E-04kg from Acetic acid,
ethoxylated lauryl alcohol	8.19E+00	8.19E+00	1.09E-01kg from Reusable Gown, Cleaned,
ethyl butanol	1.37E-03	1.37E-03	1.37E-03kg from Acetic acid,
Ethylene glycol	8.07E-01	8.07E-01	8.07E-01kg from PET,
Ethylene Glycol, Tri	3.00E-03	3.00E-03	3.00E-03kg from Ethylene glycol,
Ethylene Glycol,di	4.22E-02	4.22E-02	4.22E-02kg from PET,
grease / oil	4.03E-03	4.03E-03	4.03E-03kg from Naphtha,
Growth Regulator	1.93E-01	1.93E-01	1.93E-01kg from Cotton,
Harvest Aid	5.32E-01	5.32E-01	5.32E-01kg from Cotton,
Herbicide	1.24E+00	1.24E+00	1.24E+00kg from Cotton,
Higher Glycols	1.46E-02	1.46E-02	1.46E-02kg from Ethylene glycol,
Hydrogen	4.60E-11	4.60E-11	4.60E-11kg from Acetic acid,
Hydrogen cyanide	4.08E-02	4.08E-02	1.38E-02kg from Hydrogen cyanide, 2.70E-02kg from Dimethyl hydantoin,
Hydrogen peroxide	6.27E+00	6.27E+00	7.44E-02kg from Reusable Gown, Cleaned, 6.84E-01kg from CotPoly Fabric Biocide,
Hydroxyethyl Cornstarch	1.15E+01	1.15E+01	1.15E+01kg from CotPoly Fabric Biocide,

Table 3.4 continued

Cradle-to-Use Gown Emissions per 1000 Reusable Gowns	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Process Emissions
Water emissions [kg]			
Linear Alkyl Benzene Sulfonate, LAS	6.55E-01	6.56E-01	8.74E-03kg from Reusable Gown, Cleaned,
Magnesium hydroxide	9.55E-07	9.55E-07	9.55E-07kg from Sodium hydroxide,
Melamine formaldehyde	3.54E-02	3.54E-02	3.54E-02kg from CotPoly Fabric Biocide,
Mercury	9.97E-10	9.97E-10	9.97E-10kg from Sodium hydroxide,
Methane	1.66E-02	1.66E-02	1.66E-02kg from Hydrogen cyanide,
Methanol	5.63E-01	5.63E-01	5.60E-01kg from Methanol, 2.92E-03kg from Acetic acid,
Methyl acetate	1.51E-02	1.51E-02	1.51E-02kg from Acetic acid,
Methyl iodide	1.17E-02	1.17E-02	1.17E-02kg from Acetic acid,
Mobile ions	7.79E-01	7.79E-01	7.79E-01kg from Naphtha,
Nonyl phenoxypolyethyleneoxy ethanol	7.98E-01	7.98E-01	7.98E-01kg from CotPoly Fabric Biocide,
Paraffin Wax	1.73E+00	1.73E+00	1.73E+00kg from CotPoly Fabric Biocide,
Pesticide	9.25E-01	9.25E-01	9.25E-01kg from Cotton,
Phenol	3.64E-02	3.64E-02	3.64E-02kg from Acetone,
Poly(vinyl alcohol)	1.15E+01	1.15E+01	1.15E+01kg from CotPoly Fabric Biocide,
Polyacrylate	4.61E+00	4.61E+00	4.61E+00kg from CotPoly Fabric Biocide,
Potassium chloride	2.91E+00	2.91E+00	2.91E+00kg from Potassium chloride,
p-Xylene	3.92E-01	3.92E-01	3.92E-01kg from p-benzenedicarboxylic acid,
pyrolysis gas	8.81E-04	8.81E-04	3.87E-05kg from Propylene, 4.09E-04kg from pyrolysis gas, 4.33E-04kg from Ethylene,
Rh-Complex	3.42E-03	3.42E-03	3.42E-03kg from Acetic acid,
Sodium	3.18E-01	3.18E-01	3.18E-01kg from Naphtha,
Sodium carbonate	6.55E-01	6.56E-01	8.74E-03kg from Reusable Gown, Cleaned,
Sodium chloride	1.11E+01	1.11E+01	2.77E-04kg from Sodium chloride, 3.08E+00kg from Potassium chloride, 7.65E-02kg from Reusable Gown, Cleaned, 2.31E+00kg from CotPoly Fabric Biocide,
Sodium hydrosulfide	5.68E-01	5.68E-01	5.68E-01kg from CotPoly Fabric Biocide,
Sodium hydroxide	1.50E+02	1.50E+02	1.60E-01kg from Reusable Gown, Cleaned, 1.38E+02kg from CotPoly Fabric Biocide,
Sodium hypochlorite	7.26E+00	7.26E+00	9.67E-02kg from Reusable Gown, Cleaned,

Table 3.4 continued

Cradle-to-Use Gown Emissions per 1000 Reusable Gowns	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Process Emissions
Water emissions [kg]			
TDS	1.93E+01	9.46E-03	6.92E-03kg from Sulfur, 2.54E-03kg from Natural gas,
Tricarboxylic Acid	5.70E-01	5.70E-01	5.70E-01kg from CotPoly Fabric Biocide,
Trisodium nitrilotriacetate	3.28E+00	3.28E+00	4.37E-02kg from Reusable Gown, Cleaned,
Total Water emissions	2.76E+02	2.53E+02	2.77E-04kg from Sodium chloride, 1.99E-05kg from Sodium hydroxide, 4.15E-02kg from Hydrogen cyanide, 3.87E-05kg from Propylene, 5.86E-01kg from Acetone, 9.35E-02kg from Dimethyl hydantoin, 4.09E-04kg from pyrolysis gas, 5.67E-01kg from Methanol, 2.59E-01kg from Acetic acid, 1.28E+01kg from p-benzenedicarboxylic acid, 1.35E+00kg from Naphtha, 4.33E-04kg from Ethylene, 1.75E-02kg from Ethylene glycol, 8.49E-01kg from PET, 1.12E-02kg from Sulfur, 7.01E-02kg from DAP, 2.58E-03kg from Natural gas, 5.99E+00kg from Potassium chloride, 6.19E-01kg from Reusable Gown, Cleaned, 1.81E+02kg from CotPoly Fabric Biocide, 2.89E+00kg from Cotton,
Solid emissions [kg]			
calcium monoxide	6.45E-02	6.45E-02	6.45E-02kg from Phosphoric acid,
Clay	2.17E+00	2.17E+00	2.17E+00kg from Potassium chloride,
CotPoly Fabric Biocide	2.50E+01	2.50E+01	2.50E+01kg from Reusable Gown,
Cotton	5.51E+00	5.51E+00	5.51E+00kg from CottonPoly Yarn,
Cotton Seed	2.19E+02	2.19E+02	2.19E+02kg from Cotton,
CottonPoly Yarn	1.43E+01	1.43E+01	7.06E+00kg from CotPoly Fabric Biocide, 7.27E+00kg from CottonPoly Yarn,
Diatomaceous earth	2.02E-02	2.02E-02	2.02E-02kg from Dimethyloldimethyl hydantoin,
Hydrogen fluoride	2.46E-04	2.46E-04	2.46E-04kg from Phosphoric acid,
Impurities	5.19E-01	5.19E-01	5.19E-01kg from Phosphoric acid,
Mud (salt process)	5.91E-04	5.91E-04	5.91E-04kg from Sodium chloride,
Organic Matter	1.75E+01	1.75E+01	1.75E+01kg from Cotton,
PET	1.32E+00	1.32E+00	1.32E+00kg from CottonPoly Yarn,
Phosphate rock	5.95E+00	5.95E+00	5.95E+00kg from Phosphate rock,

Table 3.4 continued

Cradle-to-Use Gown Emissions per 1000 Reusable Gowns	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Process Emissions
Water emissions [kg]			
Phosphate rock (pure)	1.27E+00	1.27E+00	1.27E+00kg from Phosphoric acid,
Phosphogypsum	3.32E+01	3.32E+01	3.32E+01kg from Phosphoric acid,
Phosphoric acid	3.88E-01	3.88E-01	3.88E-01kg from Phosphoric acid,
Potassium chloride	2.80E+00	2.80E+00	2.80E+00kg from Potassium chloride,
Silica	6.77E-01	6.77E-01	6.77E-01kg from Phosphoric acid,
Sodium chloride	3.68E+01	3.68E+01	3.68E+01kg from Potassium chloride,
Solid waste	5.45E+01	1.43E-01	6.47E-04kg from Naphtha, 3.44E-02kg from Sulfur, 2.64E-02kg from Water for reaction, 8.18E-02kg from Natural gas,
starch suppressant	1.01E-01	1.01E-01	1.01E-01kg from Potassium chloride,
Sulfuric acid	2.95E-03	2.95E-03	2.95E-03kg from Phosphoric acid,
Total Solid emissions	4.21E+02	3.66E+02	5.91E-04kg from Sodium chloride, 2.02E-02kg from Dimethyloldimethyl hydantoin, 6.47E-04kg from Naphtha, 3.44E-02kg from Sulfur, 5.95E+00kg from Phosphate rock, 3.61E+01kg from Phosphoric acid, 2.64E-02kg from Water for reaction, 8.18E-02kg from Natural gas, 4.19E+01kg from Potassium chloride, 2.50E+01kg from Reusable Gown, 7.06E+00kg from CotPoly Fabric Biocide, 1.41E+01kg from CottonPoly Yarn, 2.36E+02kg from Cotton,

3.6 Conclusions

Performing a cradle-to-use inventory on a reusable medical patient gown shows that 65,000 MJ of energy and 2,336 kg of natural resources (excluding water) are used per 1000 gowns produced and used 75 times. The laundry and fabric production processes could be investigated further to reduce the energy usage. In the laundry process alone, using 25% less water would reduce the energy to heat the water by 11%.

Reducing the energy consumption would also reduce the carbon dioxide emissions generated.

This inventory is part of a larger study to investigate disposable and reusable medical textiles. The GTG LCI data presented in this paper can be used by readers in other LCI studies thus increasing the international LCI database.

3.7 Acknowledgements

The authors would like to thank Drs. Marian McCord and Traci May in the College of Textiles at North Carolina State University for their expertise in medical textiles, and Drs. Evan Griffing and Yong Li for their invaluable input to the life cycle inventory database. A National Science Foundation MUSES Grant funded this work. A National Science Foundation MUSES Grant (#0424514) funded this work.

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4. Cradle-to-Use Life Cycle Inventory of Medical Gowns

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This paper was presented at the InLCA/LCM 2007 conference

Portland, Oregon, October 2007

4. Cradle-to-Use Life Cycle Inventory of Medical Gowns

Abstract

This cradle-to-use life cycle inventory compares the environmental consequences of manufacturing and using a reusable cotton/polyester medical patient gown and a disposable polypropylene SMS (spunbond-meltblown-spunbond) medical patient gown. The reusable gown is made from a larger variety of chemicals and processes than the disposable gown, but on a basis of 75,000 patient uses that includes using and laundering the reusable gown 75 times, the reusable gown requires 2,336 kg of raw materials, compared to 12,607 kg of raw materials needed for the disposable gown, mostly from coal and crude oil. However the reusable gown uses more water due to irrigation of cotton and the laundry process. The reusable gown consumes less energy, and only 10.7 uses are needed to equal the energy uses of an equivalent number of disposable gown uses. Air, water, and solid emissions for the reusable gown are also lower than for the disposable gown.

Keywords: Life cycle inventory; life cycle analysis; medical textiles; reusable; disposable; laundering; energy; emissions

4.1 Introduction

Medical textiles are an expanding sector in the textiles market with forecasts of 2.4 million tons produced worldwide by 2010, which contribute to the 3.2 million tons of medical waste generated in the US each year. Fourteen thousand tons of that medical waste come from medical garments (0.44 weight %) (Lehrburger and Mullen.,Bristol, 2007).

While reducing solid waste is a clear benefit of using reusable medical gowns, questions arise concerning the environmental impact of laundering and the sterility of a garment that has been reused. In the United States, disposable nonwoven garments dominate with 80% of the market while reusable woven garments dominate in Europe (Rutala and Weber., 2001, Bushman, 2004). Although each type – disposable and reusable – claim superiority, studies show that the infection rates for both types are similar (Garibaldi et al., 1986, Bellchambers et al., 1999). A life cycle inventory shows the complete environmental picture of a product, and can be used to improve the manufacture of a product by highlighting where changes can be made to get the most impact on reducing the resources and energy consumed. This life cycle inventory compares the environmental profiles of two medical patient gowns – a reusable gown made of a cotton/polyester blend woven fabric and a disposable polypropylene SMS (spunbond-meltblown-spunbond) gown. The biocidal finish is composed of a halamine grafted onto the fabric and activated with the application of household chlorine bleach

(Qian and Sun, 2004, Sun and Sun, 2004, Sun and Worley, 2005). This life cycle inventory is part of a larger study investigating the environmental consequences of fabric choices and biocidal finishes for medical textiles.

4.2 Goal and Scope of the Study

The intent of this work is to compare a 55% cotton/45% polyester reusable medical patient gown having a biocidal surface for nosocomial infection prevention with a polypropylene SMS disposable medical patient gown having no biocidal surface using cradle-to-use life cycle inventories. An additional goal is to increase the amount of life cycle inventory data that can be used by others. Transparent gate-to-gate (within the factory) inventories are used, and the cradle-to-use inventory is the summation of these first level inventories. For the reusable gown, the scope is from the natural resources through the manufacture of the medical gown and then use of the gown, as shown in the dotted line box in Figure 4.1. Figure 4.2 shows the scope of the disposable gown in the dotted line box. The reusable gown is used 75 times, with laundering after each use, while the disposable is used once and discarded. Disposal of the gown is not included. To compare the reusable and disposable gowns on the same basis, the functional unit is 75,000 patient gown uses, or for the reusable gown, 1000 reusable patient gowns used 75 times.

4.3 Methodology

In spite of increasing interest in LCA, the available life cycle inventory information is still far less than desired. In the chemical industry, companies have considered some information needed in life cycle studies as competitive intelligence. In this study, we use design-based approach methodology (Jimenez-Gonzalez, 2000,Overcash, 1994) to obtain most of the life cycle inventory data, in which the life cycle information of each gate-to-gate subsystem is obtained using chemical engineering design techniques reflecting well known industrial practices. Every life cycle inventory (LCI) follows a similar procedure, like an experiment in a laboratory. Information is gathered from articles, books, patents, company websites, and consultations with experts in the field, then used with established process design heuristics to arrive at the LCI results. The gate-to-gate subsystems are linked through a production chain (referred to as the chemical tree), which includes extraction of raw materials and manufacturing processes. Whenever site-specific information is available, it is applied to the process design in each study. Energy to generate the energy utilities and emissions after waste management are not included.

After selecting the generic process and creating a flow diagram, the mass balance is created. Once a gate-to-gate inventory is completed, a technical peer expert in the field reviews it, and changes are made as needed.

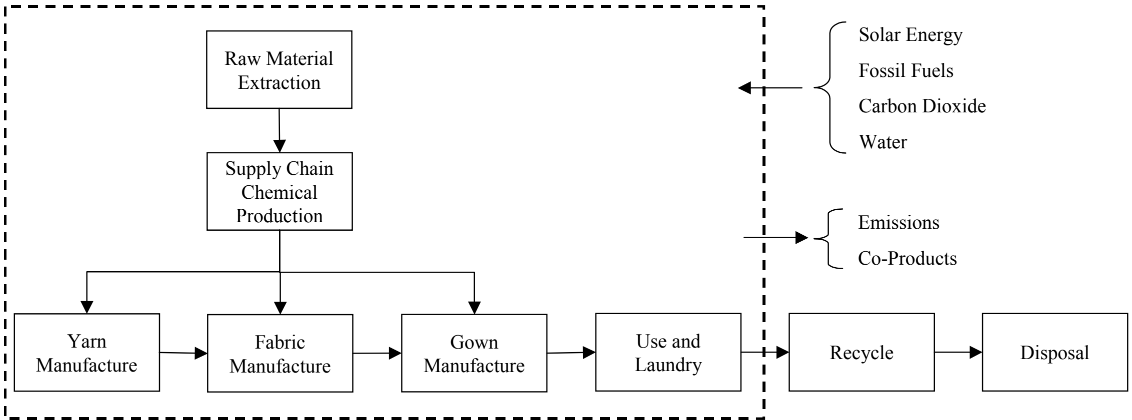


Figure 4.1. Life Cycle of Reusable Gown. Scope of inventory is in dotted line box.

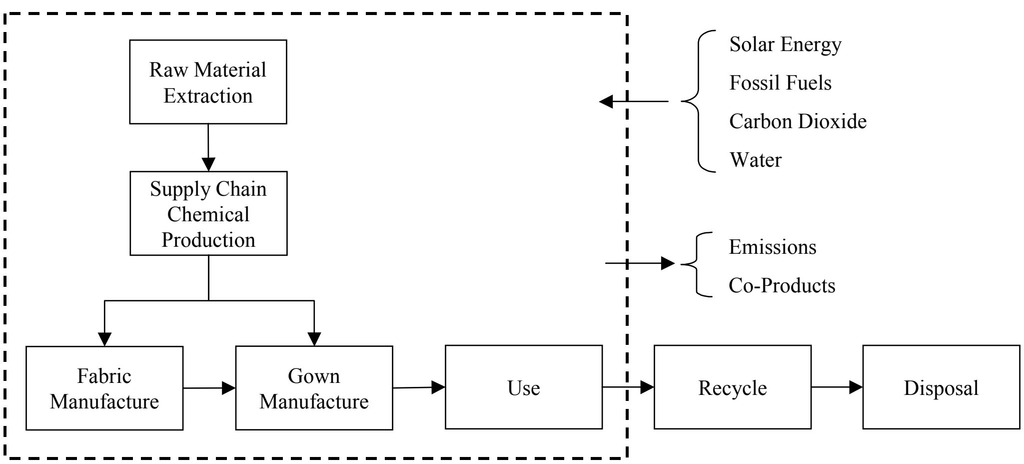


Figure 4.2. Life Cycle of Disposable Gown. Scope of inventory is in dotted line box.

4.4 Gown Manufacturing

To provide transparency of this life cycle inventory, the processes and assumptions used in this inventory are described. The processes used for the reusable gown inventory are described in Chapter 3.

4.4.1 Spunbond-Meltblown-Spunbond Fabric

The detailed process for making the SMS fabric for the disposable gown generated from research for the study is shown in Figure 4.3. Polypropylene SMS fabric is composed of a meltblown layer sandwiched between two spunbond layers. Polypropylene is colored by extruding with pigment, such as beta-copper phthalocyanine, to form concentrated color pellets (color concentrate). Extruder 2 mixes the color concentrate with polypropylene, and the polymer is forced through small holes in the spinneret plate of a spin beam. In the quench chamber (Air Quench), cool air solidifies filaments and prevents filaments from sticking together. The second air stream (Air Gun) parallel to the filaments accelerates and stretches (attenuates) filaments and orients the polymer chains, increasing the filament strength. The filaments are deposited as a random web on a moving porous belt. A vacuum under the belt (using the inlet side of a blower) removes air and assists the web formation. The web is compacted and bonded with a roller.

For the meltblown layer, polypropylene is colored in the same manner as for the spunbond layer and Extruder 4 forces the polymer through spinnerets with hot (300°C) air at a high velocity (from 20 to 100 lb/min/in^2 slot area) (Buntin, 1976). The micron-sized fibers are blown on top of the first spunbond layer, and bonding is due to self-entangling. The fiber diameter of the meltblown filament ranges from 0.5 to 15 microns, and preferably 2 to 6 microns, almost an order of magnitude smaller than spunbonded fibers.

The 2-layer laminate is then conveyed under the second spunbond station. The spunbond filaments from Extruder 6 are deposited on top of the meltblown layer. This 3-layer composite is compacted with a roller and thermally point bonded with a calendar roll heated to 133°C (Connor, 1998). Twenty percent of the fabric is bonded in a pattern such as dots or diamonds. As the fabric is wound onto rolls, 1-2 inches are trimmed from the edges (1.5 inches used in this inventory) and discarded. The fabric has a weight of 55.6 g/m^2 (1.64 oz/yd^2) and a width of 3.2 meters. Energy for unit operations in the fabric inventory is calculated based on heuristics written for each unit operation.

Unit Operation	Symbol
Blower	Blwr
Conveyor	Cnv
Compressor	Cmp
Heat Exchanger	HX

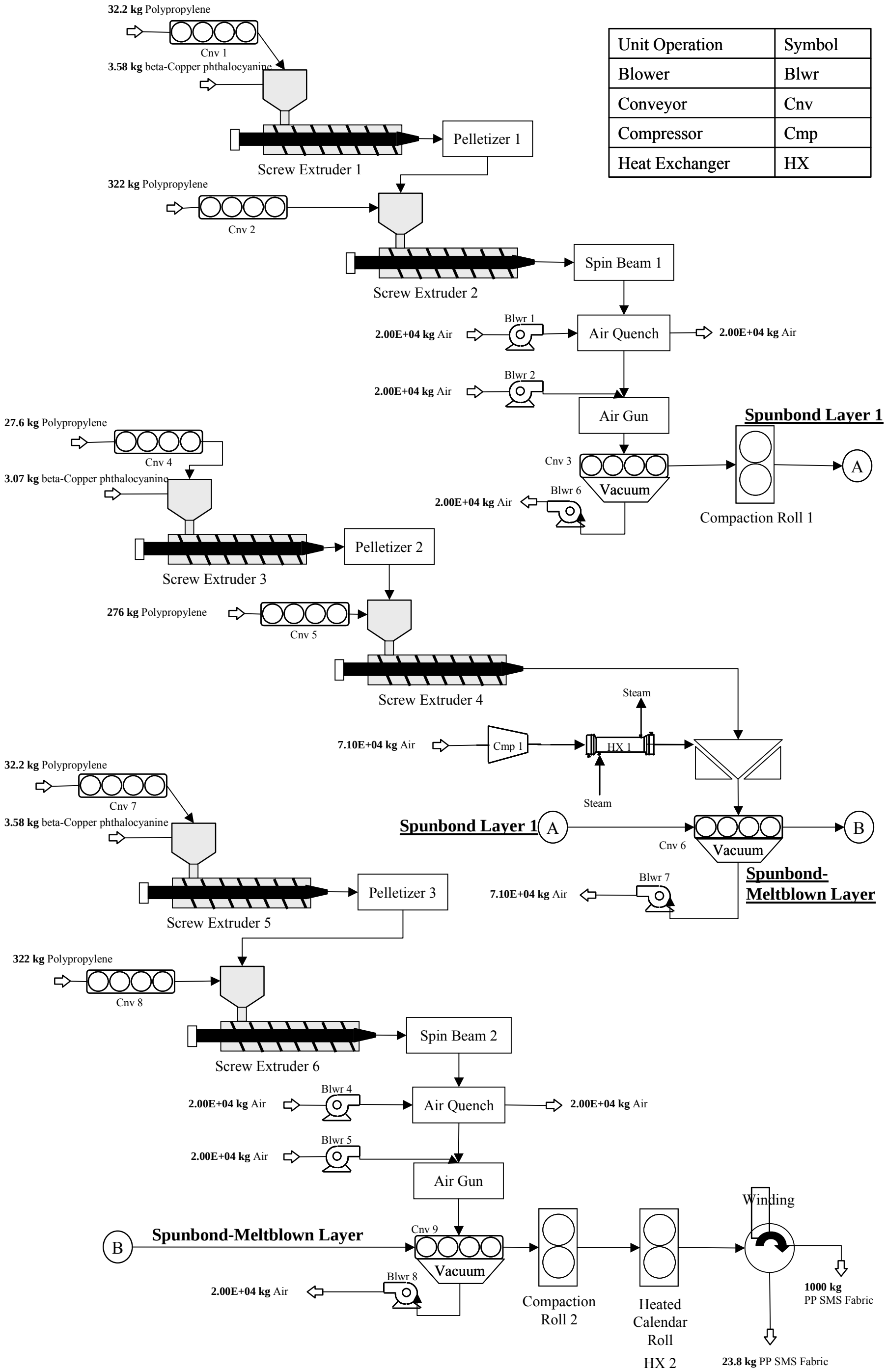


Figure 4.3. Polypropylene SMS Fabric Process Flow Diagram

4.4.2 Garment Assembly

Garment assembly is outlined in the flow diagram in Figure 4.4. Fabric from the bolt is spread in multiple layers to form a stack or ply so that multiple pieces can be cut concurrently. The pattern pieces (markers) are arranged on the fabric so that the least amount of fabric is wasted. Efficiency ranges from 65 to 90% of fabric use depending on consideration of fabric designs, fabric nap, or other constraints (Solinger, 1980). Ninety percent efficiency is use in this LCI. After cutting, the pieces are bundled according to sizes and assembled (seams are fused) into the garment. The garment is finished with a steam press. The finished patient gown weighs 60 grams, or 16,667 gowns per metric ton of gowns.

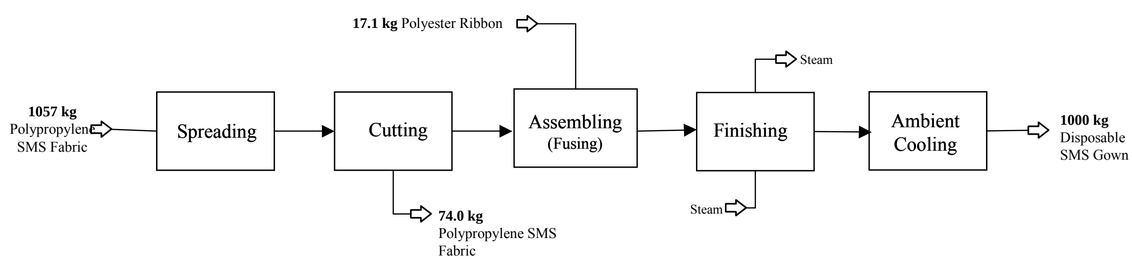


Figure 4.4. Garment Assembly Flow Diagram

4.5 Inventory Results and Discussion

The chemical tree in Figure 4.5 is a modified version of the full reusable patient gown chemical tree. It shows the product in the left-most column and the chemicals and solvents in the second column that went into direct production of the API. The fifth column shows how many chemicals (including duplicates) went into the production of those chemicals traced back to the natural resources from the ground shown in the last column. This life cycle inventory included forty-eight chemicals and the gate-to-gate inventories that were performed for each of these chemicals. Chemicals added in minor amounts, or ancillary inputs, are not shown in this chemical tree and were not included in these studies (Consoli et al., 1993).

Level 1	Level 2	Level 3	Level 4	Levels 5-11	Level 12
Reusable Gown	Cotton Polyester Fabric	Cotton Polyester Yarn	Cotton	94 chemicals	Natural Resources: Air, Coal, Cotton Seed, Crude Oil, Natural gas, Phosphate rock, Salt rock, Sand, Sylvinite ore, Water
			PET	40 chemicals	
		DMDMH	Dimethyl hydantoin	45 chemicals	
			Formaldehyde	7 chemicals	
			Sodium hydroxide	4 chemicals	

Figure 4.5. Chemical Tree of Reusable Patient Gown

Figure 4.6 shows the full disposable patient gown chemical tree. It shows the product in the left-most column. The supply chain of the disposable gown is much shorter than that of the reusable gown. Only five chemicals or products are in its supply chain compared to 47 chemicals in the reusable gown supply chain.

Level 1	Level 2	Level 3	Level 4	Level 5	Level 6
SMS Gown	Polypropylene SMS Fabric	Polypropylene	Propylene	Naphtha	oil (in ground)

Figure 4.6. Chemical Tree of Disposable Patient Gown

4.5.1 Raw Materials

In the ctu (cradle-to-use) analysis when water is not included, for 75,000 gown uses, disposable gowns required more than 5 times the raw materials of reusable gowns, as shown in Table 4.1. When water is excluded, using the gown eighty times will equal the resources used for the equivalent disposable gown uses. However, the reusable gown does require 1.4 million kg of water. Water is used mainly for irrigation of cotton (1.2 million kg) and for laundry (189,784 kg) in the reusable gown. The largest raw material inputs for the reusable gown are water, crude oil, and natural gas. Crude oil is the largest raw material since it is the natural resource for polypropylene. To produce the cotton used in the gowns, 0.41 acres of land was used.

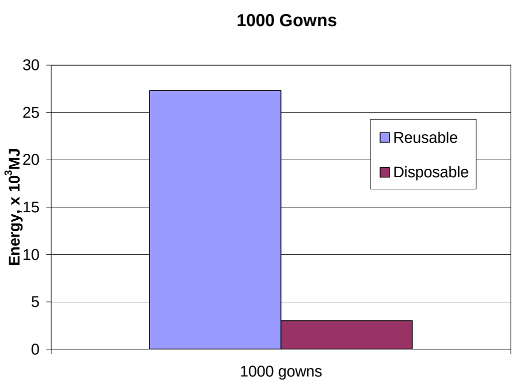
Table 4.1. Cradle-to-Use (CTU) Raw Material Consumption per 75,000 gown uses of Reusable and Disposable Gowns.

	75,000 Reusable Gown Uses			75,000 disposable gowns		
Cradle-to-use Raw Material, kg	**Total**	**Process**	**Energy-related**	**Total**	**Process**	**Energy-related**
Air	123	123	0	0	0	0
Coal	289	37	253	2,910	0	2,910
Cotton Seed	3	3	0	0	0	0
Crude Oil	1,068	728	340	5,676	5,138	345
Natural gas	752	437	315	4,019	0	4,019
Phosphate rock	27	27	0	0	0	0
Salt rock	0	0	0	0	0	0
Sand	1	1	0	0	0	0
Sylvinite ore	72	72	0	0	0	0
Water for reaction	218	218	0	0	0	0
Water for irrigation	1,183,825	1,183,825	0	0	0	0
Water for laundry	189,784	189,784	0	0	0	0
Total excluding water	2,336	1,428	907	12,605	5,138	7,274
Total including water	1,376,162	1,375,255	907	12,605	5,138	7,274

4.5.2 Energy

The energy table for the GTG chemicals/processes for the reusable gown is shown in Chapter 3. For the reusable gown, 58% of the total energy comes from the laundry process, mostly to heat water in the washing process. Fabric production and yarn production are the next largest energy consuming processes. The energy for each process for the disposable gown is shown in Table 4.2. For the disposable gown, fabric production uses 46% of the total ctu energy, primarily due to the large amount of heated air used in the web laying process.

Table 4.3 shows the energy required to manufacture 1000 reusable gowns and 1000 disposable gowns. Reusable gowns require 27,315 MJ of energy compared to 3,013 MJ for disposable gowns. However, when reusing and laundering is included, reusable gowns require less energy at 65,049 MJ compared to 225,947 MJ for disposable gowns per 75,000 gown uses. (See Figure 4.7) Based on manufacture and laundering inventories, it would take 10.7 uses for the reusable gown to equal the energy use of the same amount of single-use disposable gowns.



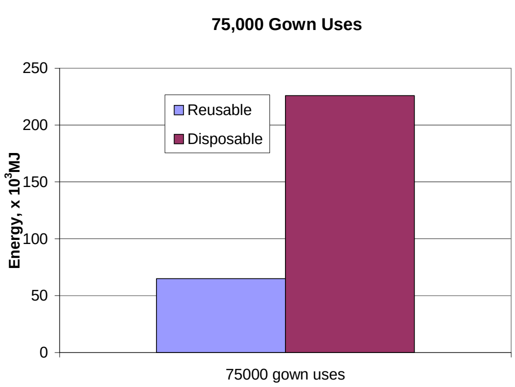


Figure 4.7. Energy Comparison for Reusable and Disposable Gowns, based on 1000 Gowns and 75,000 Gown Uses

Table 4.4 shows a breakdown of the energy used in the CTU analysis of the gowns. For reusable gowns, heating steam is the largest type of energy required, and this can be traced to the fabric dyeing, drying, and laundry processes. For the disposable gowns, dowtherm heating fluid to heat the hot air for the polypropylene web formation is the largest energy type.

4.5.3 Emissions

The ctu emissions for the disposable gown are listed in Table 4.5. The emissions come from chemical losses and energy-related emissions from each GTG inventory, and depending on the physical state, are listed as air, liquid, or solid emissions. These emissions are all process emissions and do not include the effect of waste management processes. The detailed list of the ctu emissions for the reusable gown are shown in Chapter 3, but Table 4.6 shows the total air, water, and solid emissions for both gowns per 75,000 gown uses. The disposable gown emits 3.6 times as much air emissions as the reusable gown, mostly from carbon dioxide. The disposable gown also emits twice the amount of solid emissions, but half the amount of water emissions compared to the reusable gown. These solid emissions do not include the 4,500 kg of solid waste from disposing of 75,000 disposable gowns.

Table 4.2. Cradle-to-Use (CTU) Energy Consumption for 75,000 Disposable Gown Uses.

				CTU Energy, MJ/75,000 Disposable Gown Uses[a]							
Chemicals, gate-to-gate	Mass, kg/1000 kg Gown[b]	By-products, kg/kg chemical[c]	Allocation factor[d]	Electricity	Dowtherm	Steam	Fuel, Non-transport	Fuel, Transport	Potential recovery[e]	Total net energy	% of Total
PP SMS Gown	1,000		1.000	3,593	0	1,309	0	1,980	0	6,882	3%
PP SMS Fabric	1,057		1.000	8,321	92,684	246	0	2,093	0	103,344	46%
Polypropylene	1,071		1.000	40,417	0	347	0	2,121	-3,480	39,405	17%
Propylene	1,105	C4 stream; Ethylene; fuel oil; Hydrogen; Methane; pyrolysis gas;	0.165	7,069	0	11,766	57,585	2,189	-14,075	64,534	29%
Naphtha	1,127	heavy gas oil, from distillation; kerosene, from distillation; light gas oil, from distillation; residuum, from distillation;	0.225	1,212	0	568	10,002	0	0	11,782	5%
Total Energy				60,613	92,684	14,237	67,587	8,382	-17,556	225,947	100%

[a] Amount of energy used cradle-to-gate to produce mass of chemical used in inventory.
[b] Amount used cradle-to-gate to produce 1000 kg product.
[c] By-products generated during the gate-to-gate manufacture of chemical.
[d] Mass allocation is used to distribute the inputs, energy, and emissions to each product formed in that gate-to-gate inventory. Allocation factor will be less than 1.0 when by-products are generated.
[e] Energy that can be recovered from sources requiring cooling.

Table 4.3. Cradle-to-Gate (CTG) Energy Consumption for 1000 Gowns Manufactured

CTG Energy	MJ/1000 Reusable Gowns	MJ/1000 Disposable Gowns
Electricity	5,229.49	808.17
Dowtherm	176.37	1,235.78
Heating steam	17,475.11	189.83
Fuel	3,674.09	1,012.93
Energy input	29,421.57	3,246.70
Cooling water	-4,342.99	-638.35
Refrigeration	1.42	0.01
Potential recovery[a]	-2,106.98	-234.07
Net energy (Input - Potential recovery)	27,314.60	3,012.63

[a] Energy that can be recovered from sources requiring cooling.

Table 4.4. Cradle-to-Use (CTU) Energy Consumption for 75,000 Gown Uses

CTU Energy	MJ/75,000 Reusable Gown Uses	MJ/75,000 Disposable Gown Uses
Electricity	5,994.30	60,612.67
Dowtherm	176.37	92,683.57
Heating steam	46,956.49	14,236.97
Fuel	14,029.10	75,969.59
Energy input	67,156.26	243,502.80
Cooling water	-4,342.99	-47,876.33
Refrigeration	1.42	0.88
Potential recovery[a]	-2,106.98	-17,555.57
Net energy (Input - Potential recovery)	65,049.29	225,947.23

[a] Energy that can be recovered from sources requiring cooling.

Table 4.5. Cradle-to-Use Emissions for 75,000 disposable gowns used.

	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Emissions
Air Emissions			
1,3-butadiene	9.85E-01	9.85E-01	Propylene
Acetylene	1.32E-01	1.32E-01	Propylene
Benzene	1.09E-03	1.09E-03	Naphtha
Butane	5.73E-01	5.73E-01	Propylene, Naphtha
Butene	1.71E+00	1.71E+00	Propylene
Carbon dioxide	2.05E+04	1.53E+02	Naphtha
Carbon monoxide	1.05E+01	7.46E-03	Propylene
Ethane	1.59E+00	1.59E+00	Propylene, Naphtha
Ethylene	6.45E+00	6.45E+00	Propylene
Heptane	1.26E-01	1.26E-01	Naphtha
Hydrogen	3.05E-01	3.05E-01	Propylene
Isobutane	4.35E-03	4.35E-03	Naphtha
Methane	6.61E+01	6.87E+00	Propylene, Naphtha
Naphtha	9.95E+01	9.95E+01	Propylene
n-Hexane	1.08E-01	1.08E-01	Naphtha
NMVOC	6.49E+01	2.39E-02	Naphtha
NOx	7.00E+01	0.00E+00	
n-Pentane	6.09E-02	6.09E-02	Naphtha
Octane	9.46E-02	9.46E-02	Naphtha
Polypropylene	4.83E+00	4.83E+00	Polypropylene
Propane	1.10E-01	1.10E-01	Propylene, Naphtha
Propylene	1.66E+02	1.66E+02	Polypropylene, Propylene
Propyne	1.18E-01	1.18E-01	Propylene
pyrolysis gas	1.34E+01	1.34E+01	Propylene
SOx	3.56E+01	0.00E+00	
Total Air emissions	2.11E+04	4.56E+02	Polypropylene, Propylene, Naphtha
Water Emissions			
Arsenic	3.86E-05	3.86E-05	Naphtha
Benzene	9.07E-04	9.07E-04	Naphtha
BOD	1.28E+00	0.00E+00	
Boron	1.91E-02	1.91E-02	Naphtha
Chloride	1.41E+01	1.41E+01	Naphtha
COD	3.05E+01	0.00E+00	
grease / oil	2.29E-01	2.29E-01	Naphtha
Mobile ions	4.44E+01	4.44E+01	Naphtha
pyrolysis gas	1.07E-01	1.07E-01	Propylene
Sodium	1.81E+01	1.81E+01	Naphtha
TDS	2.74E+01	0.00E+00	
Total Water emissions	1.36E+02	7.69E+01	Propylene, Naphtha

Table 4.5 continued

	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Emissions
Solid Emissions			
Polypropylene SMS Fabric	4.46E+02	4.46E+02	Polypropylene SMS Fabric
Solid waste	4.70E+02	3.69E-02	Naphtha
Total Solid emissions	9.16E+02	4.46E+02	Polypropylene SMS Fabric, Naphtha

Table 4.6. Comparison of Emissions from Reusable and Disposable Gowns

	Reusable Gown Emissions, kg	Disposable Gown Emissions, kg
Total Air emissions	5,827	21,092
Total Water emissions	276	136
Total Solid emissions	421	916

4.6 Conclusions

Cradle-to-use inventories for a reusable medical patient gown and a disposable patient gown show the reusable gown uses fewer raw materials (excluding water), but more water than the disposable gown per 75,000 gown uses. When the reusable gown is used and laundered more than ten times, the reusable gown requires less energy than the disposable gown. The reusable gown emits significantly fewer emissions than the disposable gown. The application and use of the biocidal surface account for 11%, 13%, and 5% of the total gown raw material usage, energy consumption, and emissions generated, respectively. Possible areas to reduce energy use are in the laundry process to reduce water usage, which will in turn reduce energy usage, and steam energy in the fabric dyeing and drying processes. Also a 100% polyester reusable gown would require less water since water is required for irrigation of cotton.

4.7 Acknowledgements

The authors would like to thank Dr. Don Shiffler and Steve Sharp in the College of Textiles at North Carolina State University for his expertise in the nonwoven fabrics, and Drs. Evan Griffing and Yong Li for their invaluable input to the life cycle inventory database. A National Science Foundation MUSES Grant funded this work. A National Science Foundation MUSES Grant (#0424514) funded this work.

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5. Cradle-to-Gate Life Cycle Inventory of Vancomycin Hydrochloride

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Manuscript submitted for publication to The Science of the Total Environment

This paper was presented at the 2008 AIChE Annual Meeting, Philadelphia, Pennsylvania, November 2008

5. Cradle-to-Gate Life Cycle Inventory of Vancomycin Hydrochloride

Abstract

A life cycle analysis on the cradle-to-gate production of vancomycin hydrochloride, which begins at natural resource extraction and spans through factory (gate) production, not only shows all inputs, outputs, and energy usage to manufacture the product and all related supply chain chemicals, but can highlight where process changes would have the greatest impact on reducing raw material and energy consumption and emissions. Vancomycin hydrochloride is produced by a low-yield fermentation process that accounts for 47% of the total cradle-to-gate energy. The fermentation step consumes the most raw materials and energy cradle-to-gate. Over 75% of the total cradle-to-gate energy consumption is due to steam use; sterilization within fermentation is the largest user of steam. Aeration and agitation in the fermentation vessels use 65% of the cradle-to-gate electrical energy. To reduce raw materials, energy consumption, and the associated environmental footprint of producing vancomycin hydrochloride, other sterilization methods, fermentation media, nutrient sources, or synthetic manufacture should be investigated. The reported vancomycin hydrochloride life cycle inventory is a part of a larger life cycle study of the environmental consequences of the introduction of biocide-coated medical textiles for the prevention of MRSA (methicillin-resistant Staphylococcus aureus) nosocomial infections.

Keywords: Life cycle inventory; life cycle analysis; vancomycin hydrochloride; fermentation; energy; emissions

5.1 Introduction

Vancomycin hydrochloride, also referred to as vancomycin (Figure 5.1), is a glycopeptide antibiotic used to treat resistant infections such as methicillin-resistant Staphylococcus aureus (MRSA). Vancomycin is active against gram-positive bacteria and gram-negative cocci by inhibiting bacterial cell wall peptidoglycan synthesis (McCormick et al., 1955). Vancomycin was first isolated in 1956 by Eli Lilly, and it was referred to as Mississippi Mud due to the brown color from fermentation impurities. After the 1980s, purification methods improved, and the crystals were a pure white solid. Vancomycin is currently produced in low yield by aerobic fermentation using Amycolatopsis orientalis.

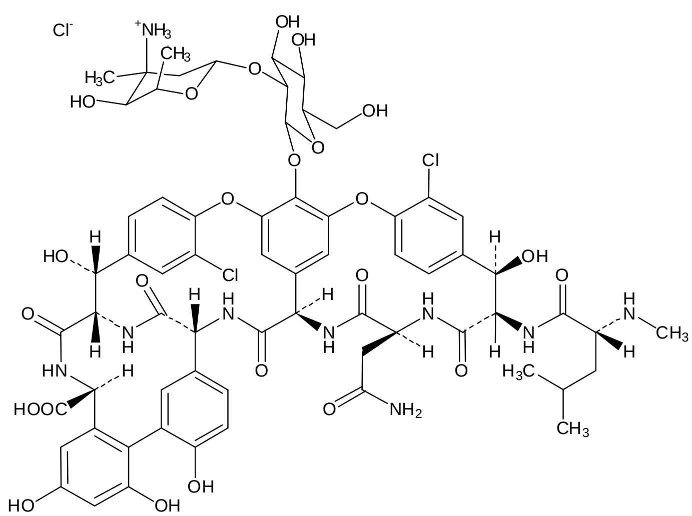

Figure 5.1. Chemical Structure of Vancomycin Hydrochloride

The cradle-to-gate (CTG) life cycle inventory (LCI) for vancomycin hydrochloride presented here was completed as part of a larger life cycle inventory investigating the environmental footprint of treating a nosocomial MRSA infection. Vancomycin hydrochloride is also the third active pharmaceutical ingredient studied by this research group. Life cycle inventories for the synthetic production of sertraline hydrochloride and paroxetine were preciously investigated, and the LCI showed solvent and energy usage to have the greatest impacts on the life cycle assessment (Jimenez-Gonzalez and Overcash., 2000). This finding has led to the development of tools to help scientist select "greener" solvents for pharmaceutical manufacturing (Curzons et al., 2007, Slater and Savelski, 2007).

A life cycle assessment (LCA) is a "methodological framework for estimating and assessing the environmental impacts attributable to the life cycle of a product." (Hendrickson et al., 2006) The ISO 14040 series outlines the requirements for conducting life cycle inventory and assessment studies (International Standard Organization, 1997). The backbone of the LCA is the life cycle inventory, or a compilation of all inputs, outputs, and energy use of a product from resource extraction, manufacture, product use, recycling, and disposal (Rebitzer et al., 2004). A life cycle inventory gives the complete environmental picture of a product, and can be used to improve the manufacture of a product by highlighting where changes can be made to make the most impact on reducing raw material and energy usage and emissions.

5.2 Goal and Scope of the Study

The intent of this work is to analyze the cradle-to-gate inventory for production of vancomycin hydrochloride (vancomycin HCl) as part of a larger life cycle inventory investigating the environmental burden of treating a nosocomial MRSA infection. An additional goal is to provide the life cycle community with usable process information for other future life cycle studies. The scope is from the natural resources through the manufacture of the active pharmaceutical ingredient (API) vancomycin hydrochloride (cradle-to-gate). Use and disposal of the API are not included in this LCI analysis.

In this study, transparent gate-to-gate (within the factory) inventories are used, and the cradle-to-gate inventory is the summation of these first level inventories of each chemical in the supply chain. The functional unit, or basis of all analysis, is 1000 kg vancomycin hydrochloride crystals.

5.3 Methodology

The design-based LCI methodology (Jimenez Gonzalez, 2000) using process flow diagrams and engineering design principles is used to collect inventory data (e.g., process inputs, process operations, waste generated, etc.) and complete gate-to-gate inventories for each chemical in the supply chain of the API. After selecting a generic manufacturing process and creating a flow diagram for each chemical input, the mass and energy balances are created to get the total raw materials input, energy consumption, and waste generated. Information is gathered from articles, books, patents, company websites, and consultations with experts in the field, and then used with established process design heuristics to arrive at the LCI results. Once each gate-to-gate inventory is completed, a technical peer expert in the field reviews it, and changes are made as needed.

5.4 Vancomycin Production

For the gate-to-gate inventory of vancomycin, aerobic fermentation using Amycolatopsis orientalis (formerly Nocardia orientalis and Streptomyces orientalis) is the general manufacturing process selected, and the process flow diagram generated from research is shown in Figure 5.2. Although a variety of nutrient sources can be used, this inventory uses glucose (dextrose) and soy flour for fermentation (Jung et al., 2007). A. orientalis spores are transferred to flasks to inoculate starter nutrient medium and incubated for 2 days. Fresh nutrient broth consisting of dextrose and soy flour as carbon and nitrogen sources, respectively, is added to Fermentor 1 and sterilized with steam for 15 min at 120ºC. Inoculum from the flask is then added to the cooled reactor medium and allowed to ferment for 24 hours at 30ºC as air is sparged into the vessel. Fresh nutrient broth is then added to progressively larger bioreactors (Fermentors 2 and 3) and sterilized before the contents of the smaller bioreactors are added. The fermentation is four to six days. Air is added at a rate of 0.4 to 0.8 volumes of air per volume broth per minute, and the temperature is held at 30ºC (Cinar et al., 2003).

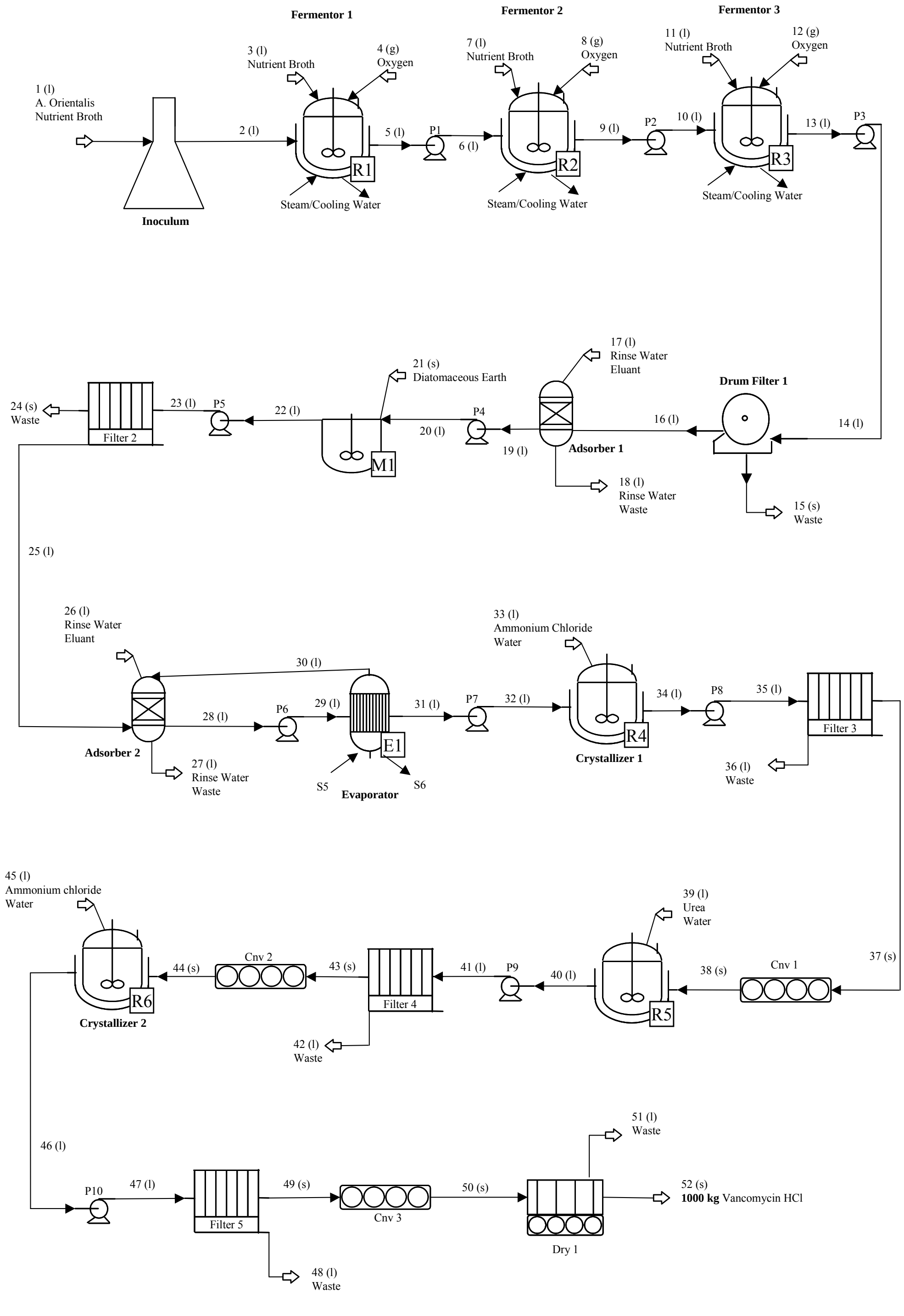

Figure 5.2. GTG Process Flow Diagram of Vancomycin Hydrochloride Production

The fermentation broth, containing from 4 to 11 g Vancomycin/L broth (Jung et al., 2007), is filtered and passed through two adsorbers (Adsorbers 1 and 2) using Dowex 50 and Amberlite XAD-16 resins to separate the active ingredient vancomycin B and to decolorize and remove impurities. The solution is concentrated in an evaporator (E1). To further purify, vancomycin hydrochloride is then crystallized (in Crystallizer 1) using ammonium chloride, converted to the base vancomycin using urea (in R5), and crystallized again as vancomycin hydrochloride using ammonium chloride (in Crystallizer 2). The vancomycin hydrochloride crystals are filtered and dried.

To calculate the energy used, it is assumed that 25% of the glucose is converted to vancomycin, according to the reaction mechanism of Dunstan et al (Dunstan et al., 2000) showing 24 moles of glucose are converted to 1 mole of vancomycin, while 75% is converted to exothermic energy by glycolysis (McIntyre et al., 1996). The fermentation energy (used to calculate cooling water requirements) is calculated from the heats of reaction for the dextrose glycolysis and dextrose-to-vancomycin reactions.

5.5 Inventory Results

The chemical tree in Figure 5.3 is a condensed version of the full vancomycin hydrochloride chemical tree. The full tree includes all of the chemicals in the supply chain of the final product. To abbreviate the chemical tree, only the first two levels are shown, along with the number of chemicals that went into the production of the second level chemicals. The natural resources are on the far right. For example, twenty-eight chemicals are in the CTG supply chain to manufacture dextrose. This number includes duplicates, as a chemical input may be used to manufacture more than one chemical product. This life cycle inventory included thirty-eight different chemicals and the gate-to-gate inventories that were completed for each of these chemicals. Chemicals added in minor amounts, or ancillary inputs, are not shown in this chemical tree and were not included in these studies (Consoli et al., 1993).

Level 1	**Level 2**		**Natural Resources**
Vancomycin HCl	Dextrose	28 chemicals	Natural Resources: Air, Coal, Crude oil, Natural gas, Phosphate rock, Salt rock, Sand, Sylvinite ore, Water
	Soy Flour	25 chemicals	
	Ammonia	4 chemicals	
	Isopropanol	7 chemicals	
	Ammonium chloride	7 chemicals	
	Urea	6 chemicals	

Figure 5.3. Chemical Tree of Vancomycin Hydrochloride

The basis for this inventory is 1000 kg vancomycin hydrochloride, and all raw material and energy consumption and emissions shown in this inventory are based on this functional unit. In the gate-to-gate (GTG) production of vancomycin hydrochloride, 155,000 kg of raw materials were consumed to directly produce the product, as shown in Table 5.1. The majority of this water is used for fermentation and other aqueous media and not directly consumed in the reactions. Other than water, the carbon and nitrogen sources dextrose and soy flour are the largest inputs by mass.

Table 5.1. Gate-to-Gate Raw Material Consumption for 1000 kg Vancomycin Hydrochloride

GTG Raw Material	kg/1000kg Vancomycin HCl	PMI
Ammonia	1,000	1.16
Ammonium chloride	1,132	1.32
Dextrose	12,099	1.31
Isopropanol	100	2.92
Soy Flour	4,625	1.12
Urea	1,200	1.39
Water (fermentation)	73,305	
Water (aqueous media)	61,947	
Total	155,408	

As an environmental measure of the process, process mass intensity (PMI) (Constable et al., 2002) can be calculated using the GTG inputs as shown below:

$$\text{Process Mass Intensity (PMI)} = \frac{\text{Total GTG Raw Materials Mass}}{\text{Product Mass}} \qquad (6.1)$$

The Process Mass Intensity ideally approaches one when the raw material input equals the product mass; thus, no waste is generated. In the case of vancomycin HCl, the PMI equals 155. In contrast, the PMI is 20 if water is not included. Henderson et al

(Henderson et al., 2007) studied mass intensity for the pharmaceutical industry, and found mass intensity to range from 25 to 200 for synthetic processes, in which water was included in the raw materials. However, fermentation processes were not included in the pharmaceutical industry study. Table 5.1 shows the PMIs for the GTG raw materials range from 1.12 to 2.92, which is much lower than those from the pharmaceutical industry study.

In the cradle-to-gate analysis, 585,000 kg of raw materials are used to make 1000 kg of the API (see Table 5.2), with most of that being water from fermentation and irrigation of crops. Dextrose and cornstarch are derived from corn, and soy flour is derived from soybeans; irrigation water is used during the growth of these crops. Crude oil and natural gas are the next largest inputs by mass.

Table 5.2. Cradle-to-Gate Raw Material Consumption for 1000 kg Vancomycin Hydrochloride

CTG Raw Material	**kg/1000 kg Vancomycin HCl**
Air	2,783
Coal	1,749
Crude Oil	7,415
Natural gas	6,826
Phosphate rock	1,619
Salt rock	837
Sand	67
Soybean Seed	158
Sylvinite ore	1,135
Water (fermentation)	73,305
Water (reacting)	64,297
Water (irrigation)	424,622
Total	584,814

The life cycle inventory also shows that the cradle-to-gate production of vancomycin hydrochloride uses 566 MJ of energy. The heat from streams that must be cooled can provide heat in another part of the process. When this recovered energy is included in the inventory total, the energy consumption is reduced to 480 MJ. Table 5.3 compares the GTG production energy to the CTG energy, and shows the GTG production of the API accounts for 48% of the total CTG energy consumed and most of the electricity, steam, and cooling water. The remaining energy comes from production of the supply chain chemicals. Coal is used in sulfur processing, and sulfur is used in the supply chains of dextrose, soy flour, and isopropanol. Corn and soybean production use farm equipment that requires diesel and gasoline (direct fuel). One third of the diesel consumption is due to farm equipment and naphtha processing, and the remaining comes from transportation of chemicals to factories. Naphtha is used in isopropanol, soy, and dextrose processing.

Table 5.3. CTG and GTG Energy Consumption for 1000 kg Vancomycin Hydrochloride

Energy [MJ/1000 kg Vancomycin HCl]	Total Vancomycin HCl CTG	Total Vancomycin HCl GTG	GTG% of CTG
Electricity	35,267	23,691	67%
Heating steam	436,802	248,073	57%
Direct fuel	21,169	0	0%
Natural gas	34,522	0	0%
Coal	64	0	0%
Diesel[a]	35,154	440	1%
Other	3,340	0	0%
Energy input	566,318	272,204	48%
Cooling water	-452,137	-349,190	77%
Potential recovery[b]	-86,724	-48,485	56%
Net energy (Input - Potential recovery)	479,595	223,719	47%

[a] One third of the diesel energy is due to farm equipment.
[b] Energy that can be recovered from sources requiring cooling.

Table 5.4 shows the CTG energy for each chemical in the supply chain of the API based on the GTG inventory of each chemical. As stated previously, the GTG production of the API uses nearly half of the CTG energy. The fermentation step consumes 45% of the total CTG energy. Table 5.5 shows which processes or chemicals use the most energy in the CTG production of the API. Fermentation nutrients, such as corn, dextrose, cornstarch, soybean, soy meal, and soy flour account for 41% of the total CTG energy. The remaining energy is consumed in the production of the remaining chemicals in the CTG inventory.

Table 5.4. Cradle-to-Gate Vancomycin Hydrochloride Production Energy for 1000 kg Vancomycin Hydrochloride

				Energy with allocation, MJ/ 1000kg Vancomycin HCl[a]							
Chemicals	**Mass, kg[b]**	**By-products, kg/kg chemical[c]**	**Allocation factor[d]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Potential recovery[e]**	**Total net energy**	**% of Total net energy**
Vancomycin HCl	1,000		1.000	2.37E+04	0	2.48E+05	0	440	-4.85E+04	2.24E+05	46.65%
Ammonia	2,368	1.18 kg Carbon dioxide	0.459	761	0	9,781	1.07E+04	1,042	-9,944	1.24E+04	2.58%
Natural gas	799		1.000	0	0	0	2,726	0	0	2,726	0.57%
Nitrogen from air	1,499	0.358 kg Oxygen from air	0.736	0	0	0	0	0	0	0	0.00%
Oxygen from air	1,284	2.79 kg Nitrogen from air	0.264	0	0	0	0	0	0	0	0.00%
Water for reaction	1,861	0.0000 kg Water	1.00	1.50	0	0	0	0	0	1.50	0.00%
Ammonium chloride	1,132	0.961 kg Sodium carbonate	0.510	227	0	3,203	0	498	-57.7	3,871	0.81%
Carbon dioxide	1,530	0.848 kg Ammonia	0.541	492	0	6,321	6,925	673	-6,427	7,985	1.66%
Sodium chloride	656		1.000	2.96	0	3,193	52.8	289	0	3,537	0.74%
Dextrose	1.21E+04		1.000	569	0	1.45E+05	859	5,323	-8,106	1.44E+05	29.99%
corn starch	1.16E+04	0.329 kg corn fiber; 0.0801 kg corn germ; 0.156 kg corn gluten	0.639	1,249	0	1.10E+04	2.51E+04	5,121	-7,371	3.51E+04	7.32%

Table 5.4 continued

				Energy with allocation, MJ/ 1000kg Vancomycin HCl[a]							
Chemicals	**Mass, kg[b]**	**By-products, kg/kg chemical[c]**	**Allocation factor[d]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Potential recovery[e]**	**Total net energy**	**% of Total net energy**
Corn	1.37E+04		1.000	472	0	0	1.19E+04	2,060	0	1.44E+04	3.01%
K in fertilizer	193		1.000	0	0	0	0	0	0	0	0.00%
Potassium chloride	387		1.00	57.3	0	88.4	0	170	-18.8	297	0.06%
Sylvinite ore	1,135		1.000	37.2	0	0	21.3	151	0	210	0.04%
N in fertilizer	313		1.000	0	0	0	0	0	0	0	0.00%
N in DAP	31.0	1.10 kg P in DAP	0.475	0	0	0	0	0	0	0	0.00%
DAP	632		1.000	49.6	0	139	0	278	0	466	0.10%
Phosphoric acid	619	0.0849 kg Fluorosilicic acid	0.922	151	0	1,950	0	273	-820	1,554	0.32%
Phosphate rock	1,343	0.0550 kg Phosphate rock large	0.948	169	0	0	699	591	-272	1,187	0.25%
Sulfuric acid	1,226		1.000	0.0926	0	884	0	540	-390	1,034	0.22%
Sulfur trioxide	996	0.989 kg Sulfur dioxide; 0.506 kg Sulfuric acid	0.401	505	0	190	558	438	-4,097	-2,407	-0.50%
Sulfur	429	already allocated	1.00	0	0	0	2,104	189	0	2,293	0.48%
Urea	1,450		1.000	1,914	0	0	0	638	0	2,551	0.53%
P in fertilizer	248		1.000	0	0	0	0	0	0	0	0.00%

Table 5.4 continued

				Energy with allocation, MJ/ 1000kg Vancomycin HCl[a]							
Chemicals	**Mass, kg[b]**	**By-products, kg/kg chemical[c]**	**Allocation factor[d]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Potential recovery[e]**	**Total net energy**	**% of Total net energy**
P in DAP	248	0.905 kg N in DAP	0.525	0	0	0	0	0	0	0	0.00%
Hydrogen chloride	19.4	1.71 kg Vinyl Chloride	0.368	0.841	0	7.98	25.7	8.52	-25.0	18.0	0.00%
Chlorine	14.0	0.0295 kg Hydrogen; 1.18 kg Sodium hydroxide	0.453	79.0	0	0	0	6.14	-2.85	82.3	0.02%
Ethylene	5.50	0.480 kg C4 stream; 0.0881 kg fuel oil; 0.0484 kg Hydrogen; 0.569 kg Methane; 0.634 kg Propylene; 1.03 kg pyrolysis gas	0.260	7.82	0	13.0	63.7	2.42	-15.6	71.4	0.01%

Table 5.4 continued

				Energy with allocation, MJ/ 1000kg Vancomycin HCl[a]							
Chemicals	Mass, kg[b]	By-products, kg/kg chemical[c]	Allocation factor[d]	Electricity	Dowtherm	Steam	Fuel, Non-transport	Fuel, Transport	Potential recovery[e]	Total net energy	% of Total net energy
Naphtha	145	1.55 kg heavy gas oil, from distillation; 0.644 kg kerosene, from distillation; 0.542 kg light gas oil, from distillation; 0.711 kg residuum, from distillation	0.225	34.7	0	16.3	287	0	0	338	0.07%
Sodium hydroxide	21.2	0.848 kg Chlorine; 0.0250 kg Hydrogen	0.534	120	0	0	0	9.32	-4.32	125	0.03%
Isopropanol	100		1.000	4.80	0	3,040	0	44.0	-160	2,929	0.61%
Propylene	92.0	0.756 kg C4 stream; 1.58 kg Ethylene; 0.139 kg fuel oil; 0.0762 kg Hydrogen; 0.898 kg Methane; 1.63 kg pyrolysis gas	0.165	131	0	218	1,065	40.5	-260	1,194	0.25%

Table 5.4 continued

				Energy with allocation, MJ/ 1000kg Vancomycin HCl[a]							
Chemicals	Mass, kg[b]	By-products, kg/kg chemical[c]	Allocation factor[d]	Electricity	Dowtherm	Steam	Fuel, Non-transport	Fuel, Transport	Potential recovery[e]	Total net energy	% of Total net energy
Soy Flour	4,625		1.000	4,374	0	2,238	0	2,035	-264	8,383	1.75%
Soy meal	4,829	0.234 kg Soybean oil	0.811	83.2	0	1,198	1,086	0	0	2,367	0.49%
n-Hexane	46.0	1.63 kg C5 from naphtha; 4.61 kg C7 from Naphtha	0.138	1.45E-03	0	32.7	0	20.2	-3.99	49.0	0.01%
Soybean	5,479	0.0453 kg Soybean Seed	0.957	85.0	0	0	6,795	2,411	0	9,290	1.94%
Soybean Seed	158		1.000	0	0	0	0	0	0	0	0.00%
Total energy				3.53E+04	0	4.37E+05	7.09E+04	2.33E+04	-8.67E+04	4.80E+05	

[a] Amount of energy used cradle-to-gate to produce mass of chemical used in inventory. [b] Amount used cradle-to-gate to produce 1000 kg product.
[c] By-products generated during the gate-to-gate manufacture of chemical.
[d] Mass allocation is used to distribute the inputs, energy, and emissions to each product formed in that gate-to-gate inventory. Allocation factor will be less than 1.0 when by-products are generated.
[e] Energy that can be recovered from sources requiring cooling.
*The elemental fertilizers, N, P, K are the notations used in agriculture. The actual fertilizers are DAP, potassium chloride, ammonia, and urea.

Table 5.5. CTG Energy by Process or Chemical for 1000 kg Vancomycin Hydrochloride

Process	MJ/1000kg Vancomycin HCl	% of Total
Fermentation (Sterilization, Agitation, Blower)	253,033	44.7%
Sterilization (Total)	230,181	40.6%
Fermentor 1	618	
Fermentor 2	12,352	
Fermentor 3	217,212	
Agitation (Total)	22,725	4.0%
Fermentor 1	28	
Fermentor 2	349	
Fermentor 3	22,348	
Blower (Total)	124	0.02%
Fermentor 1	0.05	
Fermentor 2	0.82	
Fermentor 3	123	
Separation of Vancomycin	17,303	3.1%
Recovery of Vancomycin HCl	1,428	0.3%
Corn	14,427	2.5%
Dextrose (& Cornstarch) from Corn	194,409	34.3%
Soybean	9,290	1.6%
Soy Flour (& Soy meal) from Soybean	11,014	1.9%
Solvent Chemicals for Vancomycin GTG	19,089	4.0%
Other Chemicals in CTG	65,414	7.5%
Total	566,318	100%

As highlighted in Table 5.5, the fermentation process includes 3 steps: sterilization, agitation, and aeration. The largest energy user is sterilization as the three fermentors and the contents must be sterilized by heating to 120 ºC for 15 minutes with steam. The contents are then cooled to 30 ºC and held at 30 ºC for a day or more for fermentation. The fermentors are continuously stirred during each step, and air is sparged through the fermentation broth, accounting for more energy, usually electrical. Of the electrical energy consumption in the fermentation processes, 65% comes from agitation and aeration. This is consistent with other fermentation processes (Shields and Kao, 1994).

Separation and recovery processes use 3.4% of the cradle-to-gate energy, while the solvent chemicals account for 4%. (See Table 5.6) This contrasts with results from other pharmaceutical life cycle inventories showing solvent usage to consume up to 60% of the CTG energy (Jimenez-Gonzalez et al., 2004). In this process, ammonia, isopropanol, and hydrogen chloride were used as adsorption solvents, and ammonium chloride and urea for crystallization.

Table 5.6. Solvent Energy for 1000kg Vancomycin Hydrochloride

Solvents		**Mass, kg**	**Energy, MJ/1000kg VancomycinHCl**
Adsorption Solvents	Aq. Ammonia	1000	12,356
	Isopropanol	100	293
	Hydrogen Chloride	10	18.0
Crystallization Solvents	Ammonium Chloride	1132	3871
	Urea	1200	2551
Total Energy			19,089

The total CTG emissions listed in Table 5.7 come from chemical losses, energy-related emissions, and transportation-related emissions from each GTG inventory, and depending on the physical state, are listed as air, liquid, or solid emissions. These emissions do not include the effect of waste management processes. Process emissions only include the chemical losses from each GTG inventory. Carbon dioxide was the largest contributor to air emissions at 57,200 kg per 1000 kg API, primarily due to energy-related emissions. Total water emissions were 8,508 kg and total solid emissions were 10,680 kg per 1000 kg API.

Table 5.7. Emissions from CTG Production of 1000 kg Vancomycin Hydrochloride

	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Emissions
Air Emissions			
1,3-butadiene	1.93E-02	1.93E-02	1.09E-03kg from Ethylene, 1.82E-02kg from Propylene,
2,2-Dimethylpentane	2.75E-03	2.75E-03	2.75E-03kg from n-Hexane,
2-Methylpentane	9.80E-03	9.80E-03	9.80E-03kg from n-Hexane,
3-Methylpentane	9.50E-03	9.50E-03	9.50E-03kg from n-Hexane,
Acetylene	2.59E-03	2.59E-03	1.46E-04kg from Ethylene, 2.44E-03kg from Propylene,
Ammonia	4.80E+01	4.80E+01	5.20E+00kg from Vancomycin HCl, 6.98E+00kg from Ammonia, 4.51E+00kg from Carbon dioxide, 2.16E+01kg from Corn, 5.05E-01kg from DAP, 9.28E+00kg from Urea,
Ammonium chloride	8.97E+00	8.97E+00	8.97E+00kg from Vancomycin HCl,
Argon	2.38E+01	2.38E+01	1.44E+01kg from Ammonia, 9.33E+00kg from Carbon dioxide,
Benzene	5.35E-03	5.35E-03	3.12E-05kg from Naphtha, 5.32E-03kg from n-Hexane,
Butane	1.20E-02	1.20E-02	5.45E-04kg from Ethylene, 2.31E-03kg from Naphtha, 9.11E-03kg from Propylene,
Butene	3.34E-02	3.34E-02	1.89E-03kg from Ethylene, 3.15E-02kg from Propylene,
C5 from naphtha	1.69E-01	1.69E-01	1.69E-01kg from n-Hexane,
C7 from Naphtha	2.49E-01	2.49E-01	2.49E-01kg from n-Hexane,
Carbon dioxide	5.72E+04	1.63E+04	1.58E+04kg from Vancomycin HCl, 5.71E+01kg from Ammonia, 2.12E-01kg from Natural gas, 2.40E+02kg from Ammonium chloride, 3.69E+01kg from Carbon dioxide, 5.78E+01kg from Phosphoric acid, 1.25E+02kg from Sulfur, 5.36E+00kg from Urea, 4.39E+00kg from Naphtha,
Carbon monoxide	4.21E+01	5.44E+00	3.15E+00kg from Ammonia, 2.21E-01kg from Natural gas, 2.04E+00kg from Carbon dioxide, 3.53E-02kg from Sulfur, 8.25E-06kg from Ethylene, 1.38E-04kg from Propylene,

Table 5.7 continued

	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Emissions
Chlorine	7.03E-01	7.03E-01	9.84E-03kg from Sodium chloride, 6.94E-02kg from Hydrogen chloride, 2.48E-01kg from Chlorine, 3.76E-01kg from Sodium hydroxide,
Cyclohexane	2.24E-02	2.24E-02	2.24E-02kg from n-Hexane,
Dichloroethane,-1,2	3.03E-01	3.03E-01	3.03E-01kg from Hydrogen chloride,
Diisopropyl Ether	6.00E-01	6.00E-01	6.00E-01kg from Isopropanol,
Dimethylbutane, -2,3	4.29E-03	4.29E-03	4.29E-03kg from n-Hexane,
Ethane	3.18E-02	3.18E-02	1.68E-03kg from Ethylene, 1.99E-03kg from Naphtha, 2.82E-02kg from Propylene,
Ethylene	3.54E-01	3.54E-01	2.74E-02kg from Hydrogen chloride, 7.14E-03kg from Ethylene, 2.00E-01kg from Isopropanol, 1.19E-01kg from Propylene,
Heptane	3.62E-03	3.62E-03	3.62E-03kg from Naphtha,
Hydrogen	5.50E+00	5.50E+00	3.34E+00kg from Ammonia, 2.16E+00kg from Carbon dioxide, 1.40E-03kg from Chlorine, 3.37E-04kg from Ethylene, 2.12E-03kg from Sodium hydroxide, 5.64E-03kg from Propylene,
Hydrogen chloride	5.78E-01	5.78E-01	5.42E-01kg from Vancomycin HCl, 3.57E-02kg from Hydrogen chloride, 7.56E-05kg from Chlorine, 1.15E-04kg from Sodium hydroxide,
Hydrogen fluoride	7.31E-05	7.31E-05	7.31E-05kg from Phosphoric acid,
Hydrogen sulfide	4.28E-01	4.28E-01	4.28E-01kg from Sodium chloride,
Hypochlorous acid	4.88E-04	4.88E-04	1.94E-04kg from Chlorine, 2.94E-04kg from Sodium hydroxide,
Isobutane	1.25E-04	1.25E-04	1.25E-04kg from Naphtha,
Isopropanol	1.20E+01	1.20E+01	1.00E+01kg from Vancomycin HCl, 2.00E+00kg from Isopropanol,
Methane	9.88E+01	1.67E+01	2.42E+00kg from Ammonia, 1.12E+01kg from Natural gas, 1.57E+00kg from Carbon dioxide, 1.38E+00kg from Sulfur, 3.94E-03kg from Ethylene, 9.49E-02kg from Naphtha, 6.58E-02kg from Propylene,
Methylcyclopentane	2.64E-02	2.64E-02	2.64E-02kg from n-Hexane,

Table 5.7 continued

	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Emissions
Naphtha	1.95E+00	1.95E+00	1.10E-01kg from Ethylene, 1.84E+00kg from Propylene,
n-Hexane	4.60E+01	4.60E+01	3.09E-03kg from Naphtha, 4.60E+01kg from Soy meal, 4.78E-02kg from n-Hexane,
Nitrogen dioxide	9.64E+00	9.64E+00	5.86E+00kg from Ammonia, 3.79E+00kg from Carbon dioxide,
Nitrogen monoxide	6.30E+00	6.30E+00	3.83E+00kg from Ammonia, 2.47E+00kg from Carbon dioxide,
Nitrous oxide	3.05E+00	3.05E+00	3.05E+00kg from Corn,
NMVOC	1.81E+02	4.05E+00	3.53E-01kg from Natural gas, 3.69E+00kg from Sulfur, 6.86E-04kg from Naphtha,
NOx	1.68E+02	2.02E+00	7.71E-01kg from Natural gas, 1.25E+00kg from Sulfur,
n-Pentane	1.75E-03	1.75E-03	1.75E-03kg from Naphtha,
Octane	2.71E-03	2.71E-03	2.71E-03kg from Naphtha,
Particulate matter	1.60E+01	1.60E+01	1.60E+01kg from Phosphate rock,
Propane	3.14E-03	3.14E-03	1.42E-06kg from Ethylene, 3.12E-03kg from Naphtha, 2.37E-05kg from Propylene,
Propylene	9.32E+00	9.32E+00	1.80E-02kg from Ethylene, 9.00E+00kg from Isopropanol, 3.01E-01kg from Propylene,
Propyne	2.32E-03	2.32E-03	1.31E-04kg from Ethylene, 2.18E-03kg from Propylene,
pyrolysis gas	2.63E-01	2.63E-01	1.49E-02kg from Ethylene, 2.48E-01kg from Propylene,
SOx	1.72E+02	2.01E+01	8.87E-01kg from Natural gas, 1.84E+01kg from Sulfur trioxide, 7.84E-01kg from Sulfur,
Soybean oil	9.88E+00	9.88E+00	9.88E+00kg from Soy meal,
Sulfur	2.05E+00	2.05E+00	2.05E+00kg from Sulfur trioxide,
Sulfur dioxide	1.73E-01	1.73E-01	1.73E-01kg from corn starch,
Sulfur trioxide	5.96E+00	5.96E+00	5.96E+00kg from Sulfuric acid,
Urea	4.04E+00	4.04E+00	2.03E+00kg from Vancomycin HCl, 2.02E+00kg from Urea,
Vinyl Chloride	6.11E-02	6.11E-02	6.11E-02kg from Hydrogen chloride,

Table 5.7 continued

	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Emissions
Total Air emissions	5.81E+04	1.66E+04	1.58E+04kg from Vancomycin HCl, 9.71E+01kg from Ammonia, 1.36E+01kg from Natural gas, 2.40E+02kg from Ammonium chloride, 6.28E+01kg from Carbon dioxide, 4.38E-01kg from Sodium chloride, 1.73E-01kg from corn starch, 2.46E+01kg from Corn, 5.05E-01kg from DAP, 5.78E+01kg from Phosphoric acid, 1.60E+01kg from Phosphate rock, 5.96E+00kg from Sulfuric acid, 2.04E+01kg from Sulfur trioxide, 1.33E+02kg from Sulfur, 1.67E+01kg from Urea, 4.96E-01kg from Hydrogen chloride, 2.49E-01kg from Chlorine, 1.60E-01kg from Ethylene, 4.50E+00kg from Naphtha, 3.78E-01kg from Sodium hydroxide, 1.18E+01kg from Isopropanol, 2.67E+00kg from Propylene, 5.58E+01kg from Soy meal, 5.46E-01kg from n-Hexane,
Water Emissions			
Ammonia	1.03E+03	1.03E+03	1.02E+03kg from Vancomycin HCl, 3.46E+00kg from Ammonium chloride,
Ammonium chloride	1.05E+03	1.05E+03	1.05E+03kg from Vancomycin HCl,
Arsenic	1.11E-06	1.11E-06	1.11E-06kg from Naphtha,
Atrazine	3.16E-02	3.16E-02	3.16E-02kg from Corn,
BaSO4	1.18E-01	1.18E-01	4.68E-02kg from Chlorine, 7.09E-02kg from Sodium hydroxide,
Benzene	2.60E-05	2.60E-05	2.60E-05kg from Naphtha,
BOD	3.19E+00	1.05E-04	1.05E-04kg from Natural gas,
BOD5	8.63E-02	8.63E-02	8.63E-02kg from Sulfur,
Boron	5.47E-04	5.47E-04	5.47E-04kg from Naphtha,
Calcium carbonate	5.02E-02	5.02E-02	1.99E-02kg from Chlorine, 3.02E-02kg from Sodium hydroxide,
Calcium dichloride	1.22E-02	1.22E-02	1.22E-02kg from Vancomycin HCl,
Chloride	4.04E-01	4.04E-01	4.04E-01kg from Naphtha,
COD	2.64E+01	1.84E-01	1.45E-03kg from Natural gas, 1.82E-01kg from Sulfur,

Table 5.7 continued

	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Emissions
DAP	4.17E+00	4.17E+00	4.17E+00kg from DAP,
Diisopropyl Ether	1.40E+00	1.40E+00	1.40E+00kg from Isopropanol,
grease / oil	6.57E-03	6.57E-03	6.57E-03kg from Naphtha,
Hydrogen chloride	2.42E+01	2.42E+01	2.42E+01kg from Vancomycin HCl,
Isopropanol	1.03E+02	1.03E+02	1.00E+02kg from Vancomycin HCl, 3.10E+00kg from Isopropanol,
Magnesium hydroxide	8.44E-03	8.44E-03	3.35E-03kg from Chlorine, 5.09E-03kg from Sodium hydroxide,
Magnesium Sulfate	2.22E-01	2.22E-01	2.22E-01kg from Vancomycin HCl,
Malt Extract	6.35E-03	6.35E-03	6.35E-03kg from Vancomycin HCl,
Mercury	8.81E-06	8.81E-06	3.50E-06kg from Chlorine, 5.31E-06kg from Sodium hydroxide,
Mobile ions	1.27E+00	1.27E+00	1.27E+00kg from Naphtha,
Nitrate-N	8.80E+00	8.80E+00	8.80E+00kg from Corn,
Peptone	2.33E-02	2.33E-02	2.33E-02kg from Vancomycin HCl,
Phosphate-P	8.56E-01	8.56E-01	8.56E-01kg from Corn,
Potassium chloride	4.57E+01	4.57E+01	4.57E+01kg from Potassium chloride,
pyrolysis gas	2.10E-03	2.10E-03	1.18E-04kg from Ethylene, 1.98E-03kg from Propylene,
Sodium	5.20E-01	5.20E-01	5.20E-01kg from Naphtha,
Sodium chloride	1.07E+02	1.07E+02	5.90E+01kg from Sodium chloride, 4.84E+01kg from Potassium chloride,
Soy Flour	4.62E+03	4.62E+03	4.62E+03kg from Vancomycin HCl,
Sulfuric acid	3.59E+01	3.59E+01	3.59E+01kg from Isopropanol,
TDS	1.66E+02	5.29E-01	9.03E-02kg from Natural gas, 4.38E-01kg from Sulfur,
Urea	1.20E+03	1.20E+03	1.20E+03kg from Vancomycin HCl,
Vancomycin	3.18E+01	3.18E+01	3.18E+01kg from Vancomycin HCl,
Vancomycin HCl	5.26E+01	5.26E+01	5.26E+01kg from Vancomycin HCl,
Yeast Extract	6.35E-03	6.35E-03	6.35E-03kg from Vancomycin HCl,

Table 5.7 continued

	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Emissions
Total Water emissions	8.51E+03	8.31E+03	8.10E+03kg from Vancomycin HCl, 9.19E-02kg from Natural gas, 3.46E+00kg from Ammonium chloride, 5.90E+01kg from Sodium chloride, 9.69E+00kg from Corn, 9.41E+01kg from Potassium chloride, 4.17E+00kg from DAP, 7.07E-01kg from Sulfur, 7.00E-02kg from Chlorine, 1.18E-04kg from Ethylene, 2.20E+00kg from Naphtha, 1.06E-01kg from Sodium hydroxide, 4.04E+01kg from Isopropanol, 1.98E-03kg from Propylene,
Solid Emissions			
Calcium dichloride	1.23E-05	1.23E-05	1.23E-05kg from Vancomycin HCl,
Cell Mass	5.39E+03	5.39E+03	5.39E+03kg from Vancomycin HCl,
Clay	3.41E+01	3.41E+01	3.41E+01kg from Potassium chloride,
corn starch	7.80E+02	7.80E+02	7.80E+02kg from Dextrose,
debris from corn	7.00E+01	7.00E+01	7.00E+01kg from corn starch,
Diatomaceous earth	5.14E+01	5.14E+01	5.14E+01kg from Vancomycin HCl,
Glucoamylase	1.21E+01	1.21E+01	1.21E+01kg from Dextrose,
Herbicide	9.45E+00	9.45E+00	9.45E+00kg from Soybean,
Hydrogen fluoride	1.46E-02	1.46E-02	1.46E-02kg from Phosphoric acid,
Impurities	3.09E+01	3.09E+01	3.09E+01kg from Phosphoric acid,
lime	3.84E+00	3.84E+00	3.84E+00kg from Phosphoric acid,
Magnesium Sulfate	2.22E-04	2.22E-04	2.22E-04kg from Vancomycin HCl,
Malt Extract	6.36E-06	6.36E-06	6.36E-06kg from Vancomycin HCl,
Mud (salt process)	1.26E+02	1.26E+02	1.26E+02kg from Sodium chloride,
Organic Matter	1.10E+02	1.10E+02	1.10E+02kg from Soy meal,
Peptone	2.33E-05	2.33E-05	2.33E-05kg from Vancomycin HCl,
Phosphate rock	3.54E+02	3.54E+02	3.54E+02kg from Phosphate rock,
Phosphate rock (pure)	7.58E+01	7.58E+01	7.58E+01kg from Phosphoric acid,
Phosphogypsum	1.97E+03	1.97E+03	1.97E+03kg from Phosphoric acid,
Phosphoric acid	2.31E+01	2.31E+01	2.31E+01kg from Phosphoric acid,
Potassium chloride	4.39E+01	4.39E+01	4.39E+01kg from Potassium chloride,
Silica	4.02E+01	4.02E+01	4.02E+01kg from Phosphoric acid,
Sodium chloride	6.14E+02	6.14E+02	3.63E+01kg from Dextrose, 5.78E+02kg from Potassium chloride,

Table 5.7 continued

	Total Emissions, kg	Process Emissions, kg	Chemicals Contributing to Emissions
Solid waste	3.58E+02	5.48E+00	2.91E+00kg from Natural gas, 3.91E-01kg from Water for reaction, 2.18E+00kg from Sulfur, 1.06E-03kg from Naphtha,
Soy Flour	4.63E+00	4.63E+00	4.63E+00kg from Vancomycin HCl,
Soy Hulls	3.74E+02	3.74E+02	3.74E+02kg from Soy meal,
Soybean	1.99E+02	1.99E+02	1.99E+02kg from Soybean,
starch suppressant	1.59E+00	1.59E+00	1.59E+00kg from Potassium chloride,
Sulfuric acid	1.75E-01	1.75E-01	1.75E-01kg from Phosphoric acid,
Vancomycin	2.08E+00	2.08E+00	2.08E+00kg from Vancomycin HCl,
Yeast Extract	6.36E-06	6.36E-06	6.36E-06kg from Vancomycin HCl,
Total Solid emissions	1.07E+04	1.03E+04	5.45E+03kg from Vancomycin HCl, 2.91E+00kg from Natural gas, 3.91E-01kg from Water for reaction, 1.26E+02kg from Sodium chloride, 8.28E+02kg from Dextrose, 7.00E+01kg from corn starch, 6.58E+02kg from Potassium chloride, 2.15E+03kg from Phosphoric acid, 3.54E+02kg from Phosphate rock, 2.18E+00kg from Sulfur, 1.06E-03kg from Naphtha, 4.83E+02kg from Soy meal, 2.09E+02kg from Soybean,

5.6 Conclusions and Future Work

Performing a life cycle inventory provides a more complete picture of energy and raw material usage for manufacture of a product tracing back to the cradle, or the natural resources, and it highlights areas that can be targeted for improvement to get the most impact on reducing the environmental performance. The LCI for this batch fermentation process shows different results than other pharmaceuticals studied. Fermentation is actually the largest consumer of raw materials and energy in the cradle-to-gate manufacture of vancomycin hydrochloride. Specifically, sterilization and fermentation nutrient production each consume 41% of the total CTG energy due to the low product yield. In the synthetic production of sertraline, solvent usage was more important. Energy consumption is the largest contributor to the emissions generated.

To reduce energy and raw material consumption, other fermentation methods should be investigated, such as continuous culture fermentation, using solid substrates instead of aqueous media, and using bacteria strains that give higher product yields. Synthetic manufacture could also be investigated; however, this may increase solvent usage, and water may be replaced with more hazardous solvents. Improving the GTG vancomycin yield by just 10% can reduce the cradle-to-gate energy consumption by 4% and the CTG raw material consumption by 6%. Other sterilization techniques, such as continuous sterilization, should be investigated to reduce the energy required for this step. A 10% reduction in sterilization steam energy yields a 4% reduction in the overall CTG energy consumption.

The life cycle inventory of vancomycin hydrochloride will be incorporated in the life cycle inventory of treating a hospital-acquired MRSA infection. This work can be extended to include life cycle inventories of several different carbon and nitrogen sources for fermentation to allow microbiologists to select nutrient raw materials with the smallest environmental profile. The LCI results of the nutrient database can then be weighed against product yield obtained from using different nutrient sources, as different nutrient sources may provide a different yield of vancomycin.

5.7 Acknowledgements

This work was supported by a National Science Foundation Materials Use: Science, Engineering, and Society (NSF-MUSES) grant (#0424514). The authors would like to thank Dr. Michael Flickinger at North Carolina State University for his invaluable input to this research in the area of microbiology and Drs. Evan Griffing and Yong Li for sharing their knowledge in the area of life cycle inventory analysis.

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6. Cradle-to-Gate Life Cycle Inventory of Treating a Hospital-Acquired MRSA Infection

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6. Cradle-to-Gate Life Cycle Inventory of Treating a Hospital-Acquired MRSA Infection

Abstract

When a patient contracts an infection, materials are used to test the patient, to provide contact isolation, and to treat the patient. All of these materials have environmental consequences. The results from a cradle-to-gate life cycle inventory analysis for treating a hospital-acquired infection are presented, including all raw material and energy consumption and emissions generated for the products used. Due to the use of disposable gowns and gloves, contact isolation uses the most raw material and energy resources and generates the most emissions. Fabric manufacture for the disposable gowns alone accounts for 38% of the CTG energy consumption for treating an infection. Energy use is the largest contributor to raw material consumption and emissions generation. Improving the efficiency of the fabric manufacturing process or using reusable gowns should be investigated. Preventing or reducing the rate of infections would also reduce the yearly environmental impact of treating infections.

Keywords: Life cycle inventory; environmental; nosocomial infection; MRSA; energy; emissions

6.1 Introduction

The healthcare industry is becoming increasingly aware of its environmental impact. In 2000, an environmental audit was conducted at University Hospital in Germany (Dettenkofer et al., 2000); the US EPA and the American Hospital Association also partnered that year to form Hospitals for a Healthy Environment (H2E) with aims of reducing total solid waste and toxic waste; and in 2001, an ecological footprint of Lionsgate Hospital in British Colombia was conducted (Germain, 2000). Each year, hospitals use 2931 MJ of energy per patient per day and generate 11 kg solid waste per patient per day (Hospitals for a Healthy Environment, Garvin, 1995). Once the environmental footprint is known, areas can be addressed to reduce it. One area is to prevent conditions, such as nosocomial infections, that necessitate or increase a patient's hospital stay.

When a patient contracts an infection while in the hospital, in addition to the economic costs, the products used to test and treat the patient impact the environment in natural resource costs, energy consumed, and emissions generated. After a patient acquires an infection in a hospital, the patient is tested, placed in contact isolation that requires healthcare workers and visitors to wear protective clothing, and the patient receives drug therapy. All of this treatment and required personnel is in addition to the normal medical treatment for which the patient entered the hospital. The life cycle inventory (LCI) is a tool that can be used to quantify the environmental impact of the acquisition and treatment of these infections. The results will be used in a future study to compare the environmental costs of preventing an infection utilizing a reusable medical patient gown containing a biocidal finish versus treating an infection using the procedures outlined in this paper.

A life cycle assessment (LCA) is a "methodological framework for estimating and assessing the environmental impacts attributable to the life cycle of a product" (Hendrickson et al., 2006). ISO 14040 outlines the requirements for conducting life cycle inventory and assessment studies (International Standard Organization, 1997). The backbone of the LCA is the life cycle inventory, or a compilation of all inputs, outputs, and energy use of a product from resource extraction, manufacture, product use, recycling, and disposal (Rebitzer et al., 2004). A life cycle inventory gives the complete environmental picture of a product, and can highlight where changes can be made to make the most impact on reducing resource consumption and emissions generated.

6.2 Goal and Scope of the Study

The intent of this work is to analyze the cradle-to-gate (CTG) life cycle inventory for treating a hospital-acquired infection – MRSA (Methicillin-resistant Staphylococcus aureus) – with vancomycin hydrochloride. The study scope starts from extracting the natural resources (cradle) and spans through treating an infection in the hospital (gate).

The functional unit, or basis, is treating one thousand hospital-acquired infections for a ten-day period.

In this study, the life cycle inventory (LCI) begins with a baseline of patients requiring hospitalization; a portion is severely ill (e.g., ICU, end-stage disease, etc.) and a large number have less life-threatening conditions (e.g., common surgery like gall bladder, obstetrics, etc.). In this study, some of the hospital patients who arrive infection-free contract a nosocomial infection that extends their hospital stay and places an increased demand on materials, supplies, and pharmaceuticals. There is a range of nosocomial infections (e.g., coagulase-negative staphylococci, staphylococcus aureus, enterococcus species, candida, Escherichia coli, etc.) (Hidron et al., 2008), but MRSA has been selected for this study. The LCI impact of contracting and being treated for a nosocomial infection is based only on the incremental items resulting from the treatment of the nosocomial infection during the extended stay, and not the entire hospital stay that includes treatment for the original hospitalized condition. That is, the patient bed would be occupied (at typical occupancy rating) whether the nosocomial-infected patient was there or not (although with a new patient, a new billing cycle would begin). Thus the LCI is solely aimed at the environmental consequences of the nosocomial infection. An economic analysis of treating nosocomial infections is outside of the scope of this work, but has been studied by others previously (Scott, 2009, Roberts et al., 2003, Engemann et al., 2003, Kim, 2001, Abramson and Sexton, 1999, Rubin et al., 1999, Wenzel, 1995, Wakefield et al., 1988).

6.3 Methodology

To begin the LCI, all chemical and product inputs for the infection treatment component of the hospital stay are determined. For each of these chemicals and products, transparent gate-to-gate (within the factory) inventories are completed. The design-based methodology developed by Jimenez-Gonzalez (Jimenez-Gonzalez, 2000) utilizing process flow diagrams and engineering design principles is used to collect inventory data (for mass and energy balances) for each gate-to-gate inventory incorporated to complete the final CTG inventory. Similar to laboratory experiments, every LCI completed follows a similar procedure. Information gathered from articles, books, patents, company websites, and consultations with experts in the field is then used with established process design heuristics to arrive at the LCI results.

For the infection treatment LCI, the patient scenario begins with the occurrence of a MRSA nosocomial infection that is identified from many of the known methods covered in the literature (Brown et al., 2005, Velasco et al., 2005, Cauwelier et al., 2004, Stevenson et al., 2003, Kunori et al., 2002, Walsh et al., 2001). A single screening test using a disk diffusion plate confirms the MRSA nosocomial infection. The patient is then isolated and defined to be contact isolated (Muto et al., 2003). This new isolation status changes the procedures used by all who enter the patient's area in the following ways,

1. All visitors and staff now put on gloves when crossing the threshold of the patient area (with some exceptions described below) and
2. All staff with substantial patient contact (e.g., laboratory technicians taking samples; nursing staff providing patient care like turning patients, peripheral IV, injections, etc.; and family/friends visitors) are required to put on a lightweight disposable gown.

Staff personnel that are just providing salutations in conjunction with good customer care protocols simply speak with the patients and do not use isolation procedures. Therapy for treating the nosocomial infection involves the following items,

1. An antibiotic such as vancomycin is prescribed and administered for a fixed course of ten days. This is administered daily from premixed intravenous infusion bags of approximately 200 ml (Deresinski, 2005, Kollef et al., 2004, Boyce, 2001).
2. Typical staff visitation frequency is as follows:
   a. Extensive visits by staff (technicians taking laboratory samples, nurses providing patient care, doctors) every three hours, excluding six hours of sleep, give a representative patient seven visits per day. These visits average 1.5 people per visit (representing medical students, doctor/nurse visits) giving

eleven person visits per patient day (each requiring a pair of disposable gloves and a disposable gown).

b. Non-extensive visits by staff (administering pills, taking vitals, etc.) every three hours, excluding six hours of sleep, or seven person visits per patient day, each requiring a pair of gloves.

c. Family and friends are estimated at three persons per patient day requiring gloves and gowns.

3. In addition to the initial confirmative nosocomial culture test, over a typical ten-day nosocomial infection treatment period, a weekly routine culture with an additional culture at the end of the established treatment cycle results in a total of three MRSA tests (Siegel et al., 2007).

6.4 Inventory Results and Discussion

The life cycle inventories for a disposable gown and vancomycin were reported previously in Chapters 4 and 5. Inventories for disposable latex gloves and Mueller-Hinton (MH) agar plates, and their supply chain chemicals, were completed for this study. Their chemical trees are shown in Figures 6.1 and 6.2. Figure 6.1 represents a full chemical tree for latex gloves showing all chemicals in the supply chain, while Figure 6.2 is a condensed chemical tree due to the size of the full tree. There are 34 and 42 unique chemicals in the supply chains of the latex gloves and MH agar plates, respectively.

Level 1	Level 2	Level 3	Level 4	Level 5	Level 6	Level 7	Level 8	Level 9	Level 10
Latex Glove	corn starch	Corn	K in fertilizer	Potassium chloride	Sylvinite ore	sylvinite ore (in ground)			
			N in fertilizer	Ammonia	Natural gas	Natural gas (unprocessed)			
					Nitrogen from air	Air (untreated)			
					Oxygen from air	Air (untreated)			
					Water for rxn	Water (untreated)			
				N in DAP	DAP	Ammonia	Natural gas	Natural gas (unprocessed)	
							Nitrogen from air	Air (untreated)	
							Oxygen from air	Air (untreated)	
							Water for rxn	Water (untreated)	
						Phosphoric acid	Phosphate rock	Phosphate rock (in ground)	
								Sand	
								Water for rxn	Water (untreated)
							Sulfuric acid	Sulfur trioxide	Oxygen from air
									Sulfur
									Water for rxn
								Water for rxn	Water (untreated)
							Water for rxn	Water (untreated)	
				Urea	Ammonia	Natural gas	Natural gas (unprocessed)		
						Nitrogen from air	Air (untreated)		
						Oxygen from air	Air (untreated)		
						Water for rxn	Water (untreated)		
					Carbon dioxide	Natural gas	Natural gas (unprocessed)		
						Nitrogen from air	Air (untreated)		
						Oxygen from air	Air (untreated)		
						Water for rxn	Water (untreated)		
			P in fertilizer	P in DAP	DAP	Ammonia	Natural gas	Natural gas (unprocessed)	
							Nitrogen from air	Air (untreated)	
							Oxygen from air	Air (untreated)	
							Water for rxn	Water (untreated)	
						Phosphoric acid	Phosphate rock	Phosphate rock (in ground)	
								Sand	
								Water for rxn	Water (untreated)
							Sulfuric acid	Sulfur trioxide	Oxygen from air
									Sulfur
									Water for rxn
								Water for rxn	Water (untreated)
							Water for rxn	Water (untreated)	
	Styrene butadiene latex	1,3-butadiene	C4 stream	Naphtha	oil (in ground)				
			Hydrogen	Naphtha	oil (in ground)				
				Oxygen	Air (untreated)				
				Oxygen from air	Air (untreated)				
				Water for rxn	Water (untreated)				
		Styrene	Ethylbenzene	Benzene	pyrolysis gas	Naphtha	oil (in ground)		
					reformate, from naphtha	Naphtha	oil (in ground)		
				Ethylene	Naphtha	oil (in ground)			

Figure 6.1. Chemical Tree of Latex Gloves

Level 1	Level 2	Level 3		Natural Resources
MH Agar Plate	Agar	Gelidium Algae	1 chemical	Air, Coal, Crude Oil, Gelidium, Natural gas, Phosphate rock, Salt rock, Sand, Soybean seed, Sylvinite ore, Water
		Sodium carbonate	22 chemicals	
	Casein hydrolysate	Casein	286 chemicals	
	Petri Dish	Polystyrene	12 chemicals	

Figure 6.2. Chemical Tree of Mueller-Hinton Agar Plate

The chemical tree in Figure 6.3 is a condensed version of the full infection treatment chemical tree. The full tree includes all of the chemicals in the supply chain of the final product. The natural resources are on the far right. The condensed version, Figure 6.3, shows the product in the far left column and the chemicals or products that went into the production of the chemicals to the left. To abbreviate the chemical tree, only the first three levels are shown. The number of GTG inventories (or chemicals) that went into the production of the third level chemicals is shown instead. For example, ninety-three chemical life cycle inventories are in the CTG supply chain to manufacture cornstarch. This number includes duplicates, as a chemical input may be used to manufacture more than one chemical product. This life cycle inventory included sixty-five different chemicals and the gate-to-gate inventories that were performed for each of these chemicals. Chemicals added in minor amounts, or ancillary inputs, are not shown in this chemical tree and were not included in these studies (Consoli et al., 1993).

Level 1	Level 2	Level 3		Natural Resources
Infection Treatment	Latex Glove	Corn starch	93 chemicals	Air, Coal, Crude Oil, Gelidium, Natural gas, Phosphate rock, Salt rock, Sand, Soybean seed, Sylvinite ore, Water
		Styrene Butadiene Latex	25 chemicals	
	MH Agar Plate	Agar	25 chemicals	
		Casein hydrolysate	287 chemicals	
		Petri Dish	13 chemicals	
	PVC IV Bag	Vinyl Chloride	15 chemicals	
	SMS Gown	Polypropylene SMS Fabric	4 chemicals	
	Vancomycin HCl	Ammonia	8 chemicals	
		Ammonium chloride	22 chemicals	
		Dextrose	108 chemicals	
		Isopropanol	15 chemicals	
		Soy Flour	99 chemicals	
		Urea	18 chemicals	

Figure 6.3. Chemical tree of Infection Treatment

6.4.1 Raw Materials

As seen in Table 6.1, 219 pairs of gloves, 149 gowns, 20 grams of vancomycin, and 20 PVC IV bags are used to treat one infection. The cradle-to-gate (CTG) life cycle inventory is based upon these products. Tables 6.2 and 6.3 show the total CTG inventory results for the infection treatment. Table 6.2 also lists the CTG inventory results for each product used in the infection treatment, and Table 6.3 shows the inventory results for each phase of treatment – testing, contact isolation, and drug therapy. To treat an infection, 31.2 kg of raw materials are consumed. Crude oil, coal, and natural gas are the largest inputs by mass; contact isolation uses more than 90% of these resources. Gowns and gloves are the largest inputs for the infection treatment inventory and use the most raw materials cradle-to-gate.

Table 6.1. Products Used to Treat One Infection

	Item	Units	Total Mass
Infection Test	MH Agar Plate	3 units	134 g
	Gloves	9 pairs	134 g
	Disposable Gown	9 units	540 g
Treat (Contact Isolation)	Gloves	210 pairs	3129 g
	Disposable Gown	140 units	8400 g
Treat (Therapy)	Vancomycin	20 g	20 g
	Polyvinyl chloride IV Bag	20 units	141 g

Table 6.2. Cradle-to-Gate Life Cycle Inventory for Infection Treatment and Materials Used per 1000 Infections Treated

	Infection Treatment	Latex Glove	MH Agar Plate	PVC	Gown	Vancomycin HCl
Mass Used, kg		3,263.10	134.30	141.00	8,940.00	20.00
Raw material, kg						
Air	90.43	6.25	1.36	27.28	0.00	56.39
Coal	6,072.77	217.81	6.00	35.51	5,780.72	31.02
Crude Oil	14,758.00	3,179.63	52.40	103.34	11,276.87	147.28
Gelidium	4.79	0.00	4.79	0.00	0.00	0.00
Natural gas	9,998.68	1,792.87	39.21	45.47	7,985.08	135.87
Phosphate rock	37.37	1.81	1.62	0.00	0.00	33.94
Salt rock	103.83	0.00	0.20	86.89	0.00	16.74
Sand	1.56	0.08	0.07	0.00	0.00	1.41
Soybean Seed	3.45	0.00	0.07	0.00	0.00	3.38
Sylvinite ore	27.70	1.92	2.19	0.00	0.00	23.59
Water	70.81	2.63	1.42	21.21	0.00	45.55
Total Raw Materials	31,169.37	5,202.99	109.33	319.71	25,042.67	495.16
Energy, MJ						
Electricity	126,478.89	4,536.55	124.57	739.78	120,419.58	622.86
Dowtherm	185,061.07	900.30	25.72	0.00	184,135.05	0.00
Heating steam	84,372.38	45,382.05	745.75	1,138.67	28,284.67	8,797.89
Direct fuel	13,777.18	3,254.43	93.37	82.89	10,026.09	380.24
Natural gas	211,641.29	92,748.15	2,324.12	1,463.22	114,405.35	705.53
Coal	1.47	0.07	0.06	0.00	0.00	1.35
Diesel	38,409.86	10,481.21	292.19	437.68	26,497.84	703.02

Table 6.2 continued

	Infection Treatment	Latex Glove	MH Agar Plate	PVC	Gown	Vancomycin HCl
Undefined	57.35	1.37	0.98	0.00	0.00	54.71
Heavy oil: refinery	13.86	0.64	0.57	0.00	0.00	12.66
Hydro power: refinery	0.10	0.00	0.00	0.00	0.00	0.09
Nuclear power: refinery	0.10	0.00	0.00	0.00	0.00	0.09
Energy input	659,813.55	157,304.77	3,607.34	3,862.24	483,768.57	11,278.44
Cooling water	-231,264.43	-124,301.34	-2,849.03	-4,256.61	-90,840.11	-9,090.22
Refrigeration	75.02	0.00	-1.09	1.72	0.00	71.91
Potential recovery[a]	-114,357.79	-74,877.56	-1,933.69	-821.25	-34,877.76	-1,812.93
Net energy (Input - Potential recovery)	545,455.76	82,427.21	1,673.64	3,040.99	448,890.81	9,465.51
Total Air emissions	49,376.03	5,902.93	114.59	309.84	41,903.78	1,143.69
Total Water emissions	551.11	89.03	3.79	17.13	270.40	144.52
Total Solid emissions	2,133.73	54.64	17.63	24.27	1,820.19	216.60

[a] Energy that can be recovered from sources requiring cooling.

Table 6.3. Cradle-to-Gate Life Cycle Inventory for Infection Treatment and Components of Treatment per 1000 Infections Treated (as defined in Table 6.1)

	CTG Infection Treatment	Infection Testing		Contact Isolation		Therapy	
Raw material, kg	kg	kg	% of CTG Infection Treatment	kg	% of CTG Infection Treatment	kg	% of CTG Infection Treatment
Air	90.43	1.58	2%	5.18	6%	83.67	93%
Coal	6,072.77	364.14	6%	5,640.41	93%	66.53	1%
Crude Oil	14,758.00	863.98	6%	13,644.64	92%	250.62	2%
Gelidium	4.79	4.78	100%	0.00	0%		0%
Natural gas	9,998.68	595.09	6%	9,221.97	92%	181.34	2%
Phosphate rock	37.37	1.69	5%	1.74	5%	33.94	91%
Salt rock	103.83	0.20	0%	0.00	0%	103.63	100%
Sand	1.56	0.07	5%	0.07	5%	1.41	91%
Soybean Seed	3.45	0.07	2%	0.00	0%	3.38	98%
Sylvinite ore	27.70	2.26	8%	1.84	7%	23.59	85%
Water	70.81	1.52	2%	2.52	4%	66.76	94%
Total Raw Materials	31,169.37	1,835.38	6%	28,518.36	91%	814.87	3%
Energy, MJ	MJ	MJ	% of CTG Infection Treatment	MJ	% of CTG Infection Treatment	MJ	% of CTG Infection Treatment
Electricity	126,478.89	7,584.92	6%	117,496.25	93%	1,362.64	1%
Dowtherm	185,061.07	11,184.89	6%	173,876.10	94%	0.00	0%
Heating steam	84,372.38	4,316.73	5%	70,093.89	83%	9,936.56	12%

Table 6.3 continued

	CTG Infection Treatment	Infection Testing		Contact Isolation		Therapy	
Energy, MJ	MJ	MJ	% of CTG Infection Treatment	MJ	% of CTG Infection Treatment	MJ	% of CTG Infection Treatment
Direct fuel	13,777.18	831.24	6%	12,539.81	91%	463.13	3%
Natural gas	211,641.29	13,037.81	6%	196,431.30	93%	2,168.75	1%
Coal	1.47	0.06	4%	0.06	4%	1.35	91%
Diesel	38,409.86	2,321.35	6%	34,946.83	91%	1,140.70	3%
Undefined	57.35	1.04	2%	1.32	2%	54.71	95%
Heavy oil: refinery	13.86	0.59	4%	0.61	4%	12.66	91%
Hydro power: refinery	0.10	0.00	4%	0.00	4%	0.09	91%
Nuclear power: refinery	0.10	0.00	4%	0.00	4%	0.09	91%
Energy input	659,813.55	39,278.64	6%	605,386.18	92%	15,140.69	2%
Cooling water	-231,264.43	-13,432.79	6%	-204,545.26	88%	-13,346.83	6%
Refrigeration	75.02	1.38	2%	0.00	0%	73.64	98%
Potential recovery[a]	-114,357.79	-7,110.05	6%	-104,571.26	91%	-2,634.19	2%
Net energy (Input - Potential recovery)	545,455.76	32,168.59	6%	500,814.92	92%	12,506.50	2%
	kg	kg	% of CTG Infection Treatment	kg	% of CTG Infection Treatment	kg	% of CTG Infection Treatment
Total Air emissions	49,376.03	2,888.10	6%	45,032.99	91%	1,453.53	3%
Total Water emissions	551.11	23.79	4%	339.44	62%	161.65	29%
Total Solid emissions	2,133.73	129.84	6%	1,762.64	83%	240.87	11%

[a] Energy that can be recovered from sources requiring cooling.

In examining the CTG of each input to the infection treatment (e.g., the CTG inventory of producing dextrose), vancomycin has the largest supply chain with 270 chemicals (including duplicates) required for production.

6.4.2 Energy

An evaluation of the cradle-to-gate energy requirements indicates that contact isolation consumes the most energy; contact isolation uses 660 MJ of the 605 MJ of energy used to treat one infection. During chemical manufacturing, a portion of the energy lost due to cooling can be recovered, and when the recovered energy is included, the energy consumption is reduced to 545 MJ. As seen in Table 6.2 and 6.3, natural gas, Dowtherm heating fluid, and electricity are the largest sources of energy. Table 6.4 shows all sixty-five chemicals and the amounts used in the CTG inventory for the infection treatment. The total CTG energy is the summation of each chemical energy utilization, based on the GTG energy and mass consumed. Producing the polypropylene SMS fabric for the medical gowns uses the most energy. The medical gown also contributes the largest mass in the gate-to-gate infection treatment. Drug therapy used the least amount of energy.

Table 6.4. Cradle-to-Gate Energy Consumption per Chemical Used to Treat 1000 Infections

				CTG Energy, MJ/1000 Infections Treated[a]							
Chemicals, gate-to-gate	**Mass, kg[b]**	**By-products, kg/kg chemical[c]**	**Allocation factor[d]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Potential recovery[e]**	**Total net energy**	**% of Total**
Latex Glove	3,263		1.000	35.6	0	1,572	243	1,436	0	3,286	0.60%
corn starch	281	0.329 kg corn fiber; 0.0801 kg corn germ; 0.156 kg corn gluten;	0.639	30.1	0	266	605	124	-178	847	0.16%
Corn	351		1.000	12.1	0	0	304	52.6	0	369	0.07%
K in fertilizer	4.70		1.000	0	0	0	0	0	0	0	0.00%
Potassium chloride	9.45		1.00	1.40	0	2.16	0	4.16	-0.458	7.25	0.00%
Sylvinite ore	27.7		1.000	0.908	0	0	0.521	3.69	0	5.12	0.00%
N in fertilizer	8.02		1.000	0	0	0	0	0	0	0	0.00%
Ammonia	49.9	1.18 kg Carbon dioxide;	0.459	37.2	0	217	189	21.9	-178	287	0.05%
Natural gas	16.8		1.000	0	0	0	57.3	0	0	57.3	0.01%
Nitrogen from air	31.4	0.358 kg Oxygen from air;	0.736	0	0	0	0	0	0	0	0.00%
Oxygen from air	56.8	2.79 kg Nitrogen from air;	0.264	0	0	0	0	0	0	0	0.00%

Table 6.4 continued

				CTG Energy, MJ/1000 Infections Treated[a]							
Chemicals, gate-to-gate	**Mass, kg[b]**	**By-products, kg/kg chemical[c]**	**Allocation factor[d]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Potential recovery[e]**	**Total net energy**	**% of Total**
Water for rxn	62.4	0.0000 kg Water;	1.00	0.0502	0	0	0	0	0	0.0502	0.00%
N in DAP	0.794	1.10 kg P in DAP;	0.475	0	0	0	0	0	0	0	0.00%
DAP	14.6		1.000	1.15	0	3.21	0	6.41	0	10.8	0.00%
Phosphoric acid	14.3	0.0849 kg Fluorosilicic acid;	0.922	3.49	0	45.0	0	6.29	-18.9	35.9	0.01%
Phosphate rock	31.0	0.0550 kg Phosphate rock large;	0.948	5.43	0	4.91	11.0	13.6	-6.28	28.7	0.01%
Sulfuric acid	28.1		1.000	2.12E-03	0	20.2	0	12.4	-8.93	23.7	0.00%
Sulfur trioxide	22.8	0.989 kg Sulfur dioxide; 0.506 kg Sulfuric acid;	0.401	11.6	0	4.35	12.8	10.0	-93.8	-55.1	-0.01%
Sulfur	9.83	already allocated	1.00	0	0	0	48.2	4.33	0	52.5	0.01%
Urea	30.4		1.000	40.1	0	0	0	13.4	-50.8	2.74	0.00%
Carbon dioxide	31.8	0.848 kg Ammonia;	0.541	23.7	0	138	120	14.0	-114	183	0.03%
P in fertilizer	5.65		1.000	0	0	0	0	0	0	0	0.00%
P in DAP	5.65	0.905 kg N in DAP;	0.525	0	0	0	0	0	0	0	0.00%

Table 6.4 continued

				CTG Energy, MJ/1000 Infections Treated[a]							
Chemicals, gate-to-gate	**Mass, kg[b]**	**By-products, kg/kg chemical[c]**	**Allocation factor[d]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Potential recovery[e]**	**Total net energy**	**% of Total**
Styrene butadiene latex	3,215		1.000	470	0	1.35E+04	0	1,415	-4,079	1.13E+04	2.08%
1,3-butadiene	1,122	9.14E-03 kg 1,2-butadiene; 0.980 kg butenes and butanes; 0.0155 kg Propyne;	0.499	8.42	0	5,963	0	494	-1,387	5,078	0.93%
C4 stream	1,129	2.08 kg Ethylene; 0.184 kg fuel oil; 0.101 kg Hydrogen; 1.19 kg Methane; 1.32 kg Propylene; 2.15 kg pyrolysis gas;	0.125	1,604	0	2,670	1.31E+04	497	-3,194	1.46E+04	2.68%

Table 6.4 continued

				CTG Energy, MJ/1000 Infections Treated[a]							
Chemicals, gate-to-gate	**Mass, kg[b]**	**By-products, kg/kg chemical[c]**	**Allocation factor[d]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Potential recovery[e]**	**Total net energy**	**% of Total**
Naphtha	1.35E+04	1.55 kg heavy gas oil, from distillation; 0.644 kg kerosene, from distillation; 0.542 kg light gas oil, from distillation; 0.711 kg residuum, from distillation;	0.225	3,223	0	1,510	2.66E+04	0	0	3.13E+04	5.74%
Hydrogen	0.632		1.000	2.91	0	0	0	0.278	-20.9	-17.8	0.00%
Oxygen	2.21	0.0553 kg Argon; 3.26 kg Nitrogen;	0.231	1.39	0	0	0	0	-9.93E-03	1.38	0.00%

Table 6.4 continued

				CTG Energy, MJ/1000 Infections Treated[a]							
Chemicals, gate-to-gate	**Mass, kg[b]**	**By-products, kg/kg chemical[c]**	**Allocation factor[d]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Potential recovery[e]**	**Total net energy**	**% of Total**
Styrene	2,110	0.0113 kg Benzene; 0.0253 kg Hydrogen; 0.0310 kg styrene heavies; 0.0134 kg Toluene;	0.925	76.9	0	1.10E+04	6.56E+04	929	-6.02E+04	1.75E+04	3.20%
Ethylbenzene	2,111	7.20E-03 kg heavy by-products;	0.993	132	0	3,738	0	929	-1,915	2,883	0.53%
Benzene	1,568	3.40 kg Non-aromatics for gas pool; 1.41 kg Toluene; 1.46 kg Xylenes;	0.138	0.877	0	4,085	0	690	-1,253	3,523	0.65%

Table 6.4 continued

				CTG Energy, MJ/1000 Infections Treated[a]							
Chemicals, gate-to-gate	**Mass, kg[b]**	**By-products, kg/kg chemical[c]**	**Allocation factor[d]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Potential recovery[e]**	**Total net energy**	**% of Total**
pyrolysis gas	455	0.465 kg C4 stream; 0.970 kg Ethylene; 0.0854 kg fuel oil; 0.0469 kg Hydrogen; 0.552 kg Methane; 0.615 kg Propylene;	0.268	647	0	1,077	5,269	200	-1,288	5,904	1.08%
reformate, from naphtha	1,117	0.0485 kg C5 from reformate; 0.0625 kg H2 rich fuel; 9.67E-04 kg H2S rich stream;	0.899	17.6	926	553	4,209	492	-1,787	4,411	0.81%

Table 6.4 continued

				CTG Energy, MJ/1000 Infections Treated[a]							
Chemicals, gate-to-gate	**Mass, kg[b]**	**By-products, kg/kg chemical[c]**	**Allocation factor[d]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Potential recovery[e]**	**Total net energy**	**% of Total**
Ethylene	642	0.480 kg C4 stream; 0.0881 kg fuel oil; 0.0484 kg Hydrogen; 0.569 kg Methane; 0.634 kg Propylene; 1.03 kg pyrolysis gas;	0.260	912	0	1,518	7,432	282	-1,816	8,328	1.53%
MH Agar Plate	134		1.000	0.0121	0	38.7	0	59.1	0	97.8	0.02%
Agar	1.39		1.000	1.51	0	47.9	22.7	0.612	0	72.7	0.01%
Gelidium Algae	3.59		1.000	0	0	0	3.01	0.476	0	3.49	0.00%
Sodium carbonate	0.289	1.04 kg Ammonium chloride;	0.490	0.0579	0	0.818	0	0.127	-0.0147	0.989	0.00%
Sodium chloride	81.4		1.000	0.368	0	396	6.55	35.8	0	439	0.08%
Casein hydrolysate	1.43		1.00	0.549	0	19.4	18.2	0.630	-1.93	36.8	0.01%
Casein	1.85	3.50 kg Cream; 2.08 kg Whey;	0.152	0.607	0	2.95	2.80	0.812	0	7.17	0.00%

Table 6.4 continued

				CTG Energy, MJ/1000 Infections Treated[a]							
Chemicals, gate-to-gate	**Mass, kg[b]**	**By-products, kg/kg chemical[c]**	**Allocation factor[d]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Potential recovery[e]**	**Total net energy**	**% of Total**
Milk	9.79	0.0257 kg Beef; 0.163 kg Cow Manure;	0.842	1.98	0	0	0.307	4.31	0	6.60	0.00%
Cotton	2.35		1.000	3.67	0	0	28.0	1.03	0	32.7	0.01%
Soy meal	94.5	0.268 kg Soybean oil;	0.789	3.10	0	129	23.7	0	-29.5	126	0.02%
n-Hexane	0.991	1.63 kg C5 from naphtha; 4.61 kg C7 from Naphtha;	0.138	3.12E-05	0	0.706	0	0.436	-0.0861	1.06	0.00%
Soybean	119	0.0453 kg Soybean Seed;	0.957	2.83	0	0	98.7	52.5	0	154	0.03%
Soybean Seed	3.45		1.000	0	0	0	0	0	0	0	0.00%
Petri Dish	52.5		1.00	38.4	0	2.54	0	23.1	-11.0	53.0	0.01%
Polystyrene	57.8		1.000	14.1	0	8.04	0	25.4	-18.0	29.5	0.01%
PP SMS Gown	8,940		1.000	7,138	0	2,602	0	3,934	0	1.37E+04	2.51%
PP SMS Fabric	9,449		1.000	1.65E+04	1.84E+05	490	0	4,157	0	2.05E+05	37.64%
Polypropylene	9,576		1.000	8.03E+04	0	689	0	4,214	-6,914	7.83E+04	14.35%

Table 6.4 continued

				CTG Energy, MJ/1000 Infections Treated[a]							
Chemicals, gate-to-gate	Mass, kg[b]	By-products, kg/kg chemical[c]	Allocation factor[d]	Electricity	Dowtherm	Steam	Fuel, Non-transport	Fuel, Transport	Potential recovery[e]	Total net energy	% of Total
Propylene	9,885	0.756 kg C4 stream; 1.58 kg Ethylene; 0.139 kg fuel oil; 0.0762 kg Hydrogen; 0.898 kg Methane; 1.63 kg pyrolysis gas;	0.165	1.40E+04	0	2.34E+04	1.14E+05	4,349	-2.80E+04	1.28E+05	23.51%
PVC IV Bag	141		1.000	21.0	0	369	0	62.0	-3.09	448	0.08%
Vinyl Chloride	149	0.602 kg Hydrogen chloride;	0.624	8.96	0	172	350	65.5	-228	369	0.07%
Dichloroethane,-1,2	160		1.000	71.1	0	13.3	0	70.6	-268	-113	-0.02%
Hydrogen chloride	122	1.71 kg Vinyl Chloride;	0.368	5.31	0	50.4	162	53.8	-158	114	0.02%
Chlorine	88.1	0.0295 kg Hydrogen; 1.18 kg Sodium hydroxide;	0.453	499	0	0	0	38.8	-18.0	519	0.10%
Vancomycin HCl	20.0		1.000	474	0	4,961	0	8.80	-970	4,474	0.82%

Table 6.4 continued

				CTG Energy, MJ/1000 Infections Treated[a]								
Chemicals, gate-to-gate	**Mass, kg[b]**	**By-products, kg/kg chemical[c]**	**Allocation factor[d]**	**Electricity**	**Dowtherm**	**Steam**	**Fuel, Non-transport**	**Fuel, Transport**	**Potential recovery[e]**	**Total net energy**	**% of Total**
Ammonium chloride	22.6	0.961 kg Sodium carbonate;	0.510	4.54	0	64.1	0	9.96	-1.15	77.4	0.01%
Dextrose	242		1.000	11.4	0	2,904	17.2	106	-162	2,877	0.53%
Sodium hydroxide	0.423	0.848 kg Chlorine; 0.0250 kg Hydrogen;	0.534	2.40	0	0	0	0.186	-0.0865	2.50	0.00%
Isopropanol	2.00		1.000	0.0960	0	60.8	0	0.880	-3.19	58.6	0.01%
Soy Flour	92.5		1.000	1.47	0	0	0	40.7	0	42.2	0.01%
Total energy				1.26E+05	1.85E+05	8.44E+04	2.39E+05	2.50E+04	-1.14E+05	5.45E+05	100.00%

[a] Amount of energy used cradle-to-gate to produce mass of chemical used in infection treatment inventory.
[b] Amount used cradle-to-gate to treat 1000 infections.
[c] By-products generated during the gate-to-gate manufacture of chemical.
[d] Mass allocation is used to distribute the inputs, energy, and emissions to each product formed in that gate-to-gate inventory. Allocation factor will be less than 1.0 when by-products are generated.
[e] Energy that can be recovered from sources requiring cooling.

6.4.3 Emissions

The total cradle-to-gate emissions listed in Table 6.5 come from chemical losses, energy-related emissions, and transportation-related emissions from each GTG inventory. Depending on the physical state, the emissions are listed as air, liquid, or solid emissions. These emissions do not include the effect of waste management processes, and thus are direct process chemical losses. Carbon dioxide was the largest contributor to air emissions at 48 kg of the total 49.4 kg of air emissions per infection treated, primarily due to energy-related emissions. Total water emissions were 0.55 kg and total solid emissions were 2.13 kg per infection treated. The total solid emissions do not include disposal of products such as gowns and gloves. Adding this would increase the solid emission by more than 12 kg per infection treated.

Table 6.5. Cradle-to-Gate Emissions Generated to Treat One Infection

Air emissions	kg
1,2-butadiene	0.0350
1,3-butadiene	71.6
2,2-Dimethylpentane	5.94E-05
2-Methylpentane	2.11E-04
3-Methylpentane	2.05E-04
Acetylene	0.321
Ammonia	1.10
Ammonium chloride	0.179
Argon	0.498
Benzene	25.1
Butane	1.41
Butene	4.15
butenes and butanes	3.43
C5 from naphtha	3.64E-03
C7 from Naphtha	5.37E-03
Carbon dioxide	4.80E+04
Carbon monoxide	26.5
Chlorine	2.01
Chloroform	0.0132
Cream	9.83E-03
Cyclohexane	4.24
Dichloroethane,-1,2	12.6
Diisopropyl Ether	0.0120
Dimethylbutane, -2,3	9.26E-05
Ethane	3.89
Ethanol	3.85
Ethylene	24.2
Ethylene oxide	1.05E-03
Heptane	0.335
Hydrogen	1.60
Hydrogen chloride	1.17
Hydrogen fluoride	1.69E-06
Hydrogen sulfide	0.0540
Hypochlorous acid	1.23E-03

Table 6.5 continued

Air emissions	kg
Isobutane	0.0116
Isopropanol	0.240
lauroyl peroxide	0.0888
Methane	152
Methylcyclopentane	5.70E-04
Milk	0.0979
Naphtha	242
n-Hexane	6.14
Nitrogen dioxide	0.203
Nitrogen monoxide	0.132
Nitrous oxide	0.0789
NMVOC	163
NOx	173
n-Pentane	0.162
Octane	0.252
Particulate matter	0.370
Polypropylene	9.59
Propane	0.294
Propylene	338
Propyne	0.288
pyrolysis gas	32.7
Sodium hypochlorite	5.06E-07
SOx	71.3
Soybean oil	0.215
Styrene	2.66
Styrene dimer	8.09E-03
Styrene trimer	0.0139
Sulfur	0.0469
Sulfur dioxide	4.19E-03
Sulfur trioxide	0.139
t-Butyl peroxybenzoate	0.0479
Toluene	3.37
Trichloroethane,1,1,2	0.0192
Urea	0.0829
Vinyl Chloride	1.81

Table 6.5 continued

Water emissions	kg
Vinylacetylene	0.0822
Total Air emissions	4.938E+04
1,1,2,2-Tetrachloroethane	1.29
1,3-butadiene	0.437
Acrylic acid	0.0666
Alcalase	0.0551
Ammonia	20.5
Ammonium chloride	21.0
Arsenic	1.03E-04
Ash	0.279
Atrazine	8.07E-04
BaSO4	0.297
Benzene	2.41E-03
BOD	2.60
BOD5	1.98E-03
Boron	0.0508
Calcium carbonate	0.126
Calcium dichloride	2.45E-04
calcium monoxide	0.0930
Calcium Nitrate	1.63
Carbon	0.0923
Casein	0.398
Chloride	37.4
Chloroform	0.805
COD	63.6
Coke	0.0764
DAP	0.0962
Dichloroethane,-1,2	1.31
Diisopropyl Ether	0.0280
Disproportionated tall oil	0.0167
Ethylene	0.0112
grease / oil	0.610
Growth Regulator	3.26E-03
Harvest Aid	9.02E-03
Herbicide	0.0210

Table 6.5 continued

Water emissions	**kg**
Hydrogen chloride	9.97
Isopropanol	2.06
Lactose	6.44E-04
lauroyl peroxide	0.355
Magnesium hydroxide	0.0213
Magnesium Sulfate	4.44E-03
Malt Extract	1.27E-04
Mercury	2.22E-05
Milk Fat	0.0175
Mobile ions	118
Nitrate-N	0.225
Organic Matter	9.79E-03
Peptone	4.66E-04
Pesticide	0.0157
Phosphate-P	0.0219
Potassium chloride	1.12
PVC	2.95
pyrolysis gas	0.261
Sodium	48.2
Sodium carbonate	0.289
Sodium chloride	10.1
Sodium hydroxide	21.0
Soy Flour	92.4
Styrene	8.15
Styrene butadiene latex	0.0309
Styrene dimer	0.0389
Styrene trimer	0.0589
Sulfur trioxide	0.111
Sulfuric acid	0.718
TDS	56.0
Trichloroethane,1,1,2	0.0948
Urea	24.0
Vancomycin	0.635
Vancomycin HCl	1.05
Vinyl Chloride	0.211

Table 6.5 continued

Water emissions	**kg**
Yeast Extract	1.27E-04
Total Water emissions	551
Solid emissions	**kg**
1,1,2,2-Tetrachloroethane	1.83E-03
A Orientalis	108
Agar	0.0115
Aluminum chloride	9.22
Calcium dichloride	2.45E-07
calcium monoxide	0.0886
Cellulose	0.532
Clay	0.831
Coke	0.681
corn starch	15.6
Cotton Seed	3.70
debris from corn	1.69
Diatomaceous earth	1.52
Dichloroethane,-1,2	0.581
Ethylene oxide	0.209
Fatty acid	1.76E-03
Glucoamylase	0.242
Herbicide	2.06E-04
Hydrogen fluoride	3.37E-04
Impurities	0.713
Magnesium Sulfate	4.44E-06
Malt Extract	1.27E-07
Mud (salt process)	15.6
Organic Matter	2.68
Peptone	4.66E-07
Phosphate rock	8.16
Phosphate rock (pure)	1.75
Phosphogypsum	45.5
Phosphoric acid	0.532
Polyethylene	1.20
Polyglycol ether	4.99E-04

Table 6.5 continued

Solid emissions	kg
Polystyrene	5.78
Potassium chloride	1.07
PP SMS Fabric No Dye	886
PVC	4.04
Silica	0.929
Sodium chloride	14.8
Sodium hydroxide	8.81E-03
Sodium hypochlorite	5.06E-05
Solid waste	990
Soy Flour	0.0925
Soy Hulls	8.14
Soybean	4.34
starch suppressant	0.0388
Sulfuric acid	4.04E-03
Vancomycin	0.0416
Water glass	0.0499
Yeast Extract	1.27E-07
Zinc stearate	0.0606
Total Solid emissions	2,134

6.5 Conclusions

Treating one infection utilizes 545 MJ of energy, 31.2 kg of raw materials, and 52 kg emissions to the air, water, and land. Due to the high mass of disposable gowns used, contact isolation has the greatest impact on the environmental consequences of treating an infection; it uses the most raw materials and energy and generates the most emissions. Fabric manufacture for the gowns alone accounts for 38% of the CTG energy consumption. Gown usage should be reviewed to decrease the environmental impact of treating infections. Since the gown is required for the protection of the healthcare worker, other areas, such as improving the efficiency of the fabric production stage or using reusable gowns should be considered. Prevention or the reduction of the rate of infections, while not reducing the environmental impact per infection, will reduce the yearly impact due to infections.

6.6 Acknowledgements

The authors would like to thank several hospital specialists that assisted with the challenging tasks of creating this representative profile of nosocomial infections in large urban hospitals. These include E. Early (George Washington Hospital) and Dr. Zach Moore (UNC Hospitals). We would also like to acknowledge Drs. Evan Griffing and Yong Li for their foundational contributions in the area of life cycle inventories. A National Science Foundation MUSES Grant (#0424514) funded this work.

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7. Using Life Cycle Analysis to Evaluate the Environmental Benefits of Using Biocidal Medical Garments

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7. Using Life Cycle Analysis to Evaluate the Environmental Benefits of Using Biocidal Medical Garments

Abstract

In this study, life cycle inventory analysis is used to determine the resources and emissions saved by the nation-wide use of a biocidal patient gown and the subsequent reduction in nosocomial infections. Application and use (regeneration) of a biocidal finish on the medical patient gowns (176,400,000 per year at 1 gown/patient-day) will consume 1.7 million kg of raw materials, 16.7 million MJ of energy, and emit 4.05 million kg to air, water, and land. Reducing the number of nosocomial infections (where 100% is a typical nosocomial infection rate of 45 patients per 1000) by 3.1%, 1.8%, and 4.5% will just balance these same environmental factors from the application and regeneration of the biocidal surface gowns. Thus it would be environmentally beneficial to use the biocidal finish if it reduces the number of nosocomial infections by 4.5% from 1.737 million to 1.66 million infections per year. This would be a shift in the yearly nosocomial infection rate from 4.5% to 4.30%.

Keywords: Life cycle inventory; environmental; nosocomial infection; biocide; energy; medical garment

7.1 Introduction

Each year, 1.737 million nosocomial infections occur in U.S. hospitals, or for every 1000 patients, 45 patients will acquire an infection while in the hospital (Klevens et al., 2007). Infections are transmitted by contaminated hands, clothing, equipment, and the environment (Muto et al., 2003). Nicas and Sun (Nicas and Sun., 2006) have investigated the probability of reducing the infection risk to healthcare workers when textiles such as bed linens are coated with a biocidal finish and determined a 50% reduction in infection risk, similar to a 45% reduction in respiratory illness found in a study on hand washing (Ryan et al., 2001). There are also several studies that show the economic cost of implementing prevention programs is less than the cost to treat infections (Scott, 2009,Macartney et al., 2000).

Microorganisms can grow on textiles (Belkin, 2002), and Boyce and Pittet (Boyce and Pittet, 2002) cite touching patient gowns as an infection transmission source for health-care workers. Sun et al (Sun et al., 2001, Sun and Xu, 1998) have developed a biocidal finish for medical textiles to combat microbial growth on items such as patient gowns. Biocidal heterocyclic N-halamines, such as 3-allyl-5,5-dimethyl hydantoin (ADMH) and dimethylol-5,5-dimethyl hydantoin (DMDMH) (See Figure 7.1), can be grafted onto textile fibers to create clothing with biocidal properties for use in healthcare and personal protective apparel industry and for the military. The biocidal coatings protect the fabric from microbial attack, odor, and reduce microbes that cause illness.

The halamine precursors are activated by the addition of a halogen such as chlorine or bromine. Chlorine and bromine halamines are also used in the pool industry to disinfect water (Sun et al., 1995). In several studies, fabrics with grafted halamines such as dimethylol dimethylhydantoin (DMDMH) showed a 6-7 log reduction (99.9999-99.99999% reduction) of bacteria. After reacting, the halamine structure is reduced to the precursor as shown in Figure 7.2 and can then be regenerated by adding a bleach rinse to a laundering cycle. Grafted halamines are stable over long-term storage and a wide range of temperatures.

(A) 3-Allyl-5,5-dimethylhydantoin (ADMH)

(B) 1,3-dimethylol--5,5-dimethylhydantoin (DMDMH)

Figure 7.1. Chemical Structures of Allyl dimethylhydantoin (ADMH) and Dimethylol dimethylhydantoin (DMDMH)

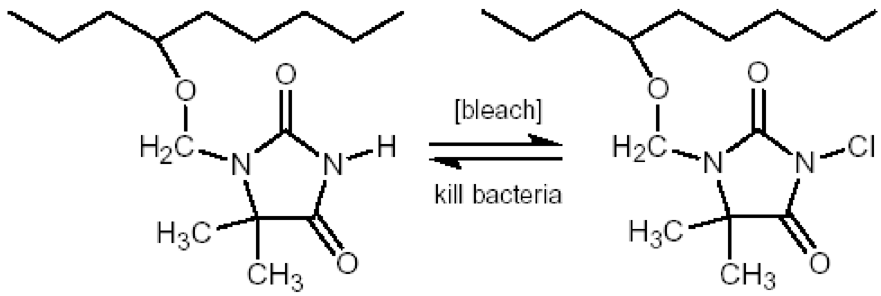

Figure 7.2. Halamine grafted onto fabric showing the reversible reaction of biocide killing bacteria and regenerating

Using medical textiles with a biocidal finish may halt the growth of microorganisms on such textiles, and thus reduce the number of nosocomial infections. When a patient contracts an infection while in the hospital, the products used to test and treat the patient impact the environment in natural resource costs, energy consumed, and emissions generated. However, the use of biocidal finishes on medical textiles is early in the transition to widespread hospital use, and no estimate of effectiveness can be verified. For the purpose of this study, the biocidal surface effectiveness was estimated at 0.1%, 1%, 2%, 5%, and 10% reduction in annual nosocomial infections. Using results from infection treatment and biocidal finish life cycle inventories reported previously, a sensitivity analysis is done to determine at what reduction in the number of infections the resources saved equal the resources used to apply and regenerate the biocidal finish. The life cycle inventory (LCI) is a compilation of all inputs, outputs, and energy use of a product from resource extraction, manufacture, product use, recycling, and disposal (Rebitzer et al., 2004).

7.2 Goal and Scope of the Study

The goal of this work is to determine whether the environmental costs of applying and regenerating a biocidal finish on medical patient gowns outweigh the resources saved by reducing the number of nosocomial infections treated through use of such gowns. The benefit, although not proven, would be a reduction in the resources used and emissions generated by reducing the number of infections treated. Since no estimate of effectiveness can be verified for the biocidal garment, the biocidal effectiveness is estimated at 0.1%, 1%, 2%, 5%, and 10% reduction in annual nosocomial infections. The study scope for the inventories starts from extracting the natural resources (cradle) and spans through treating an infection or wearing the gown in the hospital (gate). The representative infection treated is a MRSA infection treated with vancomycin. The LCI impact of being treated for a nosocomial infection is based only on the additional items resulting from the treatment of the nosocomial infection during the extended stay, and not the entire hospital stay that includes treatment for the original hospitalized condition. The functional unit, or basis, is per year.

7.3 Methodology

The cradle-to-gate (CTG) life cycle inventories for the infection treatment process and the biocidal finish application and regeneration process are the summation of the gate-to-gate (GTG, within the factory) inventories for each chemical or product that was used in the process. The design-based methodology developed by Jimenez-Gonzalez (Jimenez-Gonzalez, 2000), utilizing process flow diagrams and engineering design principles, is used to collect inventory data (for mass and energy balances) for each GTG inventory. The CTG life cycle inventory for treating an infection has previously been completed and reported in Chapter 6 based on 1000 infections treated; included are the materials used to test, isolate, and treat an infected patient (See Table 7.1). The basis of the infection treatment life cycle inventory is changed from 1000 infections to 1,737,125 infections per year.

Table 7.1. Products Used to Treat One Infection

	Item	Units	Total Mass
Infection Test	MH Agar Plate	3 units	134 g
	Gloves	9 pairs	134 g
	Disposable Gown	9 units	540 g
Treat (Contact Isolation)	Gloves	210 pairs	3129 g
	Disposable Gown	140 units	8400 g
Treat (Therapy)	Vancomycin	20 g	20 g
	Polyvinyl chloride IV Bag	20 units	141 g

Since not all patients will acquire a nosocomial infection, but all patients will wear the patient gown, the biocidal usage inventory is calculated on a yearly basis. The cradle-to-gate life cycle inventory for two biocides – 3-allyl-5,5-dimethyl hydantoin (ADMH) and dimethylol-5,5-dimethyl hydantoin (DMDMH) – have previously been completed and reported in Chapter 2, and DMDMH will be used in this study. The biocidal finish is applied once to each new garment, so the number of biocide applications equals the number of new gowns. The finish is regenerated during each laundering with a chlorine bleach rinse, and each gown is re-used seventy-five times. It is assumed that one gown is used daily by each patient. So the number of new gowns is calculated from:

$$\#\,\text{New Gowns} = \frac{(\text{Yearly Patient Days}) \times (1\,\text{Gown per Day})}{75\ \text{uses per Gown}} \qquad (7.1)$$

and the number of re-used gowns is equal to the yearly total gowns used minus the new gowns used. The biocide usage LCI is the sum of the DMDMH application for new gown inventory and the chlorine bleach rinse for re-used gowns inventory.

The patient gown usage will vary from one healthcare facility to another, depending on the location, size, and type of facility, and the services provided. For instance, patient gowns are changed daily for bed-ridden and ambulatory patients in an acute care facility. Ancillary department may have a higher gown usage. In long-term care facilities, gown usage is less than 1 per inpatient day(Moyer, 2009). In this study, 1 gown per inpatient day is used.

Klevens (Klevens et al., 2007) determined from National Nosocomial Infections Surveillance (NNIS) data that 1,737,125 nosocomial infections are contracted each year, during a yearly total of 176 million patient-days. Each year, a total of 176.4 millions gowns are used – 2.35 million new gowns and 174 million re-used gowns. The environmental costs of the biocidal finish are equal to the sum of the LCI results for the total number of biocidal applications for new gowns and biocidal regenerations for re-used gowns. The resource and emissions savings for using the biocidal finish will be calculated as the difference between the baseline infection treatment inventory and the inventory for the reduced number of infections treated. The environmental costs of the biocidal finish will be compared to this resource and emissions savings to determine at what reduction in infections the environmental savings will balance.

7.4 Inventory Results

The LCI of a representative hospital infection has been previously reported in Chapter 6 and showed that disposable gown and glove use required the most raw material and energy consumption. The products used to treat one infection are listed in Table 7.1, and the chemical tree for an infection is shown in Figure 7.3. The LCI of applying the biocidal halamine finish has also been reported previously Chapter 3. The chemical tree for DMDMH is shown in Figure 7.4.

Level 1	Level 2	Level 3		Natural Resources
Infection Treatment	Latex Glove	Corn starch	93 chemicals	Air, Coal, Crude Oil, Gelidium, Natural gas, Phosphate rock, Salt rock, Sand, Soybean seed, Sylvinite ore, Water
		Styrene Butadiene Latex	25 chemicals	
	MH Agar Plate	Agar	25 chemicals	
		Casein hydrolysate	287 chemicals	
		Petri Dish	13 chemicals	
	PVC IV Bag	Vinyl Chloride	15 chemicals	
	PP SMS Gown	Polypropylene SMS Fabric	4 chemicals	
	Vancomycin HCl	Ammonia	8 chemicals	
		Ammonium chloride	22 chemicals	
		Dextrose	108 chemicals	
		Isopropanol	15 chemicals	
		Soy Flour	99 chemicals	
		Urea	18 chemicals	

Figure 7.3. Chemical tree of Infection Treatment

Level 1	Level 2	Level 3	Level 4	Level 5	Level 6	Level 7
Dimethyloldimethyl hydantoin 1,000	Dimethyl hydantoin 696	Acetone 324	Benzene 183	pyrolysis gas 53.3	Naphtha 54.3	oil (in ground) 55.0
				reformate, from naphtha 131	Naphtha 133	oil (in ground) 134
			Oxygen 77.3	Air (untreated) 107		
			Propylene 98.4	Naphtha 100	oil (in ground) 102	
		Ammonia 104	Natural gas 21.3	Natural gas (unprocessed) 21.7		
			Nitrogen from air 39.9	Air (untreated) 39.9		
			Oxygen from air 17.7	Air (untreated) 17.7		
			Water for rxn 27.7	Water (untreated) 27.7		
		Carbon dioxide 242	Natural gas 49.6	Natural gas (unprocessed) 50.6		
			Nitrogen from air 93.1	Air (untreated) 93.1		
			Oxygen from air 41.3	Air (untreated) 41.3		
			Water for rxn 64.6	Water (untreated) 64.6		
		Hydrogen cyanide 151	Ammonia 118	Natural gas 24.2	Natural gas (unprocessed) 24.7	
				Nitrogen from air 45.5	Air (untreated) 45.5	
				Oxygen from air 20.2	Air (untreated) 20.2	
				Water for rxn 31.5	Water (untreated) 31.5	
			Natural gas 140	Natural gas (unprocessed) 143		
			Oxygen from air 527	Air (untreated) 527		
	Formaldehyde 326	Methanol 409	Natural gas 253	Natural gas (unprocessed) 258		
			Water for rxn 175	Water (untreated) 175		
		Oxygen from air 230	Air (untreated) 230			
	Sodium hydroxide 0.218	Sodium chloride 0.169	Salt rock 0.215			
		Water for rxn 0.0526	Water (untreated) 0.0526			

Figure 7.4. Chemical Tree of DMDMH. The product chemical is on the left, and natural resources to the right. The amount of each chemical used to make 1000 kg DMDMH is shown.

7.4.1 Raw Materials

As seen in Table 7.2, applying and regenerating the biocidal finish for 176,400,000 yearly gowns uses 1.7 million kg of raw materials. Salt rock accounts for 46% of the raw materials, due to the sodium hypochlorite (laundry bleach) supply chain. Oil and natural gas are the next largest raw materials consumed, due to energy consumption and not process-related. Regenerating the DMDMH biocidal finish with a bleach rinse cycle during cleaning requires 79% of the total raw materials since the garments are used 75 times. To treat 1.737 million infections, 54.1 million kg of raw materials are consumed. Energy-related raw materials utilize 53% of the total raw materials. The disposable gown materials account for 80% of the total raw materials used to treat infections.

Table 7.3 shows that raw materials consumption for using the biocidal finish will balance when the number of infections is reduced to 3.1% of the baseline number of infections, which is a reduction to 1.68 million infections treated. Table 7.4 shows the raw materials saved by treating 3.1% fewer infections yearly.

Table 7.2. Cradle-to-Gate Life Cycle Inventory for Application and Regeneration of DMDMH Biocidal Finish, Based on 1000 Gowns and the Yearly Number of Gowns Used

	Total App + Regen	Biocide App		Biocide Regen	
# gowns		1,000	2,352,000	1,000	174,048,000
Raw material, kg			Yearly		Yearly
Air	48,134	20	48,134	0	0
Coal	226,887	7	16,670	1	210,217
Crude Oil	223,247	57	133,089	1	90,158
Gelidium	0	0	0	0	0
Natural gas	208,025	53	125,092	0	82,933
Phosphate rock	0	0	0	0	0
Salt rock	772,190	5	12,331	4	759,859
Sand	0	0	0	0	0
Soybean Seed	0	0	0	0	0
Sylvinite ore	0	0	0	0	0
Water	201,332	7	15,812	1	185,520
Total Raw Materials	1,679,814	149	351,127	8	1,328,687
Energy, MJ					
Electricity	4,697,410	135	318,326	25	4,379,083
Dowtherm	4,651	2	4,651	0	0
Heating steam	10,409,722	3,193	7,510,706	17	2,899,017
Fuel	2,256,455	276	650,217	9	1,606,238
Energy input	17,368,238	3,607	8,483,901	51	8,884,337
Cooling water	-18,872,751	-531	-1,250,046	-101	-17,622,705

Table 7.2 continued

	Total App + Regen	Biocide App		Biocide Regen	
Refrigeration	118,561	2	4,062	1	114,499
Potential recovery	-626,335	-200	-469,462	-1	-156,873
Net energy (Input - Potential recovery)	16,741,903	3,407	8,014,438	50	8,727,465
Total Air Emissions, kg	1,824,228	293	688,929	7	1,135,299
Total Water Emissions, kg	2,049,148	18	41,537	12	2,007,611
Total Solid Emissions, kg	176,393	3	6,025	1	170,369
Total Emissions, kg	4,049,769	313	736,491	19	3,313,278

Table 7.3. Cradle-to-Gate Life Cycle Inventory Comparison for Application and Regeneration of DMDMH Biocidal Finish and Yearly Infection Treatment

	Biocide App + Regen	Infection Treatment	Resource and Emissions Savings[a]				
Number of Infections per year		1,737,125	1,735,388	1,719,754	1,702,383	1,650,269	1,563,413
% Reduction			0.1%	1.0%	2.0%	5.0%	10.0%
Total Number of Gowns per year	176,400,000						
Raw material, kg							
Air (untreated)	48,134	157,083	157	1,571	3,142	7,854	15,708
Coal	226,887	10,549,155	10,549	105,492	210,983	527,458	1,054,915
Crude Oil	223,247	25,636,485	25,636	256,365	512,730	1,281,824	2,563,649
Gelidium (untreated)	0	8,319	8	83	166	416	832
Natural gas	208,025	17,368,949	17,369	173,689	347,379	868,447	1,736,895
Phosphate rock (in ground)	0	64,915	65	649	1,298	3,246	6,491
Salt rock	772,190	180,373	180	1,804	3,607	9,019	18,037
Sand	0	2,705	3	27	54	135	270
Soybean Seed (Untreated)	0	5,988	6	60	120	299	599
sylvinite ore (in ground)	0	48,115	48	481	962	2,406	4,812
Water	201,332	123,007	123	1,230	2,460	6,150	12,301
Total Raw Materials	1,679,814	54,145,093	54,145	541,451	1,082,902	2,707,255	5,414,509
Energy, MJ							
Electricity	4,697,410	219,709,646	219,710	2,197,096	4,394,193	10,985,482	21,970,965
Dowtherm	4,651	321,474,211	321,474	3,214,742	6,429,484	16,073,711	32,147,421
Heating steam	10,409,722	146,565,365	146,565	1,465,654	2,931,307	7,328,268	14,656,537

Table 7.3 continued

	Biocide App + Regen	Infection Treatment	Resource and Emissions Savings[a]				
Fuel	2,256,455	458,429,386	458,429	4,584,294	9,168,588	22,921,469	45,842,939
Number of Infections per year		1,737,125	1,735,388	1,719,754	1,702,383	1,650,269	1,563,413
% Reduction			0.1%	1.0%	2.0%	5.0%	10.0%
Total Number of Gowns per year	176,400,000						
Energy input	17,368,238	1,146,178,609	1,146,179	11,461,786	22,923,572	57,308,930	114,617,861
Cooling water	-18,872,751	-401,735,222	-401,735	-4,017,352	-8,034,704	-20,086,761	-40,173,522
Refrigeration	118,561	130,321	130	1,303	2,606	6,516	13,032
Potential recovery	-626,335	-198,653,776	-198,654	-1,986,538	-3,973,076	-9,932,689	-19,865,378
Net energy (Input - Potential recovery)	16,741,903	947,524,834	947,525	9,475,248	18,950,497	47,376,242	94,752,483
Total Air Emissions, kg	1,824,228	85,772,344	85,772	857,723	1,715,447	4,288,617	8,577,234
Total Water Emissions, kg	2,049,148	957,350	957	9,573	19,147	47,867	95,735
Total Solid Emissions, kg	176,393	3,706,564	3,707	37,066	74,131	185,328	370,656
Total Emissions, kg	4,049,769	90,436,258	90,436	904,363	1,808,725	4,521,813	9,043,626

[a]Resource and Emissions Savings are the amounts of resources not consumed and emissions not generated by reducing the number of infections treated yearly.

Table 7.4 Comparison of Biocide Application and Regeneration with Resources and Emissions Saved from a 2% Reduction in Yearly Infections

	Baseline Infection Treatment	Biocide App + Regen	Resource and Emissions Savings		
Number of Infections per year	1,737,125		1,706,432	1,683,232	1,659,336
% Reduction in Yearly # of Infections			1.77%	3.10%	4.48%
Total Number of Gowns per year		176,400,000			
Total Raw Materials, kg	54,145,093	1,679,814	956,695	1,679,814	2,424,637
Net energy, MJ	947,524,834	16,741,903	16,741,903	29,396,308	42,430,513
Total Emissions, kg	90,436,258	4,049,769	1,597,927	2,805,723	4,049,769

7.4.2 Energy

Use of the biocidal finish requires 16.7 million MJ of energy yearly. The regeneration process uses 52% of this energy. The regeneration process does not require as much energy as the application process per gown. However, each gown is regenerated after use, producing a higher total regeneration energy compared to the application energy. Steam is the largest type of energy used due to drying of the fabric in the application. Electricity is the second highest due to the manufacture of the supply chain chemicals used in the regenerating process. In comparison, to treat 1.7 million infections each year, 947 million MJ of energy are consumed.

To use the biocidal finish, the energy consumption will equal the energy saved by a 1.77% reduction in infections treated to 1.71 million infections treated. Table 7.4 shows the energy saved by treating 1.77% fewer infections yearly. However, at this reduction, the raw materials consumption for using the biocide is not balanced.

7.4.3 Emissions

The total cradle-to-gate emissions listed in Tables 7.2 and 7.3 come from chemical losses, energy-related emissions, and transportation-related emissions from each GTG inventory. Use of the biocidal finish emits 4.05 million kg to air, water, and land. Most air emissions are due to carbon dioxide from energy-related emissions. Yearly, 90 million kg of waste are emitted to treat infections. To use the biocidal finish, 4.05 million kg waste emissions must be saved, and this is accomplished when the number of infections is reduced 4.5% to 1.66 million infections per year. Table 7.4 shows the emissions saved by treating 4.5% fewer infections yearly.

7.5 Conclusions and Future Work

Each year, 54.1 kg of raw materials and 947 million MJ of energy are consumed to treat nosocomial infections. Again, a reduction in nosocomial infections due to use of a biocidal gown has not been proven. However, such a biocidal gown is environmentally beneficial for a hypothetical reduction in the number of nosocomial infections by 4.5%.

At a 1.8% reduction, the energy consumption for the biocidal finish equals the energy saved from the reduction in infections. However, the raw materials consumption and emissions generated do not balance until the number of infections is reduced by 3.1% and 4.5% , respectively.

This work should be extended to include the life cycle inventory analysis of other linens such as bed sheets with a biocidal finish, and also gowns and linens of different reusable materials, such as nonwoven and 100% polyester. The next stage of the current analysis is to include disposal and reuse as a new product. When reusable healthcare gowns have reached the end of their life cycle as a gown, these products can be re-manufactured and sold as cleaning cloths. Also, the polypropylene SMS gowns can be incinerated for energy recovery. A full cradle-to-grave life cycle inventory would include this end-of-life phase.

7.6 Acknowledgements

The authors would like to thank several hospital specialists that assisted with the challenging tasks of creating this representative profile of nosocomial infections in large urban hospitals. These include E. Early (George Washington Hospital) and Dr. Zach Moore (UNC Hospitals). We would also like to acknowledge the American Reusable Textiles Association for providing hospital patient gown usage information and Drs. Evan Griffing and Yong Li for their foundational contributions in the area of life cycle inventories. A National Science Foundation MUSES Grant (#0424514) funded this work.

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8. Life Cycle Analysis of Nylon Coloration For Textile and Carpet Applications

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Manuscript submitted for publication to Dyes and Pigments May 2009

This paper was presented at the 2007 AIChE Annual Meeting, Salt Lake City, Utah, November 2007

8. Life Cycle Analysis of Nylon Coloration for Textile and Carpet Applications

Abstract

Textiles are dyed by a variety of different processes at different stages of production, including the fiber, the yarn, or textile piece, depending on the product use, economy of the process, and market demand for the color. This paper compares the environmental footprint of five carpet coloring processes using carpet as a case study. Using a life cycle approach, gate-to-gate (within the factory) inventories are created to assess resource and energy consumption and wastes associated with each of the processes. The gate-to-gate (GTG) dyeing energy is then compared to the cradle-to-gate (CTG) energy of the carpet to determine the impact the dyeing choice has on the overall cradle-to-gate carpet manufacturing energy. The CTG inventory of manufacturing the pigment/dye is not available for this analysis.

Batch processes, such as Beck and skein, consume the most water and energy, while solution coloring uses the least amount of energy. When the dye process is factored into the cradle-to-gate carpet manufacturing energy, the dyeing method accounts for 0.1% - 31% of the total carpet CTG energy, including the dyeing process. The higher dyeing energy consumption produces desirable appearances in the carpet and that is not captured in the energy per 1000 kg nylon dyed.

Keywords: Life cycle inventory; life cycle analysis; energy; carpet dyeing; nylon; fiber

8.1 Introduction

Each year 3.5 billion pounds of fiber, mostly nylon, are dyed to make 1.9 billion yards of carpet (The Carpet and Rug Institute) (See Figure 8.1 and Figure 8.2). Commercial carpet is predominantly nylon face material. The dyed carpet must resist fading from light, wetness, and friction, requiring dyes to resist degradation. Carpets and fibers are colored by a variety of different processes at different stages of production, from the fiber, the yarn, or the carpet, depending on the product use, economy of the process, and market demand for the color. Fiber can be colored as it is extruded, as in the case of solution coloring; yarn can be dyed as in skein, or space dyeing; or whole carpet pieces can be dyed as in Beck or continuous dyeing.

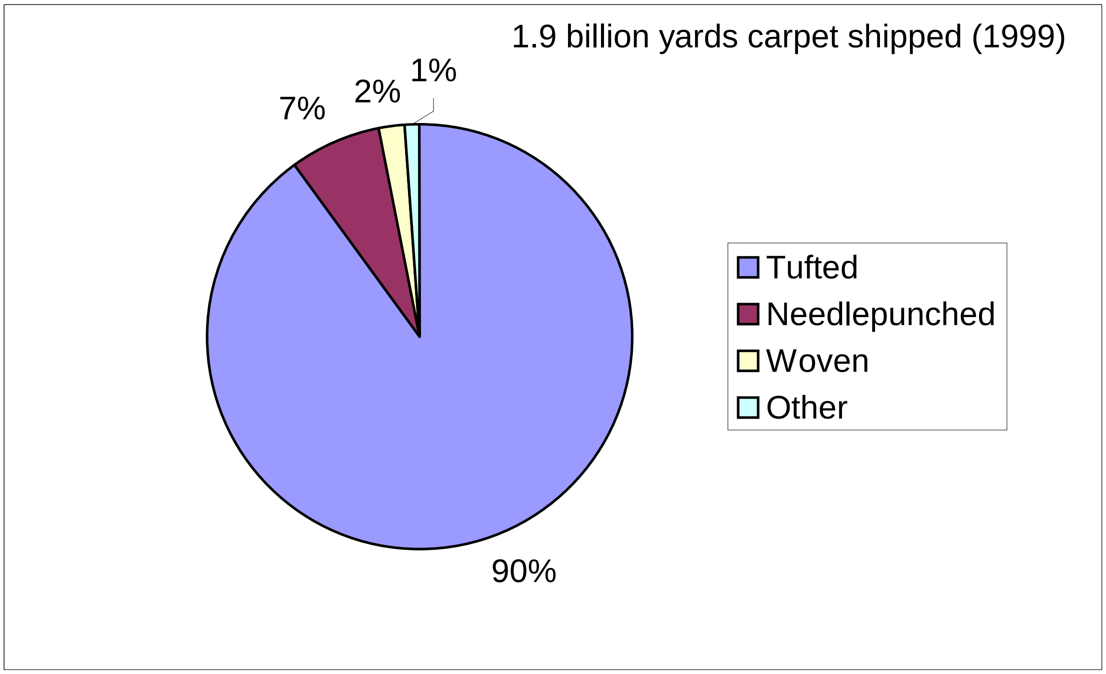

Figure 8.1. Types of Carpet Produced

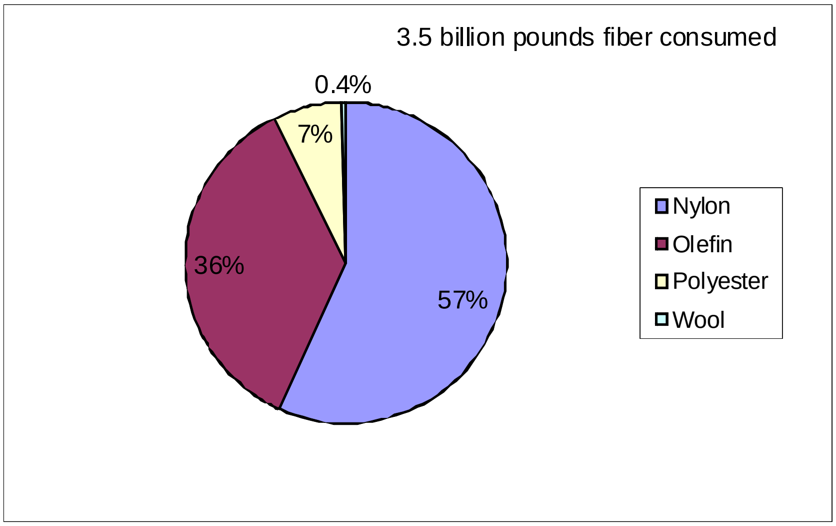

Figure 8.2. Types of Fibers used for Carpet

As more carpet is produced, more wastewater from carpet mills is discharged to publicly owned treatment works (POTW). Dyes can resist degradation in activated sludge systems, as these chemicals are not very aerobically biodegradable. Some dyes also contain heavy metals such as copper, chromium, or zinc.

Batch processes immerse yarn or carpet in a dye bath solution and heat the bath to allow penetration of the dye into the yarn. Energy is needed to heat the water, and not all of the dye in solution penetrates the yarn, thus leaving the system as waste. Dye auxiliaries are added to the dye bath to alter the pH to facilitate dye penetration.

Continuous processes aim to reduce the amount of water required and the amount of waste chemicals, but the yarn must be heated to allow penetration of the dye. The yarn is passed through steamers to open the fibers and set the dye. Energy is still required to produce the steam, but less water is discharged. Finally, pigment in solution coloring can also be added to the fiber during extrusion to color the fiber, thus avoiding pigment in the wastewater.

A life cycle assessment (LCA) is an environmental tool used to estimate and assess the environmental profile of a product over its life cycle. All raw materials and energy consumption, and waste generated during each step in the life of a product, from raw materials extraction, production, transportation, use, and disposal are tabulated and analyzed to show the total cradle-to-grave environmental impact of a product. It can allow manufacturers to select more environmentally friendly raw materials, if the raw material LCAs are known. It can also be used to improve the manufacture of a product by highlighting where changes can be made in the process to get the greatest reduction in the product's environmental performance.

8.2 Goal and Scope

The intent of this work is to investigate and analyze five carpet dyeing processes using a life cycle approach. Transparent gate-to-gate (within the factory) inventories are used to compare dyeing processes at different stages of carpet manufacture: before yarn production, after yarn production, and after tufted carpet production, depending on the dyeing process. Gate-to-gate (GTG) inventories are the first level inventories, and manufacture of the yarn, dyes, or carpet is not included, so that the GTG dyeing can be evaluated directly. The dyeing processes will be compared based on water and energy requirements and process emissions. The cradle-to-gate (CTG) life cycle inventory (LCI) for a carpet product has been done previously (Li, 2007), and includes the supply chain chemicals, excluding dyes at this time. The gate-to-gate dyeing energy is compared to the cradle-to-gate carpet energy to determine the impact the dyeing process choice has on the overall cradle-to-gate dyeing energy.

8.3 Methodology

The design-based methodology (Jiménez-González, 2000, Kim and Overcash, 2003, Jimenez-Gonzalez et al., 2001, Jimenez-Gonzalez, 2000) using process flow diagrams and engineering design principles is used to collect inventory data for each gate-to-gate inventory used to complete the carpet dyeing inventory. Industry data and literature sources (Carr and Tincher, 1983, Mock, 1997, Perkins, 1991, Tincher, 1989) are used for the carpet dyeing inventories.

All processes are compared on a basis of 1000 kg nylon fiber, so the functional unit is 1000 kg dyed nylon fiber. Only the dye mass is shown for each process since the CTG of the dye is not available for all processes. However, the cradle-to-gate carpet inventories have been calculated on the basis of one square yard of carpet, so the nylon face weight (kg/sy) is used to relate the results.

The nylon coloring processes are described below to insure transparency. Nylon fiber can be colored before it is drawn into fiber by adding pigment pellets to the nylon pellets in the extruder. The nylon can then be drawn into nylon fiber. (See Figure 8.3.) The energy for extruding the polymer is calculated from

$$\text{Extruder Energy} = 1.7301 \times \left(\int_{T_{in}}^{T_{melt}} mC_P dT + m\Delta H_{melt}(T) + \int_{T_{melt}}^{T_{out}} mC_P dT \right) \qquad (8.1)$$

where m = mass of polymer; C_p = heat capacity; T_{in}, T_{in}, T_{out} = temperature of the polymer going into, at the melting point, and coming out of the extruder, and ΔH_{melt} = heat of melting for the polymer. This calculation assumes the mechanical energy for the screw contributes 75% (the heat for melting) and the heaters to prevent cooling in the screw contribute the remaining 25% of the energy. An efficiency of 75% is assumed for the extruder drives. For the heaters, 85% heat transfer efficiency is assumed. For the mechanical energy, 85% energy conversion efficiency is assumed.

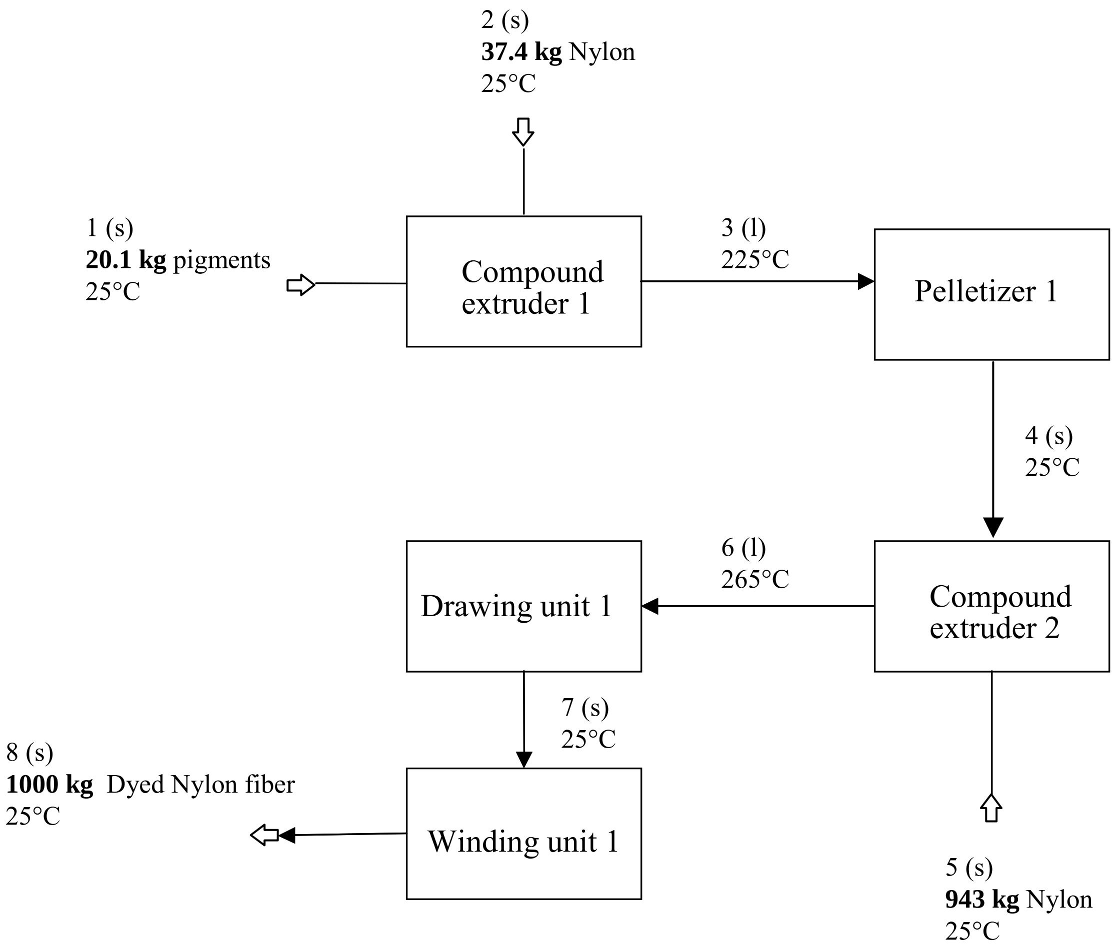

Figure 8.3. Solution Coloring Process Flow Diagram

After undyed nylon is drawn and wound into yarn, it can also be dyed by either immersion in a heated dye bath, as in skein dyeing, or printed with the dye, as in space dyeing. In skein dyeing, skeins of yarn are put on a rack and inserted into a square open tank. Water, pigments, and chemicals are added, and a lid is placed on the tank. A recirculating pump provides agitation and steam coils provide heating. After about 30 minutes, the color is checked, and if acceptable (about 40% of the time), the skeins are removed. If further color adjustment is needed a second addition and recirculating time is provided (about 60% of the time). The skeins removed are put into a centrifuge water extractor and leave at about 40 weight % water. The skeins are then placed on a short conveyor system through a hot air dryer and then are air-cooled. (See Figure 8.4.)

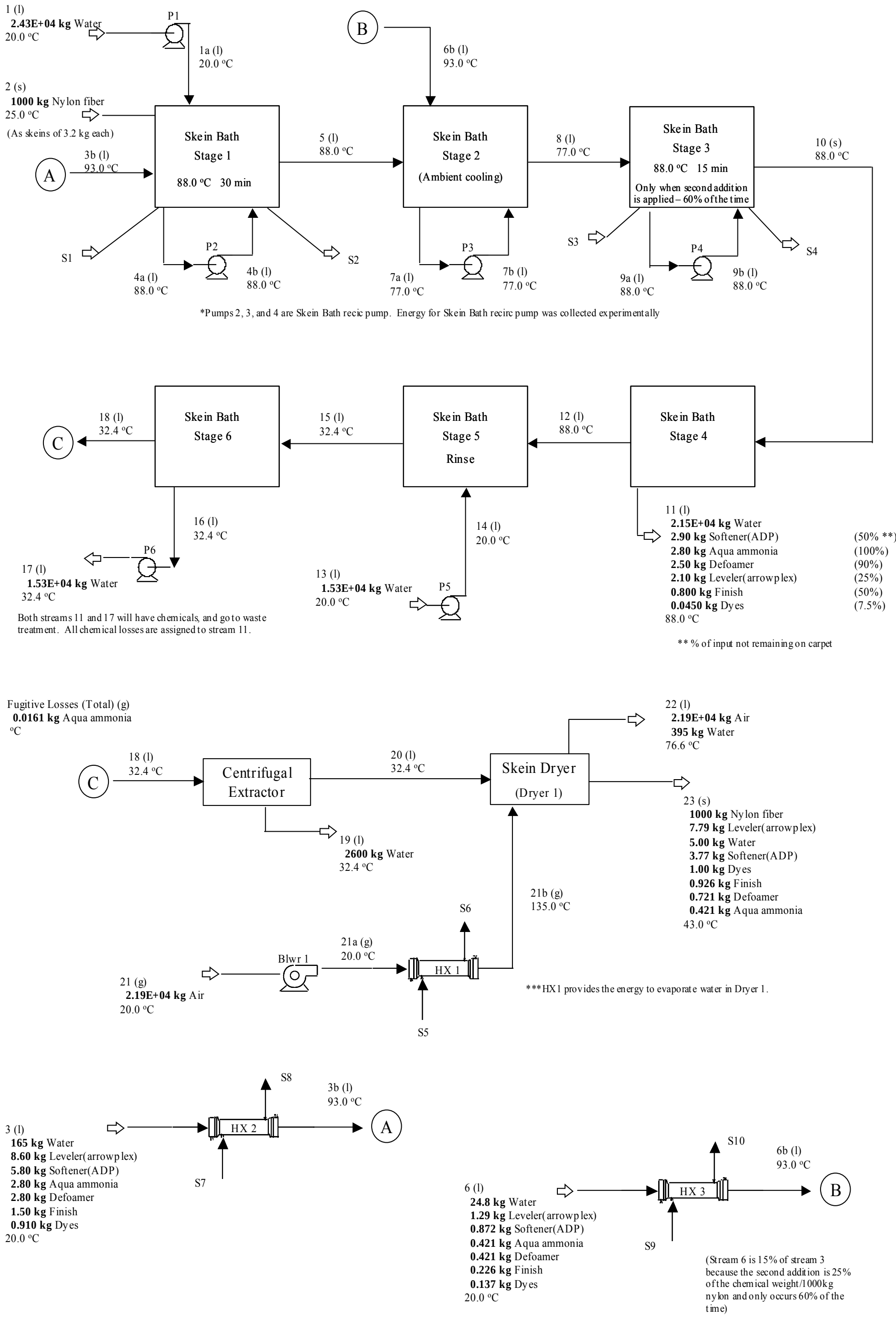

Figure 8.4. Skein Yarn Dyeing Process Flow Diagram

In space dyeing, parallel strands of nylon yarn are randomly printed with dye to create a yarn with intermittent color patterns. Next, the yarn is steamed to set the color and then excess liquid is extracted. Finally, the yarn is dried and wound for further processing. (See Figure 8.5.)

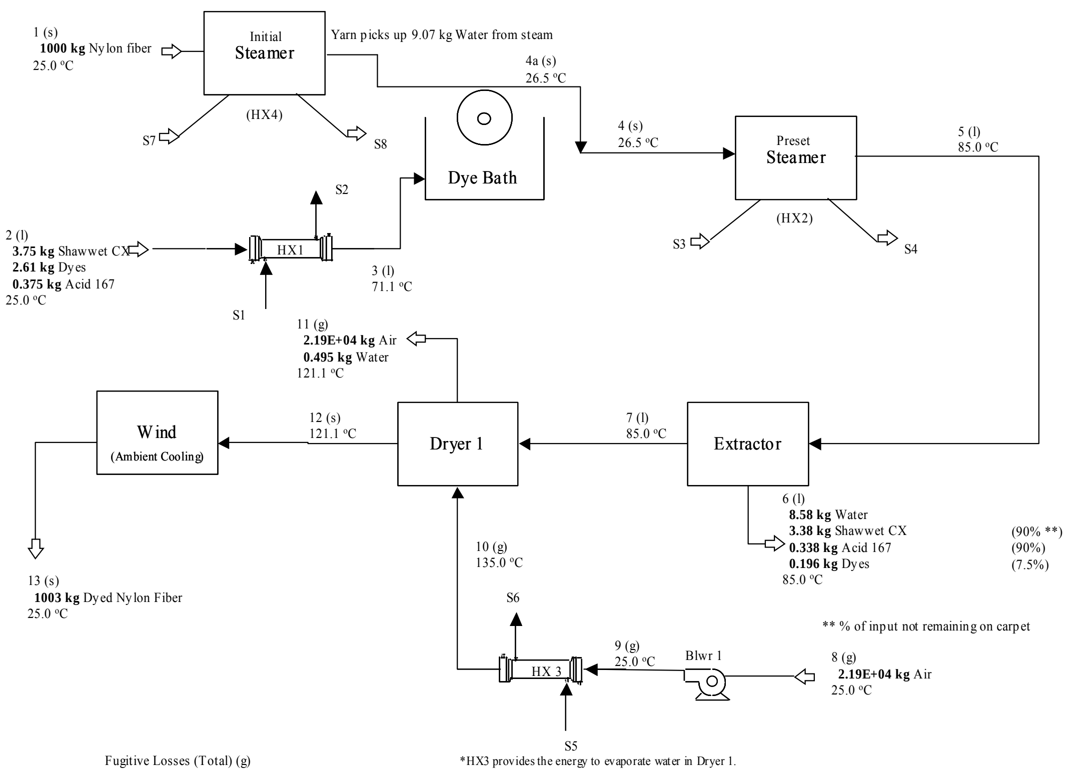

Figure 8.5. Space Yarn Dyeing Process Flow Diagram

Tufted, unfinished nylon carpet, consisting of face fiber and polypropylene backing, can be dyed either by a Beck or continuous dyeing process. In Beck dyeing, tufted carpet pieces are dipped and cycled in heated dye baths. If color is not within tolerances, a second cycle of Beck dyeing is used (~ 40% of time). Then the tufted piece is drained, excess water is extracted, and dried. (See Figure 8.6.)

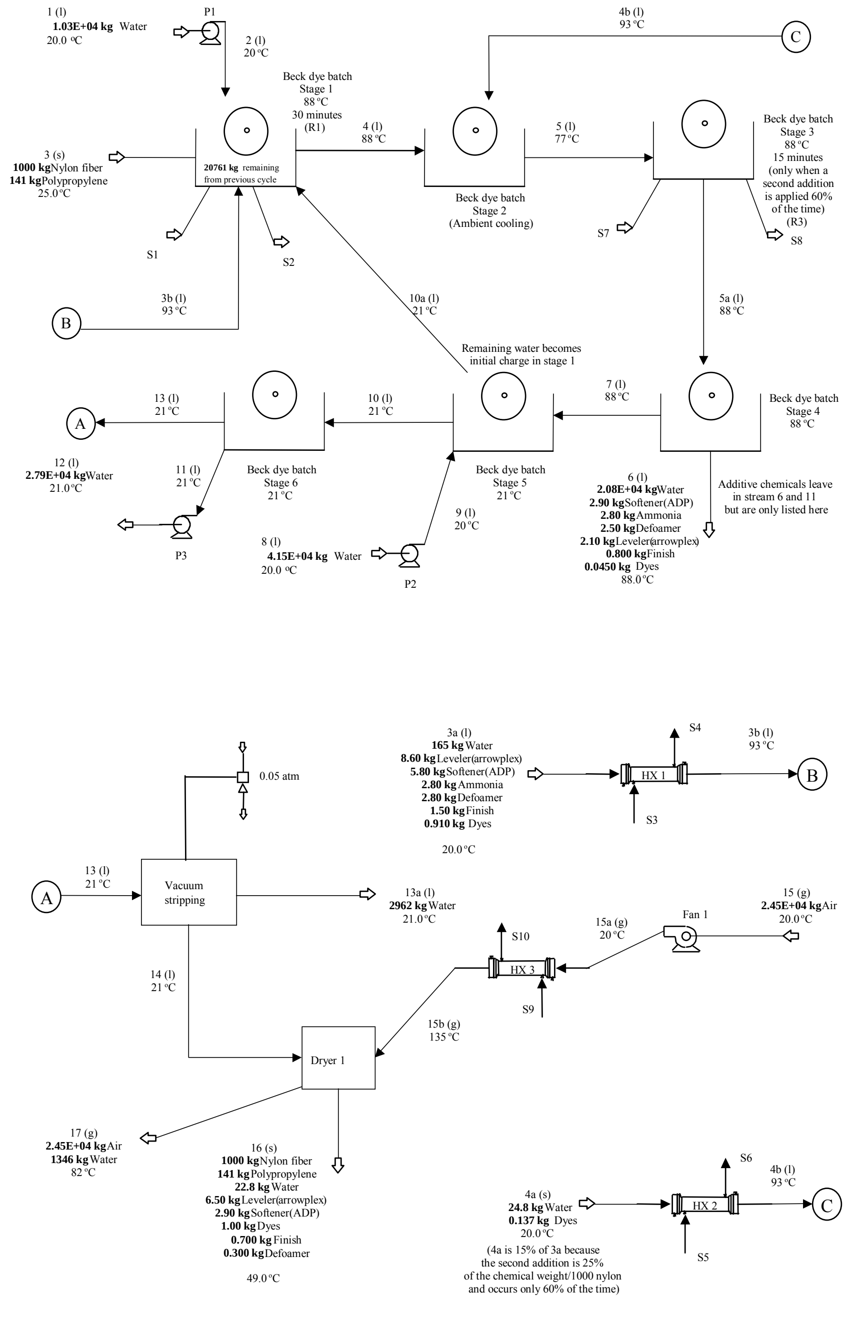

Figure 8.6. Beck Carpet Dyeing Process Flow Diagram

In the continuous carpet dyeing process tufted carpet is pre-steamed before going through a dye bath. After the dye bath, the carpet is steamed to fix the dye and excess liquid is extracted. The carpet is dried and cooled to ambient temperature. (See Figure 8.7.)

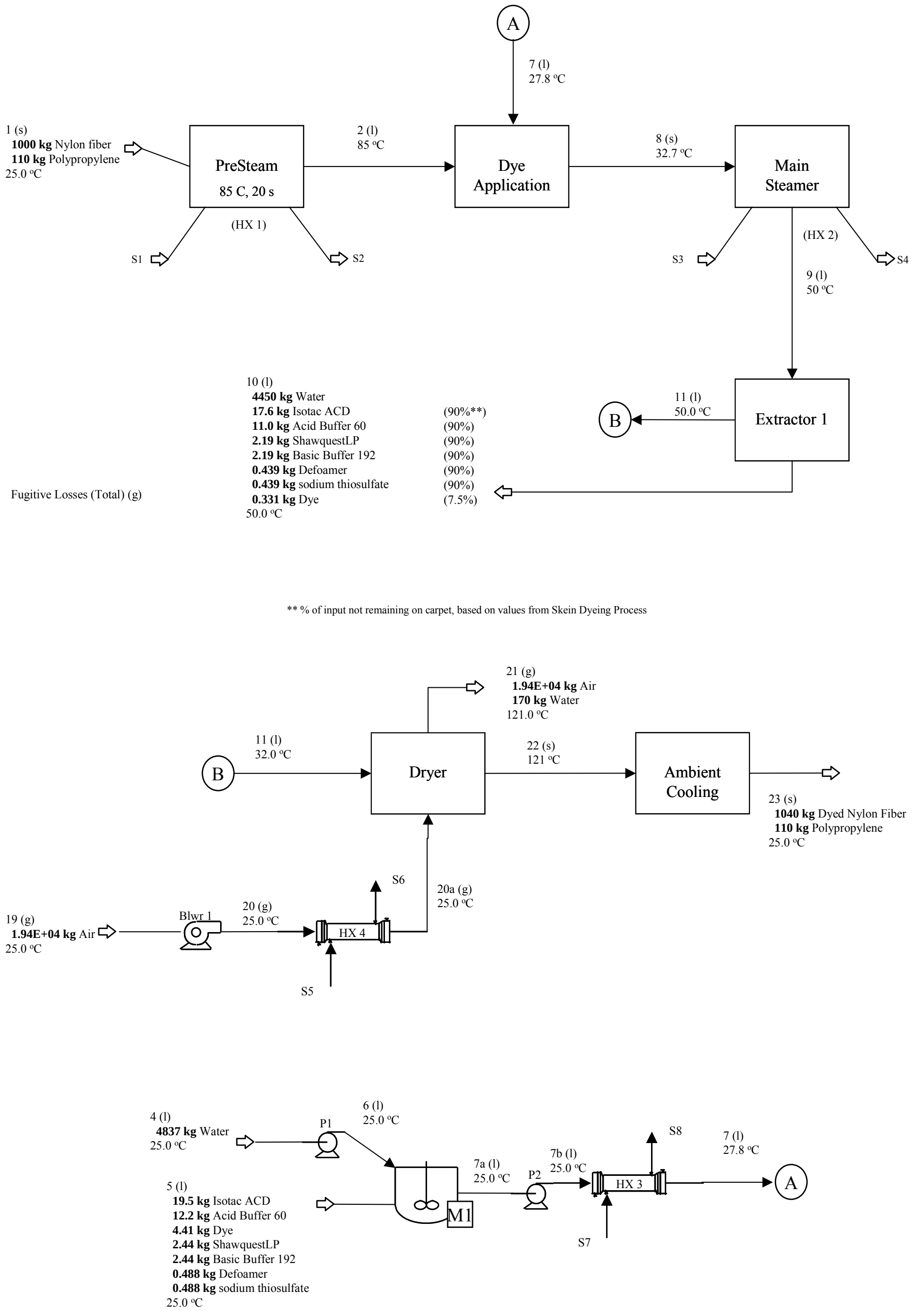

Figure 8.7. Continuous Carpet Dyeing Process Flow Diagram

While finishes such as stain resistances can be added in some of these dyeing processes, finishes were excluded in these studies to better compare the dyeing processes. Currently most finishes are foam applied in the carpet manufacturing mill and thus included in those LCI.

8.4 Results

The gate-to-gate dyeing process inputs and energy consumption for each coloring process are shown in Table 8.1. These are determined from the cumulative unit processes shown in Figures 8.3-8.7. The dyed nylon is assumed to be used in the same mill to make the final carpet product and hence no transport energy of the dyed nylon is included. All methods used the same amount of nylon. The solution coloring process only requires the electricity from the extruder and pelletizer to mix in the colorant. The remaining processes in Figure 8.3 are used in the general extrusion of nylon fiber, so micro-allocation is used to capture the energy needed solely for coloring. Since solution coloring adds pigment during the extrusion of the fiber, no water is needed. Solution coloring uses the most dye since the pigment is mixed throughout the nylon fiber during the extrusion process. In the other methods the dye is on the surface of the nylon fiber. A breakdown of the energy per process within each dyeing process is shown in Table 8.2.

Table 8.1. Inputs and Energy Required for Dyeing Processes, see explanation for exclusion of transport above.

Dyeing Process		Inputs, kg			Energy, MJ/1000 kg Nylon			Market Supply, % of Commercial Carpet Market
		Nylon	Dye	Water	Electricity	Steam	Total	
Pre-fiber	Solution	1,000	20.4	0	33.3	0	33.3	70%
Post-fiber	Skein	1,000	1.05	39,800	90.1	12,639	12,729	6%
	Space	1,000	2.61	9.1	429	5,114	5,544	9%
Post-carpet	Beck	1,000	1.05	52,100	682	19,941	20,624	14.8%
	Continuous	1,000	4.41	7,003	12.3	2,041	2,054	0.2%
Representative Commercial Carpet					168	4,300	4,470	

Table 8.2. Energy per Process within Dyeing Processes (not including diesel transport energy)

	Energy Per Process, MJ/1000 kg Nylon				
Dye Process	**Solution**	**Skein**	**Space**	**Beck**	**Continuous**
Extrusion	32.9				
Pelletizing	0.33				
Pre-Steam			17.3		135
Dye Application 1		8357	0.18	12701	67.4
Dye Application 2		1363		3932	
Rinse		1.16		1.80	
Steam			2247		447
Extraction		28.8	280	393	10.3
Drying		2979	2850	3596	1393
Winding			149		
Total	33.3	12729	5544	20624	2054

A styrene-butadiene latex-backed broadloom was selected to illustrate the inputs and emissions to manufacture a square yard of carpet (as shown in Table 8.3). Table 8.4

shows the energy for the dye process and the gate-to-gate and cradle-to-gate carpet manufacture in units of megajoules per square yard of carpet. The emissions from the cradle-to-gate carpet manufacture are shown for each type of carpet dyeing in Table 8.5. Not all of the dye and finish used in the dye bath solution remain on the dyed fiber. Of the dye and additives used, 93% of the dye and 50% of the softener and finish remain on the carpet. The balance is discharged in the wastewater to the POTW.

Table 8.3. Inputs and waste emissions for 1 square yard styrene butadiene latex-backed broadloom commercial carpet (1 square yard = 1.92 kg on the floor of a commercial building)

Inputs	kg/yd^2
(Dyed) nylon fiber	0.86
Polypropylene	0.19
Calcium carbonate	0.51
Aluminum hydroxide	0.25
Styrene butadiene latex	0.22
Total Inputs	2.03
Material Losses	kg/yd^2
(Dyed) nylon fiber	0.038
Polypropylene	0.017
Calcium carbonate	0.029
Aluminum hydroxide	0.014
Styrene butadiene latex	0.012
Total Emissions	0.111

Table 8.4. Energy for Carpet Manufacture (Styrene butadiene latex-backed broadloom)

	Energy, MJ per square yard Carpet				
	Solution	Skein	Space	Beck	Continuous
Gate-to-Gate Dye Process	0.03	11.3	3.00	16.7	1.99
Gate-to-Gate Carpet Manufacturing (no dye)	7.46	7.46	7.46	7.46	7.46
Cradle-to-Gate Carpet Manufacture	38.6	50.0	41.9	54.7	39.8

Table 8.5. Chemical Emissions from Cradle-to-Gate carpet manufacturing using each dye process

	kg Chemical Emission per square yard Carpet				
Chemical Emission	**Solution**	**Skein**	**Space**	**Beck**	**Continuous**
1,3-butadiene	1.58E+00	1.58E+00	1.58E+00	1.58E+00	1.58E+00
Acetylene	5.31E-03	5.31E-03	5.34E-03	4.49E-03	4.17E-03
Acrylic acid	1.34E-02	1.34E-02	1.34E-02	1.34E-02	1.34E-02
Aluminum chloride	1.63E-01	1.63E-01	1.63E-01	1.63E-01	1.63E-01
Aluminum hydroxide	1.01E+01	1.01E+01	1.01E+01	1.01E+01	1.01E+01
Ammonia	8.65E-01	2.10E+00	8.77E-01	2.22E+00	9.23E-01
Argon	8.98E-01	8.98E-01	9.07E-01	9.29E-01	9.43E-01
Arsenic	3.43E-06	3.43E-06	3.47E-06	3.30E-06	3.24E-06
BaSO4	3.36E-02	3.36E-02	3.36E-02	3.36E-02	3.36E-02
Benzene	3.40E+00	3.40E+00	3.45E+00	3.58E+00	3.65E+00
BOD	1.39E-01	1.74E-01	1.52E-01	1.91E-01	1.37E-01
BOD5	8.81E-03	8.82E-03	8.97E-03	9.34E-03	9.56E-03
Boron	1.70E-03	1.70E-03	1.72E-03	1.63E-03	1.61E-03
Butane	2.70E-02	2.70E-02	2.72E-02	2.36E-02	2.23E-02
Butene	6.87E-02	6.87E-02	6.90E-02	5.81E-02	5.39E-02
butenes and butanes	6.90E-02	6.90E-02	6.90E-02	6.90E-02	6.90E-02
Calcium carbonate	1.76E+01	1.76E+01	1.76E+01	1.76E+01	1.76E+01
Calcium hydroxide	2.73E+00	2.73E+00	2.73E+00	2.73E+00	2.73E+00
Caprolactam	7.64E+00	7.65E+00	7.78E+00	8.10E+00	8.30E+00
Carbon dioxide	2.31E+03	2.75E+03	2.46E+03	2.96E+03	2.34E+03
Carbon monoxide	2.60E+00	2.91E+00	2.71E+00	3.11E+00	2.71E+00
Chloride	1.25E+00	1.25E+00	1.27E+00	1.20E+00	1.18E+00
Chlorine	1.78E-01	1.78E-01	1.78E-01	1.78E-01	1.78E-01

Table 8.5 continued

	kg Chemical Emission per square yard Carpet				
Chemical Emission	**Solution**	**Skein**	**Space**	**Beck**	**Continuous**
COD	2.50E+00	2.62E+00	2.64E+00	2.72E+00	2.39E+00
Cyclohexane	6.25E+00	6.26E+00	6.36E+00	6.63E+00	6.78E+00
Cyclohexanone oxime	1.27E+00	1.27E+00	1.29E+00	1.35E+00	1.38E+00
Disproportionated tall oil	6.09E-04	6.09E-04	6.09E-04	6.09E-04	6.09E-04
Dust	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
Ethane	1.29E-01	1.29E-01	1.30E-01	1.23E-01	1.20E-01
Ethylene	3.83E-01	3.83E-01	3.84E-01	3.42E-01	3.27E-01
grease / oil	2.04E-02	2.04E-02	2.06E-02	1.96E-02	1.93E-02
Heptane	1.12E-02	1.12E-02	1.13E-02	1.08E-02	1.06E-02
HSLBLatex	6.44E+00	6.44E+00	6.44E+00	6.44E+00	6.44E+00
Hydrogen	1.05E+00	1.05E+00	1.06E+00	1.10E+00	1.13E+00
Hydrogen chloride	1.67E-01	1.67E-01	1.67E-01	1.67E-01	1.67E-01
Hydrogen sulfide	5.21E-03	5.21E-03	5.22E-03	5.22E-03	5.22E-03
Hypochlorous acid	1.39E-04	1.39E-04	1.39E-04	1.39E-04	1.39E-04
Isobutane	3.87E-04	3.87E-04	3.91E-04	3.71E-04	3.66E-04
Magnesium hydroxide	2.41E-03	2.41E-03	2.41E-03	2.41E-03	2.41E-03
Mercury	2.52E-06	2.52E-06	2.52E-06	2.52E-06	2.52E-06
Methane	5.85E+00	6.67E+00	6.20E+00	7.06E+00	5.82E+00
Mobile ions	3.95E+00	3.95E+00	3.99E+00	3.79E+00	3.73E+00
Mud (salt process)	1.49E+00	1.49E+00	1.49E+00	1.49E+00	1.49E+00
Naphtha	4.00E+00	4.00E+00	4.02E+00	3.38E+00	3.14E+00
n-Hexane	7.09E-01	7.10E-01	7.20E-01	7.46E-01	7.61E-01
Nitric oxide	3.88E-01	3.88E-01	3.94E-01	4.11E-01	4.21E-01
Nitrogen dioxide	1.11E+01	1.11E+01	1.13E+01	1.17E+01	1.20E+01
Nitrogen monoxide	2.38E-01	2.38E-01	2.40E-01	2.46E-01	2.50E-01
NMVOC	5.59E+00	7.82E+00	6.16E+00	8.75E+00	5.89E+00
Nox	8.32E+00	9.78E+00	8.79E+00	1.05E+01	8.48E+00
n-Pentane	5.41E-03	5.42E-03	5.48E-03	5.20E-03	5.12E-03
Octane	8.41E-03	8.42E-03	8.51E-03	8.08E-03	7.95E-03
Oligomer	1.64E-01	1.64E-01	1.67E-01	1.74E-01	1.78E-01
Polypropylene	9.06E+00	9.06E+00	9.06E+00	6.57E-02	5.25E-02
Propane	6.09E-02	6.10E-02	6.19E-02	6.36E-02	6.47E-02
Propylene	3.76E+00	3.76E+00	3.76E+00	2.61E+00	2.16E+00
Propyne	4.76E-03	4.76E-03	4.78E-03	4.02E-03	3.73E-03
pyrolysis gas	5.45E-01	5.45E-01	5.48E-01	4.61E-01	4.28E-01

Table 8.5 continued

	kg Chemical Emission per square yard Carpet				
Chemical Emission	Solution	Skein	Space	Beck	Continuous
Red mud	1.82E+02	1.82E+02	1.82E+02	1.82E+02	1.82E+02
Sodium	1.61E+00	1.61E+00	1.63E+00	1.55E+00	1.52E+00
Sodium chloride	7.01E-01	7.01E-01	7.01E-01	7.01E-01	7.01E-01
Sodium hydroxide	4.56E+00	4.56E+00	4.56E+00	4.56E+00	4.56E+00
sodium thiosulfate					2.09E-01
Sox	6.92E+00	8.85E+00	7.52E+00	9.87E+00	7.14E+00
Styrene	1.85E-01	1.85E-01	1.85E-01	1.85E-01	1.85E-01
Sulfur	2.09E-01	2.09E-01	2.13E-01	2.22E-01	2.27E-01
Sulfur trioxide	6.09E-01	6.09E-01	6.19E-01	6.45E-01	6.61E-01
TDS	3.33E+00	5.34E+00	3.90E+00	6.28E+00	3.41E+00
Toluene	2.58E+01	2.58E+01	2.63E+01	2.74E+01	2.80E+01
Vinylacetylene	1.65E-03	1.65E-03	1.65E-03	1.65E-03	1.65E-03

8.5 Discussion

Of the five coloring processes studied, solution coloring used the least energy and the most colorant, as shown in Table 8.1. The colorant is melted with the nylon and the fiber contains color throughout.

Batch processes that involve immersing the fiber in a dye bath, such as skein or Beck dyeing, use more water than other processes and also discharge more wastewater. This water must be heated to allow penetration and setting of the dye, causing more energy to be used for these processes. These batch processes allow rapid change of colors and small volumes of dyed fibers. As seen in Table 8.2, dye application for these processes, usually with heated aqueous baths at long residence times, requires the most energy, followed by drying. For space and continuous dyeing, steaming is used to set the dye. For these processes, drying uses the most energy, followed by steaming.

With this analysis, the variation in dyeing process energy is clarified. However, the functional unit, 1000 kg dyed nylon is actually not complete. These dyeing processes actually deliver different appearances when laid in a commercial building floor. Thus the variations in dyeing process energy should be viewed as investment in consumer preference. Table 8.6 captures the changes in appearance from the lowest energy process (solution coloring) to the highest.

Table 8.6. Appearance differences gained with increasing dyeing energy

Dyeing system	Carpet Appearance	Customer Need and Manufacturing Factors
Predyed Fiber Dyeing		
Solution dyed	Because inorganic pigments are used for coloring, this system produces the effects of resistance to change due to light and oxidizing agents such as bleaches. This is a robust feature of the carpet, but for many colors the brightness is not as high.	More stable yarn color performance used in higher traffic areas and applications. Limited number of colors available.
Skein dyed	The dyeing of individual lots of yarn can then be blended to include three to four colors and produces an important visual effect. Organic dyes are used	Picked for clear and distinct colors where any color combo can be obtained. Design appeal. Labor intensive. Big investment in equipment and floor space. Requires complex scheduling. Highest cost pre-dyed yarn method.
Space dyed	Approximately four to seven separate colors can be applied in either short or long spacing intervals. These different interval yarns can also be plied. The multi colored effect allows greater matching of accents with other aspects of a room, such as furniture, walls, and fabrics. Organic dyes are used.	Multi-color yarn effect not able to be created by another dye method. Ability to economically customize a style to meet designer accent requirements. Efficient process. Process requires little plant square footage. Not labor intensive.
Post Carpet or Piece Dyeing		
Beck	This method produces very uniform colors since the entire carpet is dyed in a batch application. With the extended residence time at the bath temperatures, close to the boil, the face fiber is more highly bulked providing a plush effect to the consumer. Typically, level dyeing acid dyes are used to promote color uniformity.	For very dark shades and custom colors this provides the most flexibility. Also, this is the only method for re-dyeing off color shades from a continuous dye line. Gives best dyeing – no sidematch issues, excellent levelness. Most expensive due to time and limited dyelot sizes. Labor intensive. Big investment in equipment and floor space. High energy costs.
Continuous	This high speed dyeing technique has variations that are hard to detect. In the typical residential uses of a single room, these variations are hard to detect, but in large commercial areas these variations are discernable. Organic dyes are used.	Lowest costs for manufacturing. Limitations are dark shades, weight of face fiber and very tight constructions. Virtually non-existent in commercial

Table 8.4 compares the dyeing process energy along with the carpet manufacture and the cradle-to-gate energy consumption. The dyeing process energy is solely the energy to dye the fiber, yarn or carpet, using one of the five processes of this article. The gate-to-gate energy is the energy to manufacture styrene butadiene latex-backed broadloom commercial carpet within the factory. The cradle-to-gate energy is the energy to manufacture styrene butadiene latex-backed broadloom commercial carpet from the factory back to the raw materials (cradle). Even though a small amount of dye is used

compared to other materials (20 or less kg dye per 1000 kg nylon), the dyeing process does have an impact on the cradle-to-gate energy consumption. If the type of dyeing process were insignificant, the CTG energy would be the same for carpet dyed using any of the five methods. The same carpet manufacturing process is used for the cradle-to-gate carpet manufacturing energy, so the amount of energy for carpet manufacturing is the same for all dyeing processes. For an energy intensive process, such as Beck dyeing, the overall CTG energy is the highest, and dyeing consumes 31% of the total CTG energy. The dyeing process energy depending on the process can range from 0.1% to 31% of the cradle-to-gate energy.

A life cycle assessment (LCA) on the cradle-to-gate carpet manufacturing using US EPA TRACI impact factors was complete for a square yard of carpet. The categories of global warming potential, acidification, eutrophication, smog, ecotoxicity, and human health noncancer are shown in Figures 8.8-8.13. Based on Bare et al (Bare, 2002), the TRACI impact factors for each impact category are multiplied by the total emissions from making the carpet cradle-to-gate, according to

$$\text{Impact Factor Potential} = \sum_i e_i \times impactfactor_i \qquad (8.1)$$

where e_i is the emission of chemical i and impact $factor_i$ is the impact factor of chemical i. The effect of dyeing method on global warming, acidification, eutrophication, and smog is not substantially different, given the LCI variability. Since dye or pigment manufacturing CTG were not included, the approximately 140-fold greater pigment/dye level in solution coloring is not fully captured. In a separate evaluation of copper pthtalocyanine pigment CTG life cycle impact categories, the larger amount of pigment in solution coloring would result in greater ecotoxicity and human health noncancer impacts.

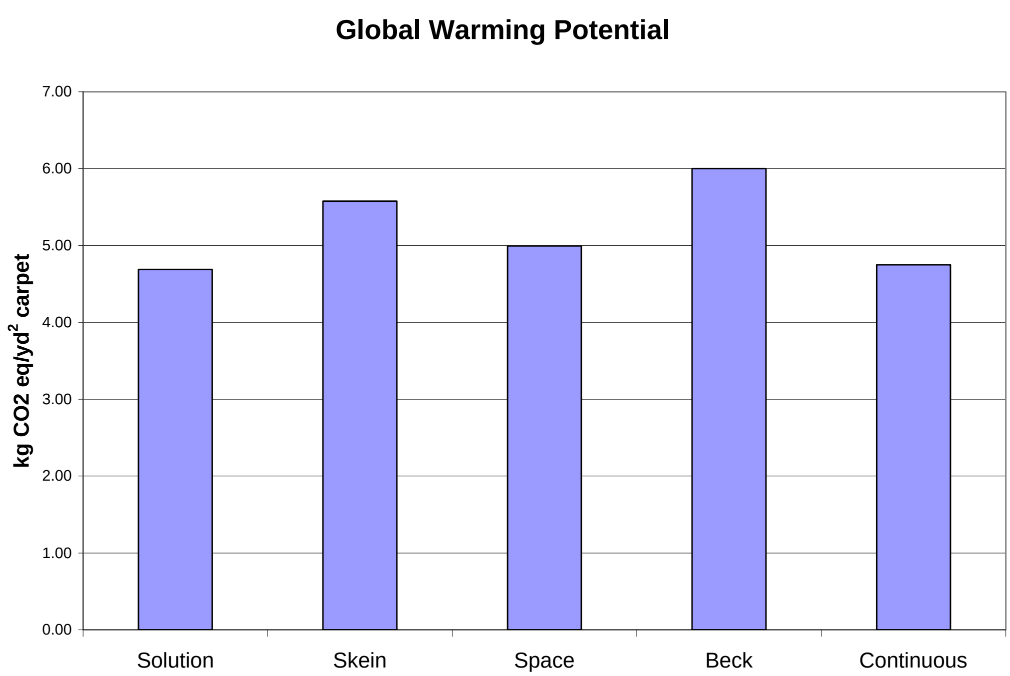

Figure 8.8. Global Warming Potential impact analysis using US EPA TRACI impact factors for the cradle-to-gate manufacture of a square yard of carpet

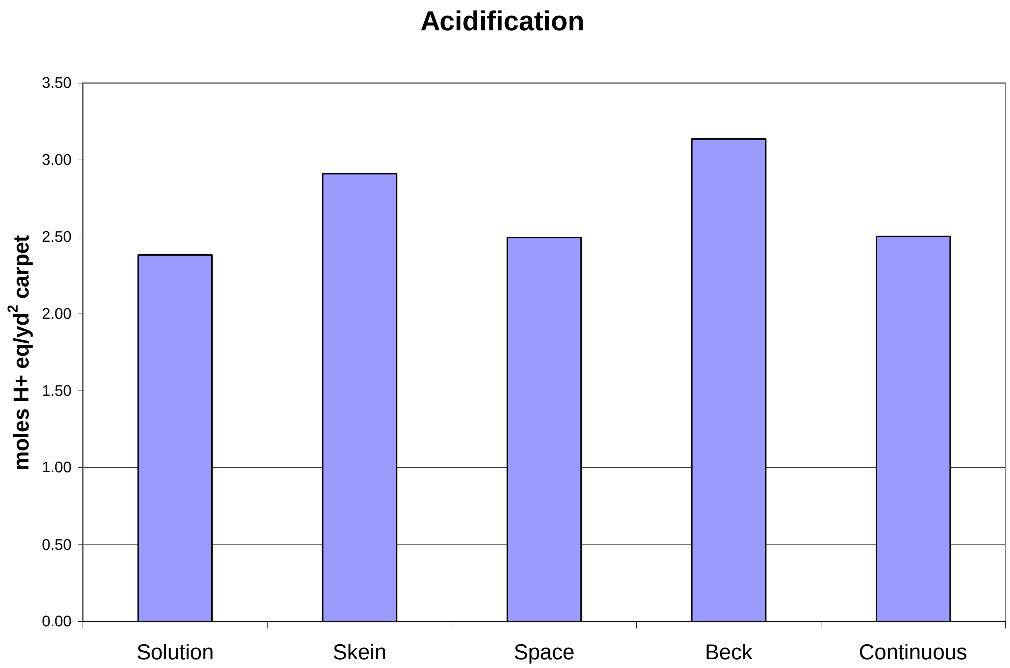

Figure 8.9. Acidification impact analysis using US EPA TRACI impact factors for the cradle-to-gate manufacture of a square yard of carpet

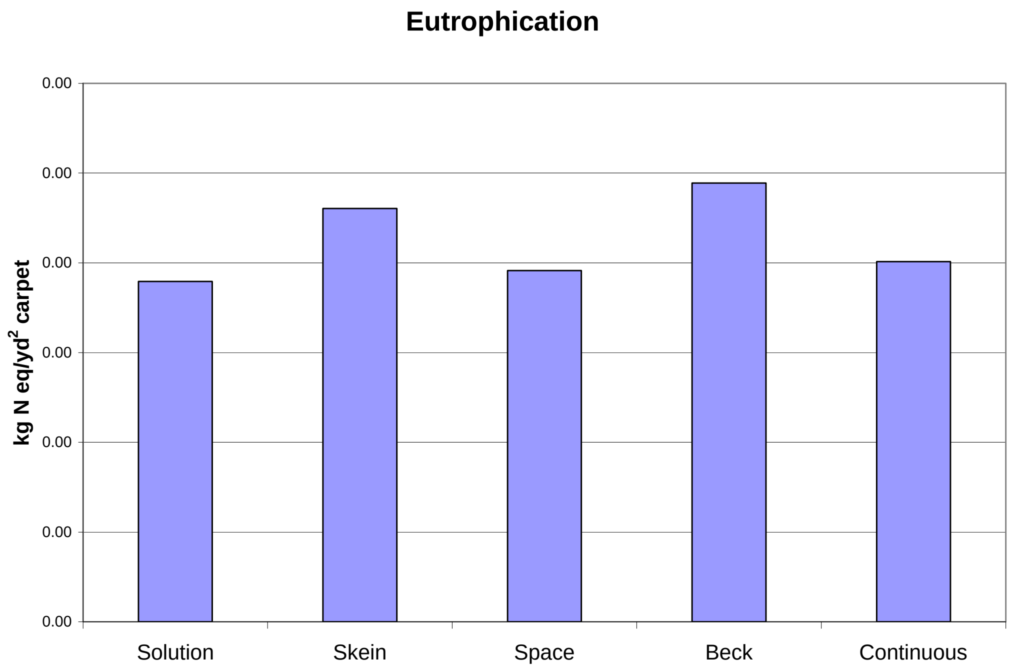

Figure 8.10. Eutrophication impact analysis using US EPA TRACI impact factors for the cradle-to-gate manufacture of a square yard of carpet

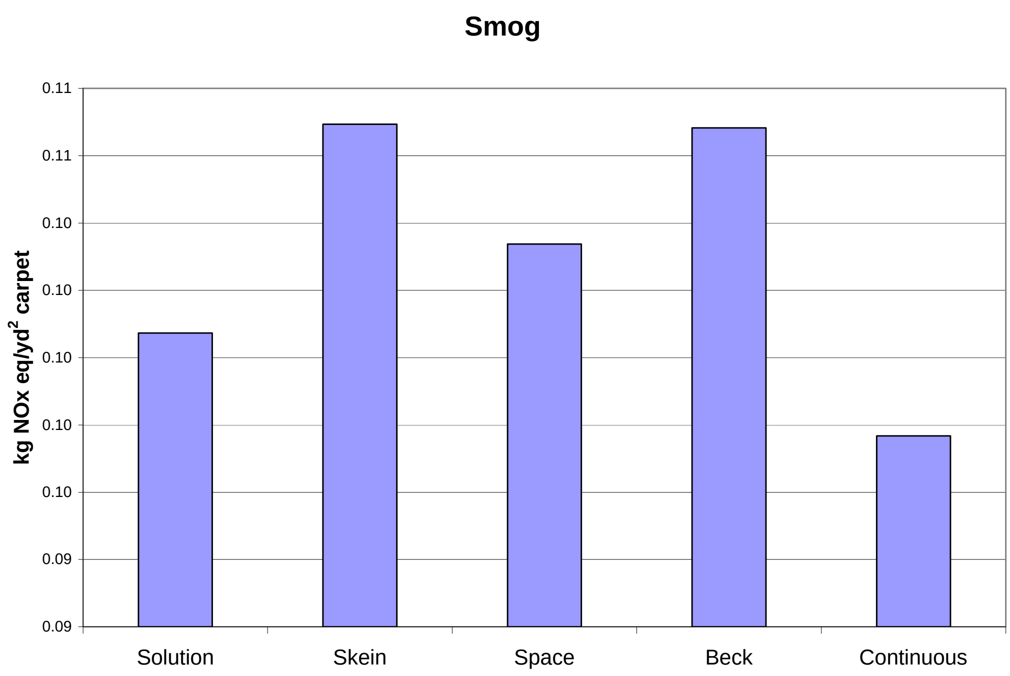

Figure 8.11. Smog impact analysis using US EPA TRACI impact factors for the cradle-to-gate manufacture of a square yard of carpet

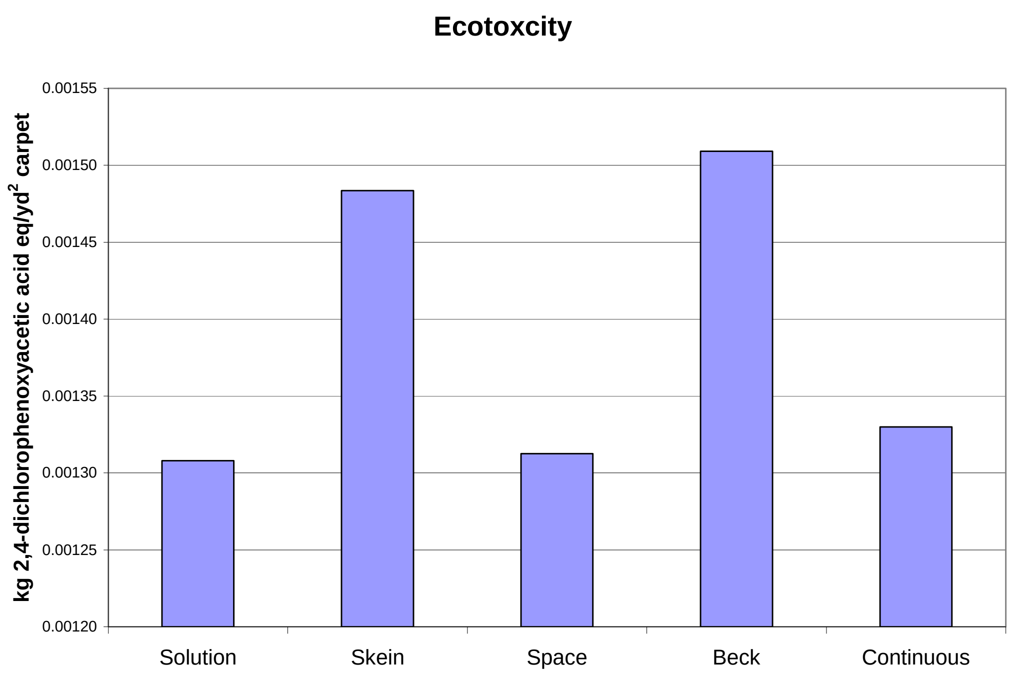

Figure 8.12. Ecotoxicity to Air impact analysis using US EPA TRACI impact factors for the cradle-to-gate manufacture of a square yard of carpet

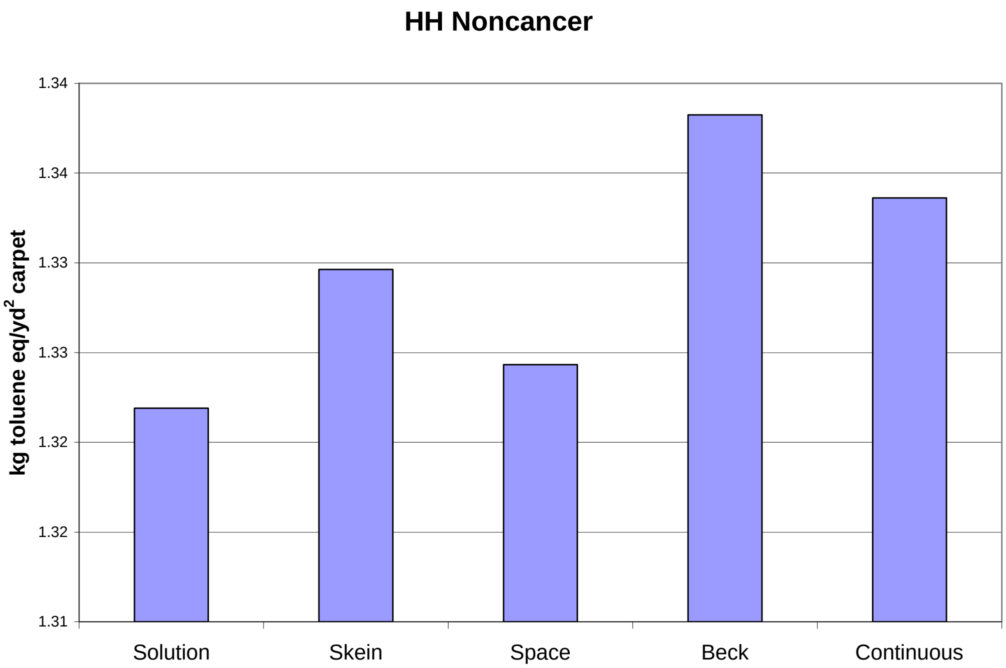

Figure 8.13. Human Health Noncancer impact analysis using US EPA TRACI impact factors for the cradle-to-gate manufacture of a square yard of carpet

8.6 Conclusions

In general, dye application and drying are the most energy intensive steps in dyeing. Batch processes consume the most water and energy, and dyeing carpet requires more water and energy than dyeing yarn only. Solution coloring used the least amount of energy, but consumed the most colorant. Solution and space dyeing required the least amount of water. The effect of dyeing process on the overall CTG of carpet manufacturing is between 0.1% - 31% with the higher energy yielding better appearance factors for customers.

8.7 Acknowledgements

The authors would like to thank Shaw Industries, Inc., J & J Invision, and the members of the Carpet and Rug Institute Sustainability Issues Management Team for their input to this work.

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9. Impact and Future Work

The aim of this body of work is to assess the environmental impact of using reusable and disposable health care garments and investigate options to reduce this environmental impact. In this research, life cycle inventories are utilized in the design of a reusable medical garment with a biocidal finish to: assess options for the biocidal chemical, compare the reusable garment with a disposable garment, and assess the use of a biocidal finish in a hospital setting. Life cycle inventories are also used to quantify the environmental impact of treating an infection once a hospital patient has become infected and the environmental impact of reducing infections. The life cycle inventories were calculated based on the process design method that uses engineering principles and rules of thumb to calculate the mass and energy balances for each unit operation in the production of each chemical used in the cradle-to-gate manufacture of the product.

The cradle-to-gate life cycle inventories of two biocidal halamines – 3-allyl-5,5-dimethyl hydantoin (ADMH) and dimethylol-5,5-dimethyl hydantoin (DMDMH) – are compared to allow the manufacturer to select the chemical that consumes less energy and raw materials and generates fewer emissions. The LCIs showed that ADMH uses four times more resources and generates ten times more emissions than DMDMH. The reusable garment is then compared with a disposable gown of similar use to determine, cradle-to-use, which has the better environmental performance. When the reusable gown is used more than ten times, the amount of energy used cradle-to-gate is less than the energy used for an equivalent number of disposable gowns.

Life cycle inventory analysis is also used to determine the resources and emissions saved by the hypothetical use of a biocidal patient gown and the subsequent reduction in nosocomial infections. This is a novel area for LCI, as no LCI has been studied for treating an infection previously. When a patient contracts an infection while in the hospital, additional materials are used to test the patient, to provide contact isolation, and to treat the patient. Inventories were analyzed for each phase of this treatment using MRSA (Methicillin-resistant Staphylococcus aureus) as the nosocomial infection contracted and treated. This analysis shows that a 5% reduction in the number of nosocomial infections can offset the manufacture and use of the biocidal finish on the patient gown.

During this analysis, waste management was not included in each gate-to-gate inventory. The process design method uses information from literature and patents, and often this waste treatment information is not included. The inclusion of waste treatment to form the complete cradle-to-grave life cycle inventory may tell a different story. Laundering during the use phase produces waste water that must be sent to a wastewater treatment plant (WWTP). Energy and additives are required during this process, and emissions are generated. This will increase the reusable gown's environmental footprint and the number of times the gown must be re-used for it to have a smaller footprint than the disposable gown. Waste treatment information can be estimated using the methodology by Jimenez-Gonzalez (Jimenez-Gonzalez et al., 2001). Inputs (oxygen, electricity, etc.) and outputs (VOC, CO_2, etc.) for wastewater treatment are based on chemical oxygen demand (COD) and total organic carbon (TOC) of the wastewater stream.

Including disposal options will show the complete environmental footprint. If waste water treatment increases the gown energy by 20%, the number of gown uses increases from 10.7 to 11.2 to equal the energy needed for an equivalent number of disposal gowns. For disposal, the garments can be incinerated, requiring energy and generating emissions. A portion of the heat generated by the incinerator can be recovered for steam production. Due to the larger mass of the 75,000 disposable gowns used, more steam will be recovered from the disposable gowns than from the 1000 reusable gowns used. The reusable gowns can also be re-manufactured into cleaning cloths, and this will allocate some of the gown resources to these products.

References

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10. Appendix

A. Life Cycle Inventories Used for this Study

Table 10.1. Gate-to-Gate Chemical Life Cycle Inventories Used in this Study

1	1,3-butadiene
2	3-Allyl-5,5-dimethylhydantoin
3	Acetic acid
4	Acetone
5	Agar
6	Allyl Alcohol
7	Allyl bromide
8	Ammonia
9	Ammonium chloride
10	Benzene
11	Brine
12	Bromine
13	C4 stream
14	Carbon dioxide
15	Carbon monoxide
16	Casein
17	Casein hydrolysate
18	Chlorine
19	Continuous Nylon Dyeing
20	Corn
21	corn starch
22	Cotton
23	Cotton Polyester Fabric
24	Cotton Polyester Yarn
25	Cotton Seed
26	DAP
27	Dextrose
28	Dichloroethane,-1,2
29	Dimethyl hydantoin
30	Dimethyloldimethyl hydantoin
31	Ethylbenzene
32	Ethylene
33	Ethylene glycol

Table 10.1 continued

34	Ethylene oxide
35	Formaldehyde
36	Gelidium Algae
37	Hydrogen
38	Hydrogen bromide
39	Hydrogen chloride
40	Hydrogen cyanide
41	Hypochlorous acid
42	Isopropanol
43	K in fertilizer
44	KOH in solution (50%)
45	Methanol
46	MH Agar Plate
47	Milk
48	N in DAP
49	N in fertilizer
50	Naphtha
51	Natural gas
52	n-Hexane
53	Nitrogen from air
54	Oxygen
55	Oxygen from air
56	P in DAP
57	P in fertilizer
58	p-benzenedicarboxylic acid
59	PET
60	Petri Dish
61	Phosphate rock
62	Phosphoric acid
63	Polypropylene
64	Polystyrene
65	Potassium chloride
66	Potassium Hydroxide
67	Propylene

Table 10.1 continued

68	Propylene oxide
69	PVC
70	p-Xylene
71	pyrolysis gas
72	Reactive Cotton Dyeing
73	reformate, from naphtha
74	Reusable Gown (Cotton Polyester Gown)
75	Skein Nylon Dyeing
76	Sodium carbonate
77	Sodium chloride
78	Sodium hydroxide
79	Soy Flour
80	Soybean Extraction (for Soy Flour)
81	Soybean
82	Soybean Seed
83	Space Nylon Dyeing
84	SMS Gown
85	SMS Polypropylene Fabric
86	Styrene
87	Styrene butadiene latex
88	Sulfur
89	Sulfur trioxide
90	Sulfuric acid
91	Sylvinite ore
92	Toluene
93	Urea
94	Vancomycin HCl
95	Vinyl Chloride
96	Water for rxn

Table 10.2. List of Life Cycle Inventories Completed for this Study

1	Acetic Peroxide
2	Agar
3	Allyl Bromide
4	Allyl dimethylhydantoin
5	Calcium hypochlorite
6	Casein
7	Casein hydrolysate
8	Continuous Nylon Dyeing
9	Cotton
10	Cotton Polyester Fabric
11	Cotton Polyester Gown (Reusable Gown)
12	Cotton Polyester Yarn
13	Dextrose
14	Dimethyl hydantoin
15	Dimethylol dimethylhydantoin
16	Disodium phosphate
17	Dodecene
18	Dodecyl benzene
19	Fluoroacrylate Stearyl Methacrylate Copolymer
20	Gelidium
21	Hexane
22	Infection Treatment
23	Latex Glove
24	Laundry Cleaning with Chlorine Bleach
25	Laundry Cleaning without Chlorine Bleach
26	Lauryl Alcohol Ethoxylate
27	Linear Alkylbenzene sulfonate
28	Milk
29	Mueller Hinton Agar Plate
30	Petri Dish
31	Polyester Spunlace Fabric

Table 10.2 continued

32	Polyester Spunlace Gown
33	Polypropylene SMS Fabric
34	Polypropylene SMS Gown
35	Potassium hypochlorite
36	Reactive Cotton Dyeing
37	Skein Nylon Dyeing
38	Soy Flour
39	Soybean
40	Soybean Extraction (for Soy Flour)
41	Space Nylon Dyeing
42	Trisodium Nitriloacetate
43	Vancomycin

B. Sample Life Cycle Inventory Report

Vancomycin hydrochloride

CONTENTS OF FACTORY GATE TO FACTORY GATE

LIFE CYCLE INVENTORY SUMMARY

Chemistry

Primary reaction:

$$24\ C_6H_{12}O_6 \quad 9\ NO_3^- + 2\ Cl^- + O_2 \rightarrow C_{66}H_{75}Cl_2N_9O_{24} + 78\ CO_2 \qquad (1)$$

Dextrose + Nitrate + Chloride + Oxygen → Vancomycin + Carbon dioxide

$$+\ 5\ ADP + 118\ NAD \quad + 118\ (NADH + H)$$

+ adenosine diphosphate + nicotinamide adenine dinucleotide   nicotinamide adenine dinucleotide

$$+\ 7\ H_20 + 5\ P_i \quad + 5\ ATP$$

+ Water + inorganic phosphate   adenosine-5'-triphosphate

$$C_{66}H_{75}Cl_2N_9O_{24} + NH_4Cl \rightarrow C_{66}H_{75}Cl_2N_9O_{24}\cdot H^- Cl^+ + NH_3 \qquad (2)$$

Vancomycin + Ammonium chloride → Vancomycin hydrochloride + Ammonia

$$C_{66}H_{75}Cl_2N_9O_{24}\cdot H^- Cl^+ + CH_4N_2O \rightarrow C_{66}H_{75}Cl_2N_9O_{24} + CH_4N_2O + HCl \qquad (3)$$

Vancomycin Hydrochloride + Urea → Vancomycin + Urea + Hydrogen chloride

$$C_{66}H_{75}Cl_2N_9O_{24} + NH_4Cl \rightarrow C_{66}H_{75}Cl_2N_9O_{24}\cdot H^- Cl^+ + NH_3 \qquad (4)$$

Vancomycin + Ammonium chloride → Vancomycin hydrochloride + Ammonia

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Net Reaction:

$$24\ C_6H_{12}O_6 \quad 9\ NO_3^- + 2\ Cl^- + O_2 \rightarrow C_{66}H_{75}Cl_2N_9O_{24}\cdot H^- Cl^+ + 78\ CO_2 \qquad (5)$$

Dextrose + Nitrate + Chloride + Oxygen → Vancomycin hydrochloride + Carbon dioxide

$$+\ 5\ ADP + 118\ NAD \quad + 118\ (NADH + H)$$

+ adenosine diphosphate + nicotinamide adenine dinucleotide   nicotinamide adenine dinucleotide

$$+\ 7\ H_20 + 5\ P_i \quad + 5\ ATP$$

+ Water + inorganic phosphate   adenosine-5'-triphosphate

$$+\ 2NH_4Cl \quad + 2NH_3 + HCl$$

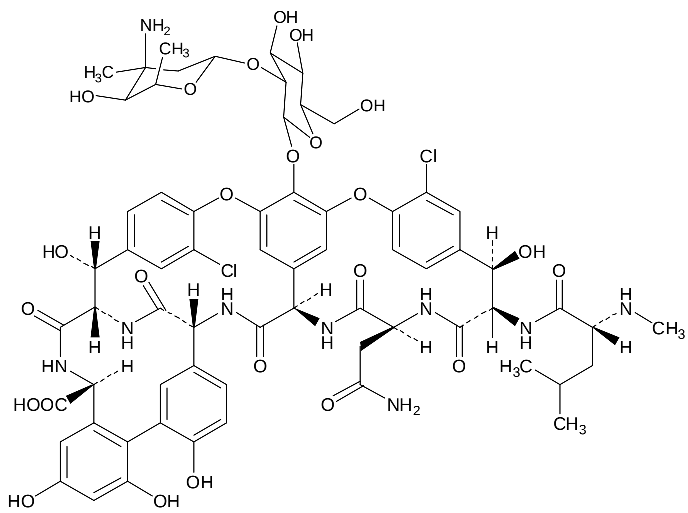
+ Ammonium chloride   + Ammonia + Hydrogen chloride

Side reactions:

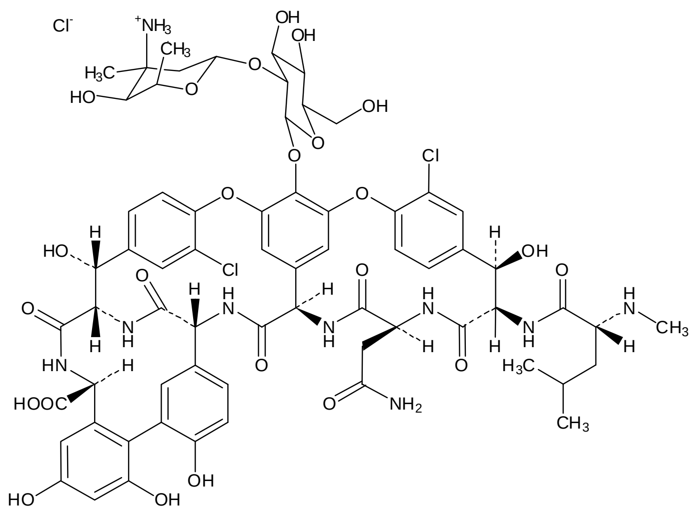
$$C_6H_{12}O_6 + 6\ O_2 \rightarrow 6\ CO_2 + 6\ H_20 \qquad (6)$$

Dextrose + Oxygen → Carbon Dioxide + Water

Vancomycin Structure



Vancomycin Hydrochloride Structure



Process Summary

Vancomycin is in the glycopeptide class of antibiotics, "with two glycosidically linked sugars, glucose and vancosamine, and a complex cyclic peptide aglycon containing aromatics residues linked together in a unique resorcinol ether system."[1] It is active against gram-positive bacteria and gram-negative cocci by inhibiting bacterial cell wall peptidoglycan synthesis.[2] Vancomycin was first isolated in 1956 by Eli Lilly and called Mississippi Mud due to its brown color from fermentation impurities; it was toxic at high doses. After the 1980s, purification methods improved, and upon purification it is a white solid. The hydrochloride form of vancomycin is administered intravenously in a dilute solution (0.5 weight % vancomycin, 5% dextrose, and 94.5% water) by slow injection or continuous infusion at a rate of two grams over 24 hours.[3]

Vancomycin is produced from aerobic fermentation using Amycolatopsis orientalis (formerly Nocardia orientalis and Streptomyces orientalis).[4] In aerobic fermentation, glucose is converted to energy by glycolysis:

$$C_6H_{12}O_6 + 6\ O_2 \rightarrow 6\ CO_2 + 6\ H_20$$

Dextrose + Oxygen → Carbon Dioxide + Water

In the reaction glucose is also converted to vancomycin:

$$24\ C_6H_{12}O_6 + 9\ NO_3 + 2\ Cl + O_2 + 5\ ADP + 118\ NAD + 7\ H_20 + 5\ Pi \rightarrow C_{66}H_{75}Cl_2N_9O_{24} + 78\ CO_2 + 118\ (NADH + H) + 5\ ATP$$

adenosine diphosphate (ADP) and nicotinamide adenine dinucleotide, (NAD^+) are stored in the microorganism, and are converted to adenosine-5'-triphosphate (ATP) and NADH using glucose and inorganic phosphate (Pi), producing energy for the organism to grow. Vancomycin production is considered a secondary metabolite, and not necessary for growth of the organism. All glucose is consumed during the glycolysis or vancomycin production steps.[5]

A. orientalis spores are grown on nutrient agar and transferred to flasks to inoculate starter nutrient medium, and incubated for 2 days. Fresh nutrient broth consisting of nitrogen and carbon sources is added to a bioreactor and sterilized with steam for 30 min at 120ºC. Inoculum from the flask is then added to the cooled medium and allowed to ferment for 24 hours. Fresh nutrient broth is then added to an industrial-sized bioreactor and sterilized before the contents of the smaller bioreactor are added. Fermentation lasts for four to six days. Air is added at a rate of 0.4 to 0.8 volumes of air per volume broth per minute, and the temperature is held at 30ºC.[6]

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[1] Wilson, C. and Gisvold, O. *Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, 11th ed.* 2004

[2] McCormick, M.H., Stark, W.M., Pittenger, G.E., Pittenger, R.C., and McGuire, J.M. *Antibiotics Annual.* 1955, 606.

[3] Baxter Healthcare Corporation. Vancomycin Injection Material Safety Data Sheet, 2005.

[4] Dunstan, G.H., Avignone-Rossa, C., Langley, D., and Bushell, M.E. The Vancomycin biosynthetic pathway is induced in oxygen-limited Amycolatopsis orientalis (ATCC 19795) cultures that do not produce antibiotic. *Enzyme and Microbial Technology.* **27**, (2000) 502-510.

[5] McIntyre, J., Bull, A.T., and Bunch, A.W. Vancomycin Production in Batch and Continuous Culture. *Biotechnology and Bioengineering.* **49**, (1996) 412-420.

[6] Cinar, A., Parulekar, S.J., Undey, C. and Birol, G. *Batch Fermentation: Modeling, Monitoring and Control.* CRC Press: New York 2003.

The fermentation broth, containing from 4 to 11 g Vancomycin/L broth[7], is filtered, and passed through adsorbents (Dowex 50 and Amberlite XAD-16 resins) to separate active ingredient vancomycin B and to decolorize and remove impurities. The solution is concentrated in an evaporator. Vancomycin is then crystallized two to three times with acetone, alcohol, or ammonium chloride, and filtered and dried to recover Vancomycin hydrochloride. Vancomycin hydrochloride is highly soluble (200 mg/mL) in water, but insoluble in organic solvents.[8]

Although a variety of nutrient sources can be used, this inventory uses glucose (dextrose) and soy flour for fermentation[7], and 25% of the glucose is converted to vancomoycin while 75% is converted to exothermic energy.[5] Ammonium chloride is used to crystallize the vancomycin hydrochloride.

The fermentation energy (used to calculate cooling water requirements) is calculated from the heats of reaction for the dextrose glycolysis and dextrose-to-vancomycin reactions. Cooney et al (1968)[9] and Luong and Volesky (1980)[10] found the heat evolution during fermentation to correlate well with oxygen consumption. Comparing the energy calculated in this inventory with their correlations in Table 1 shows a 2 and 10% difference.

Table 1. Comparison of Fermentation Energy

	net O2 consumed, kg/1000kg Product	gmol O2 consumed	Energy, MJ/1000kg Product (Cooney et al 1968)	Energy, MJ/1000kg Product (Luong and Volesky 1980)	Energy, MJ/1000kg Product (calculated from heat of rxn, used in this Inventory)
Reactor 1	8.49	265	138	122	124
Reactor 2	169	5290	2744	2434	2482
Reactor 3	9479	296231	153685	136326	139000

[7] Jung, H., Kim, S., Moon, H., Oh, D., and Lee, J. Optimization of culture conditions and scale-up to pilot and plant scales for vancomycin production by Amycolatopsis orientalis. *Appl. Microbiol. Biotechnol.* **77**, (2007) 789-795.
[8] Robison, R.L., inventor; Vancomycin-HCl Solutions and the Lyophilization Therof. US Patent 4,885,275. 1989 Dec. 5.
[9] Cooney, C., Wang, D., and Mateles, R. Measurement of Heat Evolution and Correlation with Oxygen Consumption during Microbial Growth. Biotechnology and Bioengineering **11**, (1968) 269-281.
[10] Luong, J. and B. Volesky. Heat evolution during the microbial process — Estimation, measurement, and applications. Advances in Biochemical Engineering/Biotechnology **28** (1983) 1-38.

Critical parameters

Conversion / Yield information from both reactors		
		Conversion of or Yield from Dextrose
Total conversion in reactor 1: (% of reactant entering the process that reacts)	From mass balance	100%
Total per pass conversion in reactor 1: (% of reactant entering the reactor that reacts)	From mass balance	100%
Total yield of reactor 1: (% yield ProductChem produced in the reactor based on reactant input to process)	From mass balance	25.3%
Total conversion in reactor 2: (% of reactant entering the process that reacts)	From mass balance	100%
Total per pass conversion in reactor 2: (% of reactant entering the reactor that reacts)	From mass balance	100%
Total yield of reactor 2: (% yield produced in the reactor based on reactant input to process)	From mass balance	25.3%
Total conversion in reactor 3: (% of reactant entering the process that reacts)	From mass balance	100%
Total per pass conversion in reactor 3: (% of reactant entering the reactor that reacts)	From mass balance	100%
Total yield of reactor 3: (% yield ProductChem produced in the reactor based on reactant input to process)	From mass balance	25.3%
Total per pass conversion in reactor 4: (% of reactant entering the reactor that reacts)	From mass balance	100%
Total yield of reactor 4: (% yield ProductChem produced in the reactor based on reactant input to process)	From mass balance	100%
Total per pass conversion in reactor 5: (% of reactant entering the reactor that reacts)	From mass balance	100%
Total yield of reactor 5: (% yield ProductChem produced in the reactor based on reactant input to process)	From mass balance	100%
Total per pass conversion in reactor 6: (% of reactant entering the reactor that reacts)	From mass balance	100%
Total yield of reactor 6: (% yield ProductChem produced in the reactor based on reactant input to process)	From mass balance	100%
Total yield of Process: (% yield produced by the overall process based on reactant input to process)	From mass balance	100%
Notes:		

Product purity			
	Vancomycin Hydrochloride		Comments
Used here	99.8%		

Summary of LCI Information

Inputs					
Input UID	Input Name	Input Flow	Input purity	Units	Comments
57-13-6	Urea	1200		[kg/hr]	
12125-02-9	Ammonium chloride	1132		[kg/hr]	
67-63-0	Isopropanol	100.0		[kg/hr]	
7664-41-7	Ammonia	1000		[kg/hr]	
68513-95-1	Soy Flour	4625		[kg/hr]	
50-99-7	Dextrose	1.21e+4		[kg/hr]	
	Total	2.02e+4		[kg/hr]	
Non-reacting inputs					
UID	Name	Flow	Purity	Units	Comments
7782-44-7	Oxygen	9679		[kg/hr]	
UIDAir	Air	2.00e+4		[kg/hr]	
7732-18-5	Water	1.35e+5		[kg/hr]	
	Total	1.65e+5		[kg/hr]	
Ancillary inputs					
UID	Name	Flow	Purity	Units	Comments
68855-54-9	Diatomaceous earth	51.4		[kg/hr]	
7647-01-0	Hydrogen chloride	1.00e-2		[kg/hr]	
10043-52-4	Calcium dichloride	1.23e-2		[kg/hr]	
7487-88-9	Magnesium Sulfate	0.222		[kg/hr]	
8002-48-0	Malt Extract	6.36e-3		[kg/hr]	
8013-01-2	Yeast Extract	6.36e-3		[kg/hr]	

73049-73-7	Peptone	2.33e-2		[kg/hr]	
UIDAOrientalis	A Orientalis	1.00e-3		[kg/hr]	
	Total	51.7		[kg/hr]	

Products

Product UID	Product Name	Product Flow	Purity	Units	Comments
1404-93-9	Vancomycin HCl	1000	99.8	[kg/hr]	Impurities are Ammonium chloride (0.09), Urea (0.02), and water (1.87)
	Total	1000		[kg/hr]	

Benign Outflows

UID	Name	Flow	Purity	Units	Comments
7782-44-7	Oxygen	21.8		[kg/hr]	
UIDAir	Air	2.00e+4		[kg/hr]	
7732-18-5	Water	1.41e+5		[kg/hr]	
	Total	1.61e+5		[kg/hr]	

Chemical Emissions

Emission UID	Emission Name	Gas Flow	Liquid Flow	Solid Flow	Solvent Flow	Units	Comments
124-38-9	Carbon dioxide	1.58e+4	0	0	0	[kg/hr]	
1404-93-9	Vancomycin HCl	0	52.6	0	0	[kg/hr]	
1404-90-6	Vancomycin	0	31.8	2.08	0	[kg/hr]	
57-13-6	Urea	2.03	1198	0	0	[kg/hr]	
12125-02-9	Ammonium chloride	8.97	1049	0	0	[kg/hr]	
67-63-0	Isopropanol	10.0	100.0	0	0	[kg/hr]	
68855-54-9	Diatomaceous earth	0	0	51.4	0	[kg/hr]	
7664-41-7	Ammonia	5.20	1023	0	0	[kg/hr]	
7487-88-9	Magnesium Sulfate	0	0.222	2.22e-4	0	[kg/hr]	

7647-01-0	Hydrogen chloride	0.542	24.2	0	0	[kg/hr]	
10043-52-4	Calcium dichloride	0	1.22e-2	1.23e-5	0	[kg/hr]	
68513-95-1	Soy Flour	0	4621	4.63	0	[kg/hr]	
8002-48-0	Malt Extract	0	6.35e-3	6.36e-6	0	[kg/hr]	
8013-01-2	Yeast Extract	0	6.35e-3	6.36e-6	0	[kg/hr]	
73049-73-7	Peptone	0	2.33e-2	2.33e-5	0	[kg/hr]	
UIDAOrientalis	A Orientalis	0	0	5391	0	[kg/hr]	
Totals		1.58e+4	8100	5449	0	[kg/hr]	

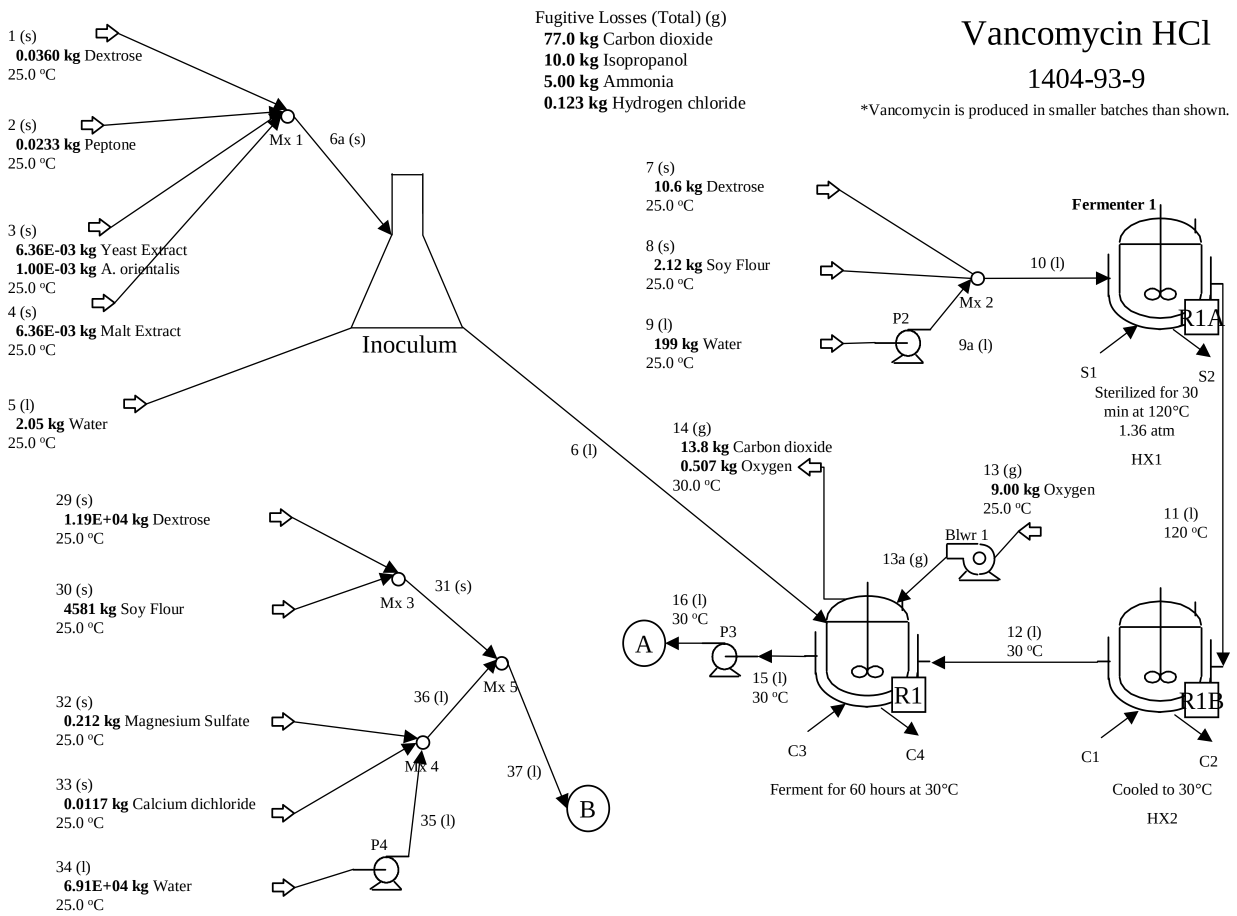
Mass Balance			
Total inputs	1.85e+5		
Total outflows	1.91e+5		
Net input	-5803		
Energy use			
Energy type	Amount	Comments	
electricity	2.37e+4	[MJ/hr]	
heating steam	2.48e+5	[MJ/hr]	
Net input requirement	2.72e+5	[MJ/hr]	Net of energies input to system
cooling water	-3.49e+5	[MJ/hr]	
potential recovery	-4.85e+4	[MJ/hr]	
Net energy	2.23e+5	[MJ/hr]	Net input requirement - potential recovery

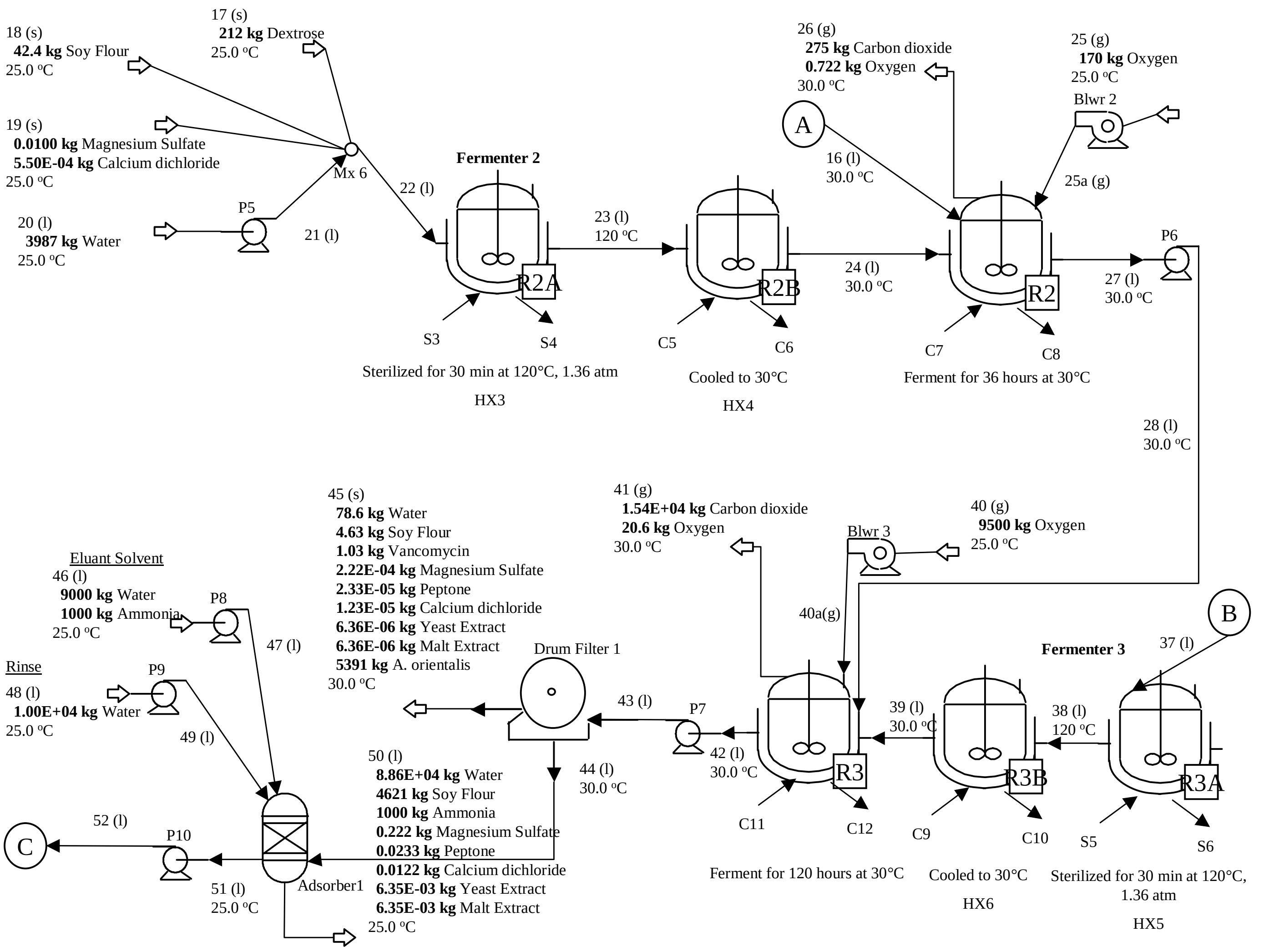
Process Diagram Interpretation Sheet

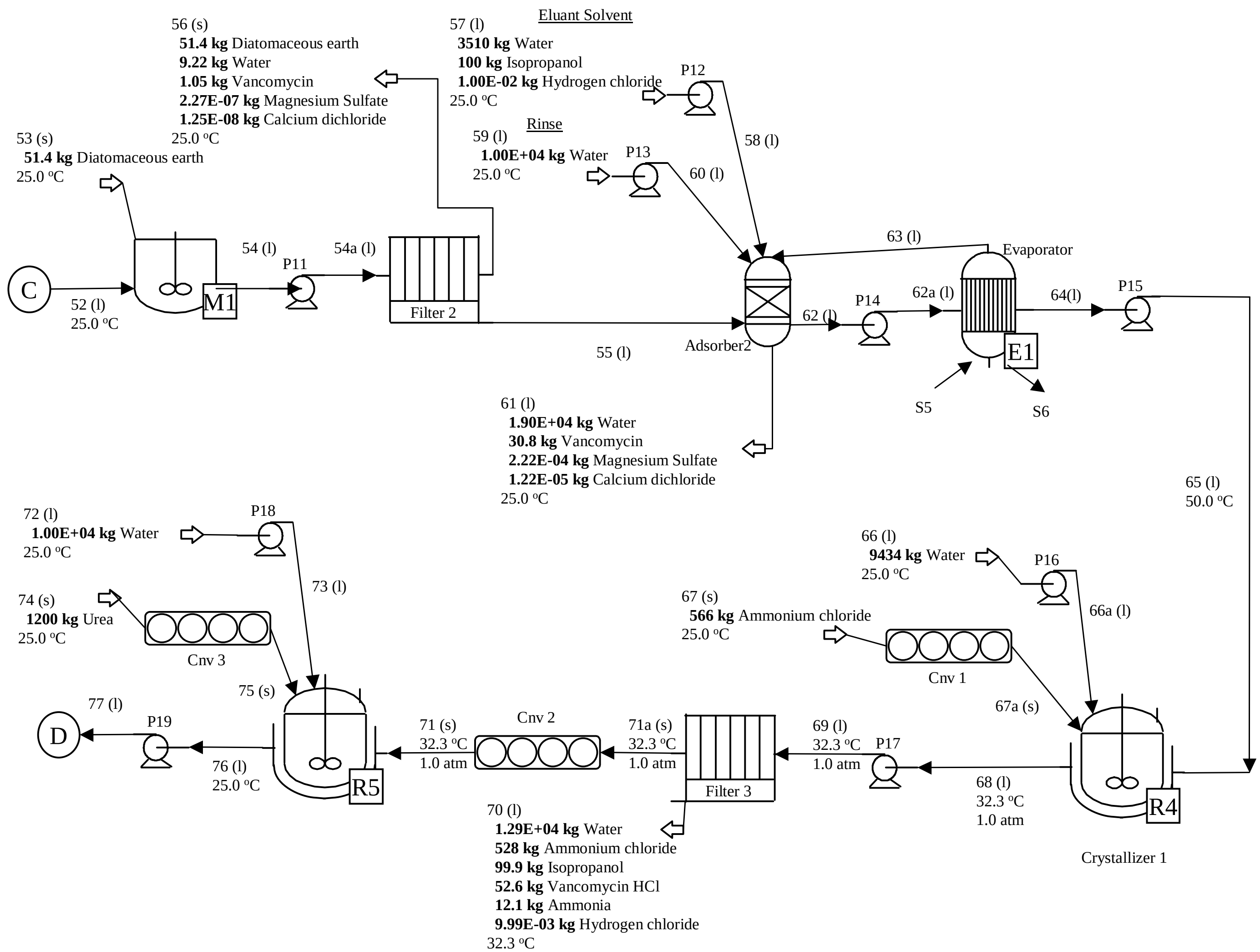
1) As much as possible, standard symbols are used for all unit processes.
2) Only overall input and output chemicals are labeled on these diagrams. All intermediate information is given on the attached Process Mass Balance sheet
3) The physical state of most streams is shown (gas, g; liquid, l; solid, s)
4) The process numbering is as follows,
   - generally numbers progress from the start to the end of the process
   - numbers are used for process streams
   - C i , i = 1,..n are used for all cooling non-contact streams
   - S j, j = 1,...n are used for all steam heating non-contact streams
5) Recycle streams are shown with dotted lines

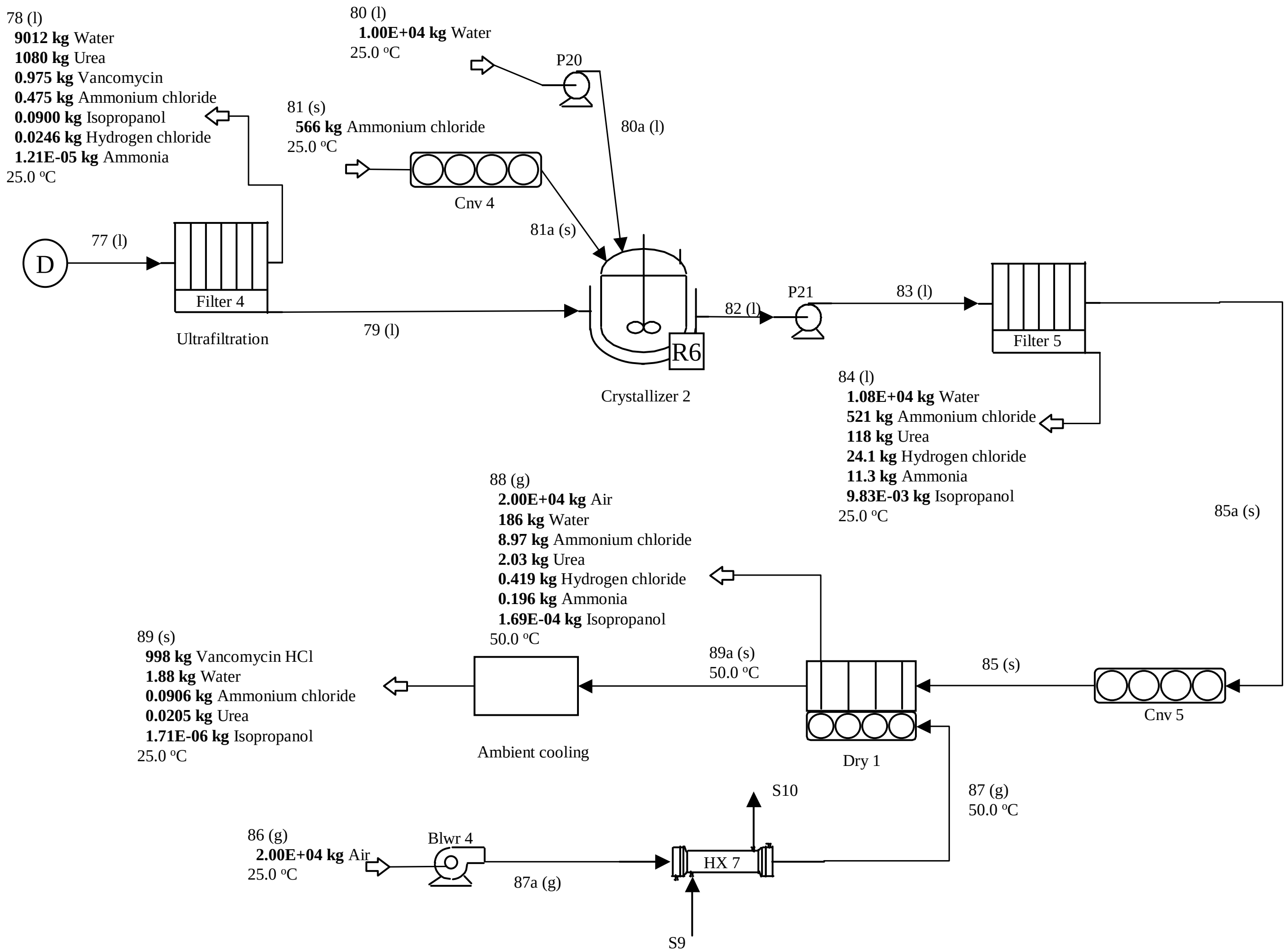
For most streams, the temperature and pressure are shown, if the pressures are greater than 1 atm

Process Diagram or Boundary of LCI




18 (s)
42.4 kg Soy Flour
25.0 ºC
17 (s)
212 kg Dextrose
25.0 ºC
19 (s)
0.0100 kg Magnesium Sulfate
5.50E-04 kg Calcium dichloride
25.0 ºC
20 (l)
3987 kg Water
25.0 ºC
P5
Mx 6
21 (l)
22 (l)
Fermenter 2
23 (l)
120 ºC
R2A
S3
S4
Sterilized for 30 min at 120°C, 1.36 atm
HX3
R2B
C5
C6
Cooled to 30°C
HX4
24 (l)
30.0 ºC
26 (g)
275 kg Carbon dioxide
0.722 kg Oxygen
30.0 ºC
A
16 (l)
30.0 ºC
25 (g)
170 kg Oxygen
25.0 ºC
Blwr 2
25a (g)
R2
C7
C8
Ferment for 36 hours at 30°C
P6
27 (l)
30.0 ºC
28 (l)
30.0 ºC
45 (s)
78.6 kg Water
4.63 kg Soy Flour
1.03 kg Vancomycin
2.22E-04 kg Magnesium Sulfate
2.33E-05 kg Peptone
1.23E-05 kg Calcium dichloride
6.36E-06 kg Yeast Extract
6.36E-06 kg Malt Extract
5391 kg A. orientalis
30.0 ºC
41 (g)
1.54E+04 kg Carbon dioxide
20.6 kg Oxygen
30.0 ºC
Blwr 3
40 (g)
9500 kg Oxygen
25.0 ºC
40a(g)
B
Fermenter 3
37 (l)
Eluant Solvent
46 (l)
9000 kg Water
1000 kg Ammonia
25.0 ºC
P8
47 (l)
Rinse
48 (l)
1.00E+04 kg Water
25.0 ºC
P9
49 (l)
Drum Filter 1
43 (l)
P7
42 (l)
30.0 ºC
44 (l)
30.0 ºC
R3
C11
C12
Ferment for 120 hours at 30°C
39 (l)
30.0 ºC
R3B
C9
C10
Cooled to 30°C
HX6
38 (l)
120 ºC
R3A
S5
S6
Sterilized for 30 min at 120°C, 1.36 atm
HX5
50 (l)
8.86E+04 kg Water
4621 kg Soy Flour
1000 kg Ammonia
0.222 kg Magnesium Sulfate
0.0233 kg Peptone
0.0122 kg Calcium dichloride
6.35E-03 kg Yeast Extract
6.35E-03 kg Malt Extract
25.0 ºC
52 (l)
C
P10
51 (l)
25.0 ºC
Adsorber1


Eluant Solvent
56 (s)
51.4 kg Diatomaceous earth
9.22 kg Water
1.05 kg Vancomycin
2.27E-07 kg Magnesium Sulfate
1.25E-08 kg Calcium dichloride
25.0 ºC
57 (l)
3510 kg Water
100 kg Isopropanol
1.00E-02 kg Hydrogen chloride
25.0 ºC
P12
53 (s)
51.4 kg Diatomaceous earth
25.0 ºC
Rinse
59 (l)
1.00E+04 kg Water
25.0 ºC
P13
58 (l)
60 (l)
63 (l)
Evaporator
C
52 (l)
25.0 ºC
M1
54 (l)
P11
54a (l)
Filter 2
Adsorber2
55 (l)
62 (l)
P14
62a (l)
E1
64(l)
P15
S5
S6
61 (l)
1.90E+04 kg Water
30.8 kg Vancomycin
2.22E-04 kg Magnesium Sulfate
1.22E-05 kg Calcium dichloride
25.0 ºC
65 (l)
50.0 ºC
72 (l)
1.00E+04 kg Water
25.0 ºC
P18
73 (l)
74 (s)
1200 kg Urea
25.0 ºC
Cnv 3
66 (l)
9434 kg Water
25.0 ºC
P16
66a (l)
67 (s)
566 kg Ammonium chloride
25.0 ºC
Cnv 1
67a (s)
75 (s)
77 (l)
D
P19
76 (l)
25.0 ºC
R5
71 (s)
32.3 ºC
1.0 atm
Cnv 2
71a (s)
32.3 ºC
1.0 atm
Filter 3
69 (l)
32.3 ºC
1.0 atm
P17
68 (l)
32.3 ºC
1.0 atm
R4
Crystallizer 1
70 (l)
1.29E+04 kg Water
528 kg Ammonium chloride
99.9 kg Isopropanol
52.6 kg Vancomycin HCl
12.1 kg Ammonia
9.99E-03 kg Hydrogen chloride
32.3 ºC


78 (l)
9012 kg Water
1080 kg Urea
0.975 kg Vancomycin
0.475 kg Ammonium chloride
0.0900 kg Isopropanol
0.0246 kg Hydrogen chloride
1.21E-05 kg Ammonia
25.0 ºC
80 (l)
1.00E+04 kg Water
25.0 ºC
P20
80a (l)
81 (s)
566 kg Ammonium chloride
25.0 ºC
Cnv 4
81a (s)
D
77 (l)
Filter 4
Ultrafiltration
79 (l)
R6
Crystallizer 2
82 (l)
P21
83 (l)
Filter 5
84 (l)
1.08E+04 kg Water
521 kg Ammonium chloride
118 kg Urea
24.1 kg Hydrogen chloride
11.3 kg Ammonia
9.83E-03 kg Isopropanol
25.0 ºC
85a (s)
88 (g)
2.00E+04 kg Air
186 kg Water
8.97 kg Ammonium chloride
2.03 kg Urea
0.419 kg Hydrogen chloride
0.196 kg Ammonia
1.69E-04 kg Isopropanol
50.0 ºC
89 (s)
998 kg Vancomycin HCl
1.88 kg Water
0.0906 kg Ammonium chloride
0.0205 kg Urea
1.71E-06 kg Isopropanol
25.0 ºC
Ambient cooling
89a (s)
50.0 ºC
Dry 1
85 (s)
Cnv 5
S10
87 (g)
50.0 ºC
86 (g)
2.00E+04 kg Air
25.0 ºC
Blwr 4
87a (g)
HX 7
S9

Mass Balance of Chemicals in Each Process Stream

All flow rates are given in kg / hr
Physical state of chemical losses:

Gas
Liquid
Solid

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
		0		1.00		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		0	0
Input		1	25.0	1.00	s	0.0360	0.0360																					
Input		2	25.0	1.00	s	0.0233		0.0233																				
Input		3	25.0	1.00	s	6.36 E-03			6.36 E-03																			
Input		4	25.0	1.00	s	6.36 E-03				6.36 E-03																		
Input		5	25.0	1.00	l	2.05					2.05																	
		6a	25.0	1.00	s	0.0720	0.0360	0.0233	6.36 E-03	6.36 E-03	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		6	25.0	1.00	l	2.12	0.0360	0.0233	6.36 E-03	6.36 E-03	2.05	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Input		7	25.0	1.00	s	10.6	10.6																					
Input		8	25.0	1.00	s	2.12						2.12																
Input		9	25.0	1.00	l	199					199																	
		9a	25.0	1.00	l	199					199																	
		10	25.0	1.00	l	212	10.6	0	0	0	199	2.12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		11	120	1.00	l	212	10.6	0	0	0	199	2.12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		12	30.0	1.00	l	212	10.6	0	0	0	199	2.12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Input		13	25.0	1.00	g	9.00											9.00											

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
		13a	25.0	1.00	g	9.00											9.00											
R1	2.70	kg	Dextrose			is converted in rxn 1 (25.3 % of reactor input)																						
	7.94	kg	Dextrose			is lost in rxn 2																						
		kg				is lost in rxn 3																						
		Input to reactor			:	223	10.6	0.0233	6.36 E-03	6.36 E-03	201	2.12	0	0	0	0	9.00	0	0	0	0	0	0	0	0	0	0	
		R1 Reaction Coefficient 1			:		-24.0				-7.00						-1.00							1.00		78.0		
		R1 Conversion 1 [kg/hr]			:	0.252	-2.70				-0.0787						-0.0200							0.904		2.14		
		R1 Conversion 1 [kgmol/hr]			:	6.24 E-04	-0.0150				-4.37E-03						-6.24 E-04							6.24 E-04		0.0487		
		R1 Reaction Coefficient 2			:		-1.00				6.00						-6.00									6.00		
		R1 Conversion 2 [kg/hr]			:	2.65 E-03	-7.94				4.77						-8.47									11.7		
		R1 Conversion 2 [kgmol/hr]			:	0.0441	-0.0441				0.265						-0.265									0.265		
		R1 Reaction Coefficient 3			:																							
		R1 Conversion 3 [kg/hr]			:																							
		R1 Conversion 3 [kgmol/hr]			:																							
		Flow out of react	0.0617		:	223	0	0.0233	6.36 E-03	6.36 E-03	206	2.12	0	0	0	0	0.507	0	0	0	0	0	0	0.904	0	13.8	0	

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
		or																										
		Primary product			:	Vancomycin																						
		Total conversion			:		NA	NA	NA	NA	-3.47E-03	-0	NA	-0	-0	-0	0.0877	-0	-0	-0	-0	-0	-0	NA	NA	NA	NA	
		Per pass conversion			:		100	-0	-0	-0	NA	-0					94.4							NA				
		Total yield from reactor			:		25.3										0.235							NA				
Waste		14	30.0	1.00	g	-14.3	0	0	0	0	0	0	0	0	0	0	-0.507	0	0	0	0	0	0	0	0	-13.8	0	0
		15	30.0	1.00	l	209	0	0.0233	6.36E-03	6.36E-03	206	2.12	0	0	0	0		0	0	0	0	0	0	0.904	0		0	
		16	30.0	1.00	l	209	0	0.0233	6.36E-03	6.36E-03	206	2.12	0	0	0	0	0	0	0	0	0	0	0	0.904	0	0	0	
Input		17	25.0	1.00	s	212	212																					
Input		18	25.0	1.00	s	42.4						42.4																
Input		19	25.0	1.00	s	0.0106									0.0100	5.50E-04												
Input		20	25.0	1.00	l	3987					3987																	
		21	25.0	1.00	l	3987					3987																	
		22	25.0	1.00	s	4242	212	0	0	0	3987	42.4	0	0	0.0100	5.50E-04	0	0	0	0	0	0	0	0	0	0	0	
		23	120	1.00	l	4242	212	0	0	0	3987	42.4	0	0	0.0100	5.50E-04	0	0	0	0	0	0	0	0	0	0	0	
		24	30.0	1.00	l	4242	212	0	0	0	3987	42.4	0	0	0.0100	5.50E-04	0	0	0	0	0	0	0	0	0	0	0	
Input		25	25.0	1.00	g	170											170											
		25a	25.0	1.00	g	170	0	0	0	0	0	0	0	0	0	0	170	0	0	0	0	0	0	0	0	0	0	
R2	53.8	kg	Dextrose			is converted in rxn 1 (25.3 % of reactor input)																						

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
	158	kg	Dextrose			is lost in rxn 2																						
		kg				is lost in rxn 3																						
		Input to reactor			:	4621	212	0.0233	6.36E-03	6.36E-03	4193	44.5	0	0	0.0100	5.50E-04	170	0	0	0	0	0	0	0.904	0	0	0	
		R2 Reaction Coefficient 1			:		-24.0				-7.00						-1.00							1.00		78.0		
		R2 Conversion 1 [kg/hr]			:	5.02	-53.8				-1.57						-0.398							18.0		42.7		
		R2 Conversion 1 [kgmol/hr]			:	0.0124	-0.299				-0.0871						-0.0124							0.0124		0.970		
		R2 Reaction Coefficient 2			:		-1.00				6.00						-6.00									6.00		
		R2 Conversion 2 [kg/hr]			:	0.0528	-158				95.0						-169									232		
		R2 Conversion 2 [kgmol/hr]			:	0.880	-0.880				5.28						-5.28									5.28		
		R2 Reaction Coefficient 3			:																							
		R2 Conversion 3 [kg/hr]			:																							
		R2 Conversion 3 [kgmol/hr]			:																							
		Flow out of reactor			:	4626	0	0.0233	6.36E-03	6.36E-03	4287	44.5	0	0	0.0100	5.50E-04	0.722	0	0	0	0	0	0	18.9	0	275	0	
		Primary product			:	Vancomycin																						
		Total conversion			:		NA	NA	NA	NA	-0.069	-0	NA	-0	-0	-0	1.75	-0	-0	-0	-0	-0	-0	NA	NA	NA	NA	

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
											1																	
		Per pass conversion			:		100	-0	-0	-0	NA	-0			-0	-0	99.6							NA		NA		
		Total yield from reactor			:		25.3										0.235							NA		NA		
Waste		26	30.0	1.00	g	-276	0	0	0	0	0	0	0	0	0	0	-0.722	0	0	0	0	0	0	0	0	-275	0	0
		27	30.0	1.00	l	4350	0	0.0233	6.36E-03	6.36E-03	4287	44.5	0	0	0.0100	5.50E-04		0	0	0	0	0	0	18.9	0		0	
		28	30.0	1.00	l	4350	0	0.0233	6.36E-03	6.36E-03	4287	44.5	0	0	0.0100	5.50E-04	0	0	0	0	0	0	0	18.9	0	0	0	
Input		29	25.0	1.00	s	1.19E+04	1.19E+04																					
Input		30	25.0	1.00	s	4581						4581																
		31	25.0	1.00	s	1.65E+04	1.19E+04	0	0	0	0	4581	0	0	0	0	0	0	0	0	0	0	0		0	0	0	
Input		32	25.0	1.00	s	0.212									0.212													
Input		33	25.0	1.00	s	0.0117										0.0117												
Input		34	25.0	1.00	l	6.91E+04					6.91E+04																	
		35	25.0	1.00	l	6.91E+04	0	0	0	0	6.91E+04	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		36	25.0	1.00	l	6.91E+04	0	0	0	0	6.91E+04	0	0	0	0.212	0.0117	0	0	0	0	0	0	0	0	0	0	0	
		37	25.0	1.00	l	8.56E+04	1.19E+04	0	0	0	6.91E+04	4581	0	0	0.212	0.0117	0	0	0	0	0	0	0	0	0	0	0	
		38	120	1.00	l	8.56E+04	1.19E+04	0	0	0	6.91E+04	4581	0	0	0.212	0.0117	0	0	0	0	0	0	0	0	0	0	0	
		39	30.0	1.00	l	8.56E+04	1.19E+04	0	0	0	6.91E+04	4581	0	0	0.212	0.0117	0	0	0	0	0	0	0	0	0	0	0	

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
Input		40	25.0	1.00	g	9500											9500											
		40a	25.0	1.00	g	9500											9500											
R3	3010	kg	Dextrose			is converted in rxn 1 (25.3 % of reactor input)																						
	8866	kg	Dextrose			is lost in rxn 2																						
		kg				is lost in rxn 3																						
		Input to reactor			:	9.94 E+04	1.19 E+04	0.0233	6.36 E-03	6.36 E-03	7.34E +04	4625	0	0	0.222	0.0123	9500	0	0	0	0	0	0	18.9	0	0	0	
		R3 Reaction Coefficient 1			:		-24.0				-7.00						-1.00							1.00		78.0		
		R3 Conversion 1 [kg/hr]			:	281	-3010				-87.8						-22.3							1010		2392		
		R3 Conversion 1 [kgmol/hr]			:	0.697	-16.7				-4.88						-0.697							0.697		54.3		
		R3 Reaction Coefficient 2			:		-1.00				6.00						-6.00									6.00		
		R3 Conversion 2 [kg/hr]			:	2.95	-8866				5320						-9457									1.30 E+04		
		R3 Conversion 2 [kgmol/hr]			:	49.3	-49.3				296						-296									296		
		R3 Reaction Coefficient 3			:																							
		R3 Conversion 3 [kg/hr]			:	0																						
		R3 Conversion 3 [kgmol/hr]			:																							
		Flow out of reactor			:	9.97 E+04	0	0.0233	6.36 E-03	6.36 E-03	7.86E +04	4625	0	0	0.222	0.0123	20.6	0	0	0	0	0	0	1029	0	1.54 E+04	0	
		Primary			:	Vancomyci																						

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
		product				n																						
		Total conversion			:		NA	NA	NA	NA	-3.87	-0	NA	-0	-0	-0	97.9	-0	-0	-0	-0	-0	-0	NA	NA	NA	NA	
		Per pass conversion			:		100	-0	-0	-0	NA	-0			-0	-0	99.8							NA		NA		
		Total yield from reactor			:		25.3										0.235							NA		NA		
Waste		41	30.0	1.00	g	-1.54E+04	0	0	0	0	0	0	0	0	0	0	-20.6	0	0	0	0	0	0	0	0	-1.54E+04	0	0
		42	30.0	1.00	l	8.43E+04	0	0.0233	6.36E-03	6.36E-03	7.86E+04	4625	0	0	0.222	0.0123		0	0	0	0	0	0	1029	0		0	
		43	30.0	1.00	l	8.43E+04	0	0.0233	6.36E-03	6.36E-03	7.86E+04	4625	0	0	0.222	0.0123	0	0	0	0	0	0	0	1029	0	0	0	
		43	30.0	1.00	m	8.43E+04	0	0.0233	6.36E-03	6.36E-03	7.86E+04	4625	0	0	0.222	0.0123	0	0	0	0	0	0	0	1029	0	0	0	
<> filter <>		solubility in solvent (g / g solvent)			:		0.160	0.400	0.400	0.400	1.00	0.400	1.00	1.00	0.272	0.420	1.00	1.00	1.00	1.00	1.00	1.00	1.00	200	1.00	1.00	1.00	
		liquid phase 43			:	8.43E+04	0	0.0233	6.36E-03	6.36E-03	7.86E+04	4625	0	0	0.222	0.0123	0	0	0	0	0	0	0	1029	0	0	0	
		solid phase 43			:	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	Water	is the solvent																										
	0.200	g liquid / g solid in sediment																										
	0.100	% of liquid phase exits in																										

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
		solid stream																										
	Liquid Out	44	30.0	1.00	l	8.42E+04	0	0.0233	6.35E-03	6.35E-03	7.86E+04	4621	0	0	0.222	0.0122	0	0	0	0	0	0	0	1027	0	0	0	
Waste	Solid Out	45	30.0	1.00	s	-84.3	0	-2.33E-05	-6.36E-06	-6.36E-06	-78.6	-4.63	0	0	-2.22E-04	-1.23E-05	0	0	0	0	0	0	0	-1.03	0	0	0	0
Input		46	25.0	1.00	l	1.00E+04					9000							1000										
		47	25.0	1.00	l	1.00E+04	0	0	0	0	9000	0	0	0	0	0	0	1000	0	0	0	0	0	0	0	0	0	
Input		48	25.0	1.00	l	1.00E+04					1.00E+04																	
		49	25.0	1.00	l	1.00E+04	0	0	0	0	1.00E+04	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Waste		50	25.0	1.00	l	-9.42E+04	0	-0.0233	-6.35E-03	-6.35E-03	-8.86E+04	-4621	0	0	-0.222	-0.0122	0	-1000	0	0	0	0	0	0	0	0	0	0
		51	25.0	1.00	l	1.00E+04					9000		0	0	2.22E-04	1.22E-05	0	0	0	0	0	0	0	1027	0	0	0	
		52	25.0	1.00	l	1.00E+04	0	0	0	0	9000	0	0	0	2.22E-04	1.22E-05	0	0	0	0	0	0	0	1027	0	0	0	
Input		53	25.0	1.00	s	51.4														51.4								
		54	25.0	1.00	l	1.01E+04	0	0	0	0	9000	0	0	0	2.22E-04	1.22E-05	0	0	0	51.4	0	0	0	1027	0	0	0	
		54a	25.0	1.00	l	1.01E+04	0	0	0	0	9000	0	0	0	2.22E-04	1.22E-05	0	0	0	51.4	0	0	0	1027	0	0	0	
	Input	54a	25.0	1.00	m	1.01E+04	0	0	0	0	9000	0	0	0	2.22E-	1.22E-05	0	0	0	51.4	0	0	0	1027	0	0	0	

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
															04													
<> filter <>		solubility in solvent (g / g solvent)			:		0.160	0.400	0.400	0.400	1.00	0.400	1.00	1.00	0.272	0.420	1.00	1.00	1.00	0	1.00	0.260	1.00	200	1.00	1.00	1.00	
		liquid phase 54a			:	1.00E+04	0	0	0	0	9000	0	0	0	2.22E-04	1.22E-05	0	0	0	0	0	0	0	1027	0	0	0	
		solid phase 54a			:	51.4	0	0	0	0	0	0	0	0	0	0	0	0	0	51.4	0	0	0	0	0	0	0	
	Water	is the solvent																										
	0.200	g liquid / g solid in sediment																										
	0.102	% of liquid phase exits in solid stream																										
	Liquid Out	55	25.0	1.00	l	1.00E+04	0	0	0	0	8991	0	0	0	2.22E-04	1.22E-05	0	0	0	0	0	0	0	1026	0	0	0	
Waste	Solid Out	56	25.0	1.00	s	-61.6	0	0	0	0	-9.22	0	0	0	-2.27E-07	-1.25E-08	0	0	0	-51.4	0	0	0	-1.05	0	0	0	0
Input		57	25.0	1.00	l	3610					3510								1.00E-02		100							
		58	25.0	1.00	l	3610	0	0	0	0	3510	0	0	0	0	0	0	0	1.00E-02	0	100	0	0	0	0	0	0	
		Stream 91:Recycle input				6400	0	0	0	0	5490	0	0	0	0	0	0	0	9.99	0	900	0	0	0	0	0	0	
		Stream 91:Recycle calculated				6400	0	0	0	0	5490	0	0	0	0	0	0	0	9.99	0	900	0	0	0	0	0	0	
		Stream 91:Recycle residue				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Input		59	25.0	1.00	l	1.00					1.00E																	

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
						E+04					+04																	
		60	25.0	1.00	l	1.00 E+04	0	0	0	0	1.00E +04	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Waste		61	25.0	1.00	l	- 1.90 E+04	0	0	0	0	- 1.90E +04	0	0	0	- 2.2 2E- 04	- 1.22 E-05	0	0	0	0	0	0	0	-30.8	0	0	0	0
		62	25.0	1.00	l	1.10 E+04	0	0	0	0	9000	0	0	0	0	0	0	0	10.0	0	1000	0	0	1026	0	0	0	
		62a	25.0	1.00	l	1.10 E+04	0	0	0	0	9000	0	0	0	0	0	0	0	10.0	0	1000	0	0	1026	0	0	0	
evaporator <>		percentage of input in vapor phase			:		0	0	0	0	61.0	0	0	0	0	0	0	0	99.9	0	90.0	0	0	0	0	0	0	
		percentage of input in solid / liquid phase			:		100	100	100	100	39.0	100	100	100	100	100	100	100	0.10 00	100	10.0	100	100	100	100	100	100	
		Boiling Temperature (Tb) [oC]			:		344				99.9	300	380		112 4	1600	-183	-33.5	-85.0	220 4	81.9	520	192	3594	3594	-78.7	-78.7	
	Gas phas e out	63	50.0	1.00	g	6400	0	0	0	0	5490	0	0	0	0	0	0	0	9.99	0	900	0	0	0	0	0	0	
	S/L phas e out	64	50.0	1.00	l	4636	0	0	0	0	3510	0	0	0	0	0	0	0	1.00 E-02	0	100	0	0	1026	0	0	0	
		65	50.0	1.00	l	4636	0	0	0	0	3510	0	0	0	0	0	0	0	1.00 E-02	0	100	0	0	1026	0	0	0	
Input		66	25.0	1.00	l	9434					9434																	
		66a	25.0	1.00	l	9434					9434																	
Input		67	25.0	1.00	s	566																566						
		67a	25.0	1.00	s	566																566						
R4	1026	kg	Vancomycin			is converted in rxn 1 (100 % of reactor input)																						
		kg				is lost in rxn																						

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
						2																						
		kg				is lost in rxn 3																						
		Input to reactor			:	1.46 E+04	0	0	0	0	1.29E +04	0	0	0	0	0	0	0	1.00 E-02	0	100	566	0	1026	0	0	0	
		R4 Reaction Coefficient 1			:													1.00				-1.00		-1.00	1.00			
		R4 Conversion 1 [kg/hr]			:	-0.333												12.1				-37.9		-1026	1052			
		R4 Conversion 1 [kgmol/hr]			:	0.708												0.708				-0.708		-0.708	0.708			
		R4 Reaction Coefficient 2			:																							
		R4 Conversion 2 [kg/hr]			:																							
		R4 Conversion 2 [kgmol/hr]			:																							
		R4 Reaction Coefficient 3			:																							
		R4 Conversion 3 [kg/hr]			:																							
		R4 Conversion 3 [kgmol/hr]			:																							
		Flow out of reactor			:	1.46 E+04	0	0	0	0	1.29E +04	0	0	0	0	0	0	12.1	1.00 E-02	0	100	528	0	0	1052	0	0	
		Primary product			:	Vancomycin HCl																						
		Total conversion			:		NA	NA	NA	NA	-0	-0	NA	-0	-0	-0	-0	-1.21	-0	-0	-0	3.35	-0	NA	NA	NA	NA	
		Per pass conversion			:						-0							NA	-0		-0	6.70		100	NA			
		Total yield from reactor			:																	100		100	NA			
		68	32.3	1.00	l	1.46	0	0	0	0	1.29E	0	0	0	0	0	0	12.1	1.00	0	100	528	0	0	1052	0	0	

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
						E+04					+04								E-02									
		69	32.3	1.00	l	1.46E+04	0	0	0	0	1.29E+04	0	0	0	0	0	0	12.1	1.00E-02	0	100	528	0	0	1052	0	0	
Waste		70	32.3	1.00	l	-1.36E+04	0	0	0	0	-1.29E+04	0	0	0	0	0	0	-12.1	-9.99E-03	0	-99.9	-528	0	0	-52.6	0	0	0
		71a	32.3	1.00	s	1013	0	0	0	0	12.9	0	0	0	0	0	0	0.0121	1.00E-05	0	0.1000	0.528	0	0	999	0	0	
		71	32.3	1.00	s	1013	0	0	0	0	12.9	0	0	0	0	0	0	0.0121	1.00E-05	0	0.1000	0.528	0	0	999	0	0	
Input		72	25.0	1.00	l	1.00E+04					1.00E+04																	
		73	25.0	1.00	l	1.00E+04					1.00E+04																	
Input		74	25.0	1.00	s	1200																	1200					
		75	25.0	1.00	s	1200																	1200					
R5	999	kg	Vancomycin HCl			is converted in rxn 1 (100 % of reactor input)																						
		kg				is lost in rxn 2																						
		kg				is lost in rxn 3																						
		Input to reactor			:	1.22E+04	0	0	0	0	1.00E+04	0	0	0	0	0	0	0.0121	1.00E-05	0	0.1000	0.528	1200	0	999	0	0	
		R5 Reaction Coefficient 1			:														1.00					1.00	-1.00			
		R5 Conversion 1 [kg/hr]			:	0.336													24.6					975	-999			
		R5 Conversion 1 [kgmol/hr]			:	0.673													0.673					0.673	-0.673			
		R5 Reaction Coefficient 2			:																							
		R5 Conversion 2 [kg/hr]			:																							

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
		R5 Conversion 2 [kgmol/hr]			:																							
		R5 Reaction Coefficient 3			:																							
		R5 Conversion 3 [kg/hr]			:																							
		R5 Conversion 3 [kgmol/hr]			:																							
		Flow out of reactor			:	1.22 E+04	0	0	0	0	1.00E +04	0	0	0	0	0	0	0.01 21	24.6	0	0.10 00	0.52 8	1200	975	0	0	0	
		Primary product			:	Vancomyci n																						
		Total conversion			:		NA	NA	NA	NA	-0	-0	NA	-0	-0	-0	-0	-0	- 2.46 E+05	-0	-0	-0	-0	NA	NA	NA	NA	
		Per pass conversion			:						-0							-0	NA		-0	-0	-0	NA	100			
		Total yield from reactor			:																			NA	100			
		76	25.0	1.00	l	1.22 E+04	0	0	0	0	1.00E +04	0	0	0	0	0	0	0.01 21	24.6	0	0.10 00	0.52 8	1200	975	0	0	0	
		77	25.0	1.00	l	1.22 E+04	0	0	0	0	1.00E +04	0	0	0	0	0	0	0.01 21	24.6	0	0.10 00	0.52 8	1200	975	0	0	0	
Wast e		78	25.0	1.00	l	- 1.01 E+04	0	0	0	0	-9012	0	0	0	0	0	0	- 1.21 E-05	- 0.02 46	0	- 0.09 00	- 0.47 5	- 1080	- 0.97 5	0	0	0	0
		79	25.0	1.00	s	2120					1001	0	0	0	0	0	0	0.01 21	24.5	0	1.00 E-02	0.05 28	120	974	0	0	0	
Input		80	25.0	1.00	l	1.00 E+04					1.00E +04																	
		80a	25.0	1.00	l	1.00 E+04	0	0	0	0	1.00E +04																	
Input		81	25.0	1.00	s	566	0	0	0	0												566						
		81a	25.0	1.00	s	566																566						
R6	974	kg	Vancomyci			is converted in rxn 1 (100 %																						

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
			n			of reactor input)																						
		kg				is lost in rxn 2																						
		kg				is lost in rxn 3																						
		Input to reactor			:	1.27 E+04	0	0	0	0	1.10E +04	0	0	0	0	0	0	0.01 21	24.5	0	1.00 E-02	566	120	974	0	0	0	
		R6 Reaction Coefficient 1			:													1.00				-1.00		-1.00	1.00			
		R6 Conversion 1 [kg/hr]			:	- 0.316												11.4				-36.0		-974	998			
		R6 Conversion 1 [kgmol/hr]			:	0.672												0.67 2				- 0.67 2		- 0.67 2	0.67 2			
		R6 Reaction Coefficient 2			:																							
		R6 Conversion 2 [kg/hr]			:																							
		R6 Conversion 2 [kgmol/hr]			:																							
		R6 Reaction Coefficient 3			:																							
		R6 Conversion 3 [kg/hr]			:																							
		R6 Conversion 3 [kgmol/hr]			:																							
		Flow out of reactor			:	1.27 E+04	0	0	0	0	1.10E +04	0	0	0	0	0	0	11.5	24.5	0	1.00 E-02	530	120	0	998	0	0	
		Primary product			:	Vancomyci n HCl																						
		Total conversion			:		0	0	0	0	-0	-0	NA	-0	-0	-0	-0	-1.14	-0	-0	-0	3.18	-0	NA	NA	NA	NA	
		Per pass conversion			:						-0							NA	-0		-0	6.35	-0	100	NA			
		Total yield from			:																	100.		100	NA			

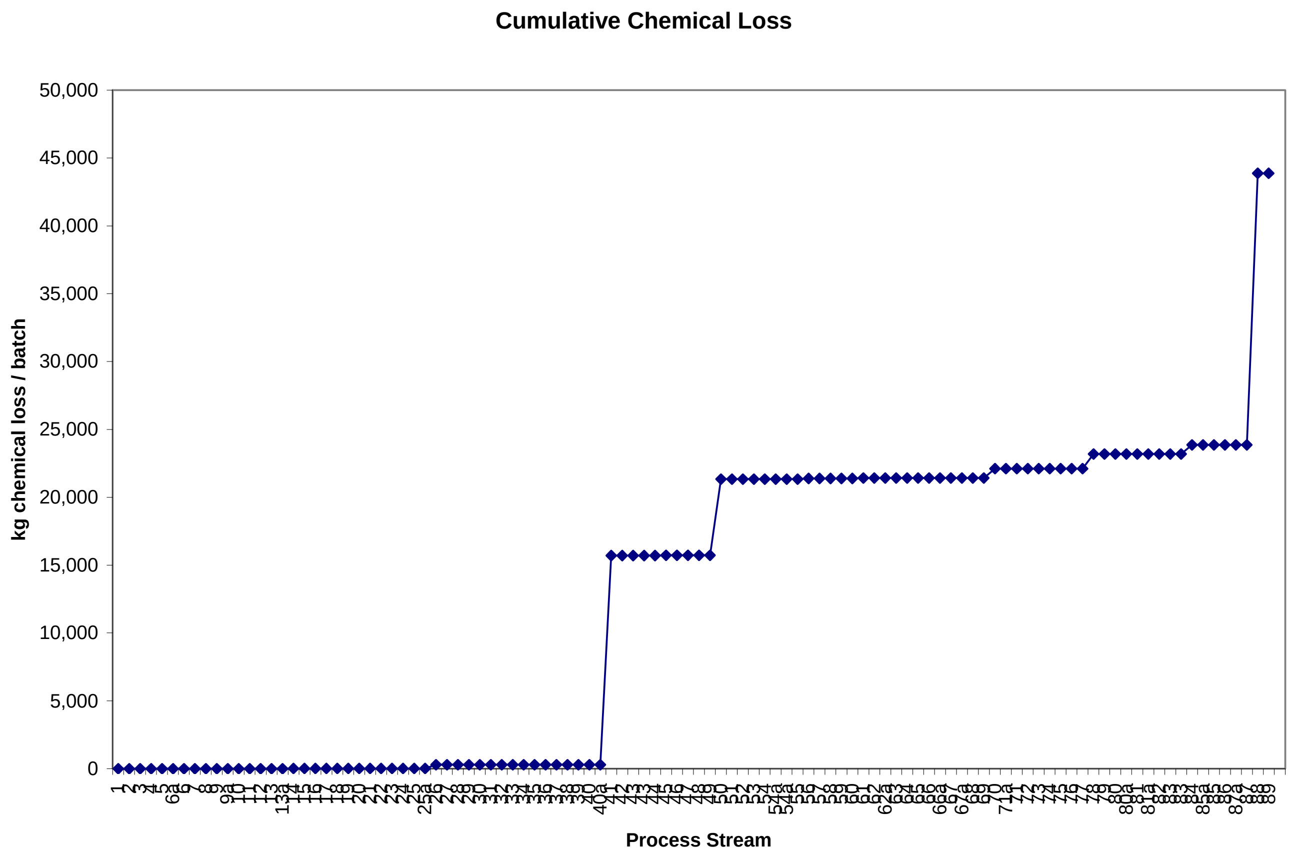
	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
		reactor																				0						
		82	25.0	1.00	l	1.27E+04	0	0	0	0	1.10E+04	0	0	0	0	0	0	11.5	24.5	0	1.00E-02	530	120	0	998	0	0	
		83	25.0	1.00	l	1.27E+04	0	0	0	0	1.10E+04	0	0	0	0	0	0	11.5	24.5	0	1.00E-02	530	120	0	998	0	0	
	Input	83	25.0	1.00	m	1.27E+04	0	0	0	0	1.10E+04	0	0	0	0	0	0	11.5	24.5	0	1.00E-02	530	120	0	998	0	0	
<> filter <>		solubility in solvent (g / g solvent)			:		0.160	0.400	0.400	0.400	1.00	0.400	1.00	1.00	0.272	0.420	1.00	1.00	1.00	0	1.00	0.260	1.00	200	0	1.00	1.00	
		liquid phase 83			:	1.17E+04	0	0	0	0	1.10E+04	0	0	0	0	0	0	11.5	24.5	0	1.00E-02	530	120	0	0	0	0	
		solid phase 83			:	998	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	998	0	0	
	Water	is the solvent																										
	0.200	g liquid / g solid in sediment																										
	1.71	% of liquid phase exits in solid stream																										
Waste	Liquid Out	84	25.0	1.00	l	-1.15E+04	0	0	0	0	-1.08E+04	0	0	0	0	0	0	-11.3	-24.1	0	-9.83E-03	-521	-118	0	0	0	0	
	Solid Out	85a	25.0	1.00	s	1198	0	0	0	0	188	0	0	0	0	0	0	0.196	0.419	0	1.71E-04	9.06	2.05	0	998	0	0	
		85	25.0	1.00	s	1199	0	0	0	0	188	0	0	0	0	0	0	0.196	0.419	0	1.71E-04	9.06	2.05	0	998	0	1.00	
Input		86	25.0	1.00	g	2.00E+04								2.00E+04														
		87a	25.0	1.00	g	2.00E+04								2.00E+04														

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
		87	50.0	1.00	g	2.00 E+04								2.00 E+04														
Waste		88	50.0	1.00	g	-2.02 E+04					-186			-2.00 E+04				-0.196	-0.419	0	-1.69 E-04	-8.97	-2.03	0				
		89a	50.0	1.00	s	1000	0	0	0	0	1.88	0	0	0	0	0	0	0	0	0	1.71 E-06	0.0906	0.0205	0	998	0	0	
Main product		89	25.0	1.00	s	1000	0	0	0	0	1.88	0	0	0	0	0	0	0	0	0	1.71 E-06	0.0906	0.0205	0	998	0	0	
		Product purity (%)				0.998																						
		Main product				Vancomycin HCl																						
		Overall Rxn coefficients					-25.0				-1.00						-7.00	2.00	1.00			-2.00			1.00	84.0		
		Total yield of process (from reactant)					25.0											NA	NA			6.35			NA	NA		
Waste		Fugitive Losses (Total)			g	-92.1	0	0	0	0	0	0	0	0	0	0	0	-5.00	-0.123	0	-10.0	0	0	0	0	-77.0	0	
		Input Sum				1.85 E+05	1.21 E+04	0.0233	6.36 E-03	6.36 E-03	1.35E +05	4625	0	2.00 E+04	0.222	0.0123	9679	1000	1.00 E-02	51.4	100	1132	1200	0	0	0	0	
		Fugitive Replacement of Reactants				0	0				0						0					0						
		Total Input (Input + Fugitive Replacement)				1.85 E+05	1.21 E+04	0.0233	6.36 E-03	6.36 E-03	1.35E +05	4625	0	2.00 E+04	0.222	0.0123	9679	1000	1.00 E-02	51.4	100	1132	1200	0	0	0	0	
		Product				1000	0	0	0	0	1.88	0	0	0	0	0	0	0	0	0	1.71 E-06	0.0906	0.0205	0	998	0	0	

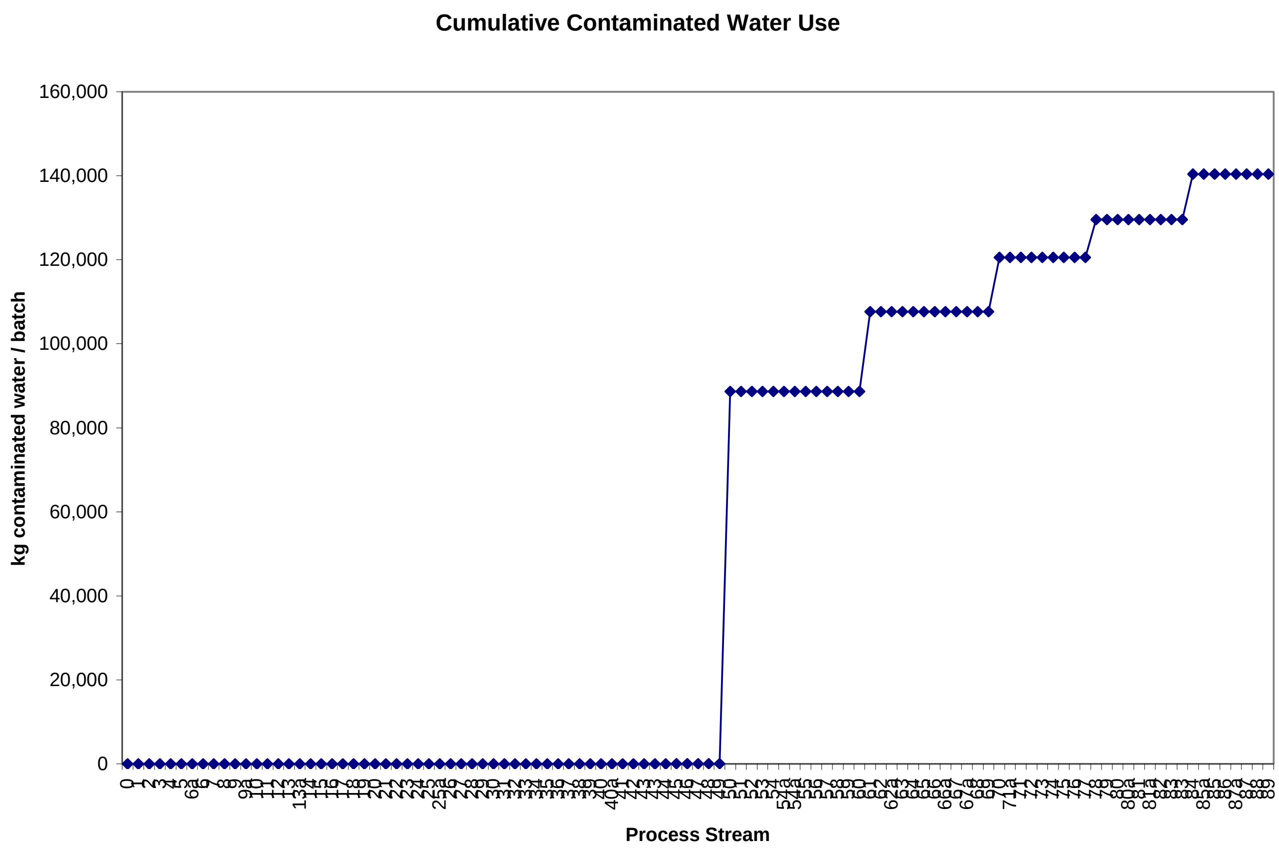
	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
		Sum																										
		Main product flow				1000	0	0	0	0	1.88	0	0	0	0	0	0	0	0	0	1.71E-06	0.0906	0.0205	0	998	0	0	
		Net Input (in - out, omitting fugitives)				-320																						
Input		C1	20.0	1.00	l	3526																						3526
Cooling out		C2	50.0	1.00	l	-3526																						-3526
Input		C3	20.0	1.00	l	843																						843
Cooling out		C4	50.0	1.00	l	-843																						-843
Input		C5	20.0	1.00	l	7.05E+04																						70518
Cooling out		C6	50.0	1.00	l	-7.05E+04																						-70518
Input		C7	20.0	1.00	l	1.68E+04																						16807
Cooling out		C8	50.0	1.00	l	-1.68E+04																						-16807
Input		C9	20.0	1.00	l	1.24E+06																						1239270
Cooling out		C10	50.0	1.00	l	-1.24E+06																						-1239270
Input		C11	20.0	1.00	l	9.41E+05																						941202
Cooling out		C12	50.0	1.00	l	-9.41E+05																						-941202
Input		S1	207	1.00	l	323																					323	

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Dextrose	Peptone	Yeast Extract	Malt Extract	Water	Soy Flour	Sodium nitrate	Air	Magnesium Sulfate	Calcium dichloride	Oxygen	Ammonia	Hydrogen chloride	Diatomaceous earth	Isopropanol	Ammonium chloride	Urea	Vancomycin	Vancomycin HCl	Carbon dioxide	Steam	Water
Steam out		S2	207	1.00	l	-323																					-323	
Input		S3	207	1.00	l	6460																					6460	
Steam out		S4	207	1.00	l	-6460																					-6460	
Input		S5	207	1.00	l	1.14E+05																					113604	
Steam out		S6	207	1.00	l	-1.14E+05																					-113604	
Input		S7	207	1.00	l	9049																					9049	
Steam out		S8	207	1.00	l	-9049																					-9049	
Input		S9	207	1.00	l	309																					309	
Steam out		S10	207	1.00	l	-309																					-309	

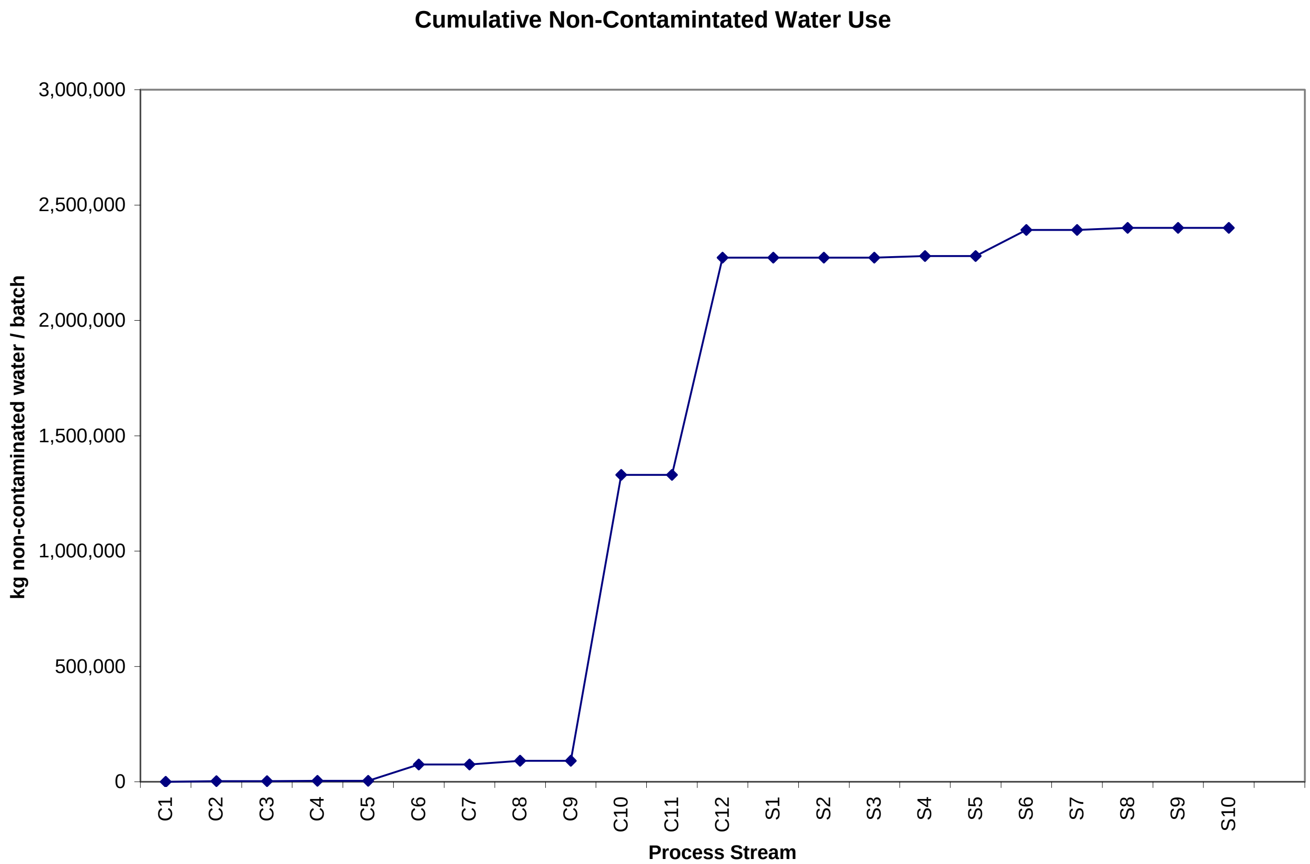
Graph of Cumulative Chemical Losses through Manufacturing Process



Graph of Cumulative Contaminated Water Use



Graph of Cumulative Non-Contaminated Water Use



Energy Input for each Unit Process, Cumulative Energy Requirements, Cooling Requirements (exotherms), and Assumed Heat Recovery from Hot Streams Receiving Cooling

Energy Input [MJ / batch]						Cooling Requirements [MJ / batch]									
Process Diagram Label	Unit	Energy input [MJ / 1000 kg Product]	Cumulative energy [MJ / 1000 kg Product]	To [C] (Used to determine	Energy Type	Process diagram label	Unit	Energy Loss	Cumulative cooling water energy	Tef [C] (for recovery	Recovery Efficiency	Energy Recovered	Cumulative recovered [MJ / 1000 kg Product]
P2	Pump 2	3.97E-06	3.97E-06		E	Hx2	Heat exchanger 2	-521	-521	120	0.250	-130	-130
Hx1	Heat exchanger 1	525	525	120	S	R1	Reactor 1	-124	-645	30.0	0	0	-130
Blw1	Blower 1	0.0451	525		E	Hx4	Heat exchanger 4	-1.04E+04	-1.11E+04	120	0.250	-2603	-2734
:	Agitator R1A	0.233	525		E	R2	Reactor 2	-2482	-1.35E+04	30.0	0	0	-2734
:	Agitator R1B	0.114	525		E	Hx6	Heat exchanger 6	-1.83E+05	-1.97E+05	120	0.250	-4.58E+04	-4.85E+04
:	Agitator R1	27.6	553		E	R3	Reactor 3	-1.39E+05	-3.36E+05	30.0	0	0	-4.85E+04
P3	Pump 3	4.51E-06	553		E	Evp1	Evaporator condenser 1	-1.37E+04	-3.49E+05	50.0	0	0	-4.85E+04
P4	Pump 4	1.42	554		E								
P5	Pump 5	0.0138	554		E								

Hx3	Heat exchanger 3	1.05E+04	1.11E+04	120	S								
Blw2	Blower 2	0.820	1.11E+04		E								
:	Agitator R2A	4.67	1.11E+04		E								
:	Agitator R2B	0.241	1.11E+04		E								
:	Agitator R2	345	1.14E+04		E								
P6	Pump 6	0.0175	1.14E+04		E								
Hx5	Heat exchanger 5	1.85E+05	1.96E+05	120	S								
Blw3	Blower 3	123	1.96E+05		E								
:	Agitator R3A	94.1	1.96E+05		E								
:	Agitator R3B	0.510	1.96E+05		E								
:	Agitator R3	2.23E+04	2.19E+05		E								
P7	Pump 7	0.849	2.19E+05		E								
P8	Pump 8	0.177	2.19E+05		E								
P9	Pump 9	0.177	2.19E+05		E								
P10	Pump 10	0.178	2.19E+05		E								
:	Agitator M1	0.212	2.19E+05		E								
P11	Pump 11	0.181	2.19E+05		E								
P12	Pump 12	0.0105	2.19E+05		E								
P13	Pump 13	0.177	2.19E+05		E								
P14	Pump 14	0.233	2.19E+05		E								
Evp1	Evaporator 1	1.47E+04	2.33E+05	50.0	S								
P15	Pump 15	0.0209	2.33E+05		E								
:	Agitator R4	309	2.34E+05		E								
P16	Pump 16	0.150	2.34E+05		E								
Cnv1	Conveyer 1	2.38E-03	2.34E+05		E								
P17	Pump 17	0.512	2.34E+05		E								
P18	Pump 18	0.177	2.34E+05		E								
Cnv2	Conveyer 2	4.25E-03	2.34E+05		E								
:	Agitator R5	258	2.34E+05		E								
P19	Pump 19	0.309	2.34E+05		E								

P20	Pump 20	0.177	2.34E+05		E								
Cnv3	Conveyer 3	5.04E-03	2.34E+05		E								
:	Agitator R6	268	2.34E+05		E								
P21	Pump 21	0.344	2.34E+05		E								
Blw4	Blower 4	1.39	2.34E+05		E								
Hx7	Heat exchanger 7	502	2.35E+05	50.0	S								
Cnv4	Conveyer 4	2.38E-03	2.35E+05		E								
Cnv5	Conveyer 5	5.03E-03	2.35E+05		E								
	Potential recovery	-4.85E+04	1.86E+05										
	Net energy		1.86E+05				Potential recovery:						-4.85E+04
	Electricity	2.37E+04	E	[MJ/hr]									
	DowTherm	0	D	[MJ/hr]									
	Heating steam	2.11E+05	S	[MJ/hr]									
	Direct fuel use	0	F	[MJ/hr]									
	Heating natural gas	0	G	[MJ/hr]									
	Energy input requirement	2.35E+05		[MJ/hr]									
	Cooling water	-3.49E+05		[MJ/hr]									
	Cooling refrigeration			[MJ/hr]									
	Potential heat recovery	-4.85E+04		[MJ/hr]									
	Net energy	1.86E+05		[MJ/hr]									

Graph of Cumulative Energy Requirements