QFL5931/MPT6009 – Química Verde

Análise de Ciclo de Vida – Aula 2

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Estudo de Caso

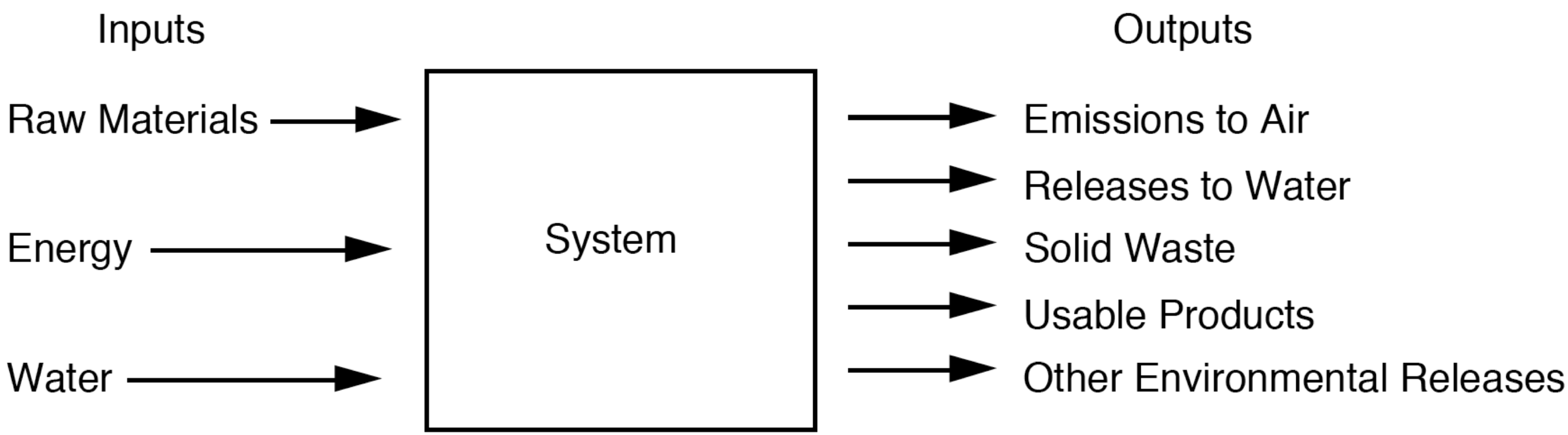
Saco de papel vs. Saco de Plástico

Material Didatico: Paper or Plastic? A LCA perspective

http://www.monroecounty.gov/Image/LESSON12.pdf

Análise de Inventário

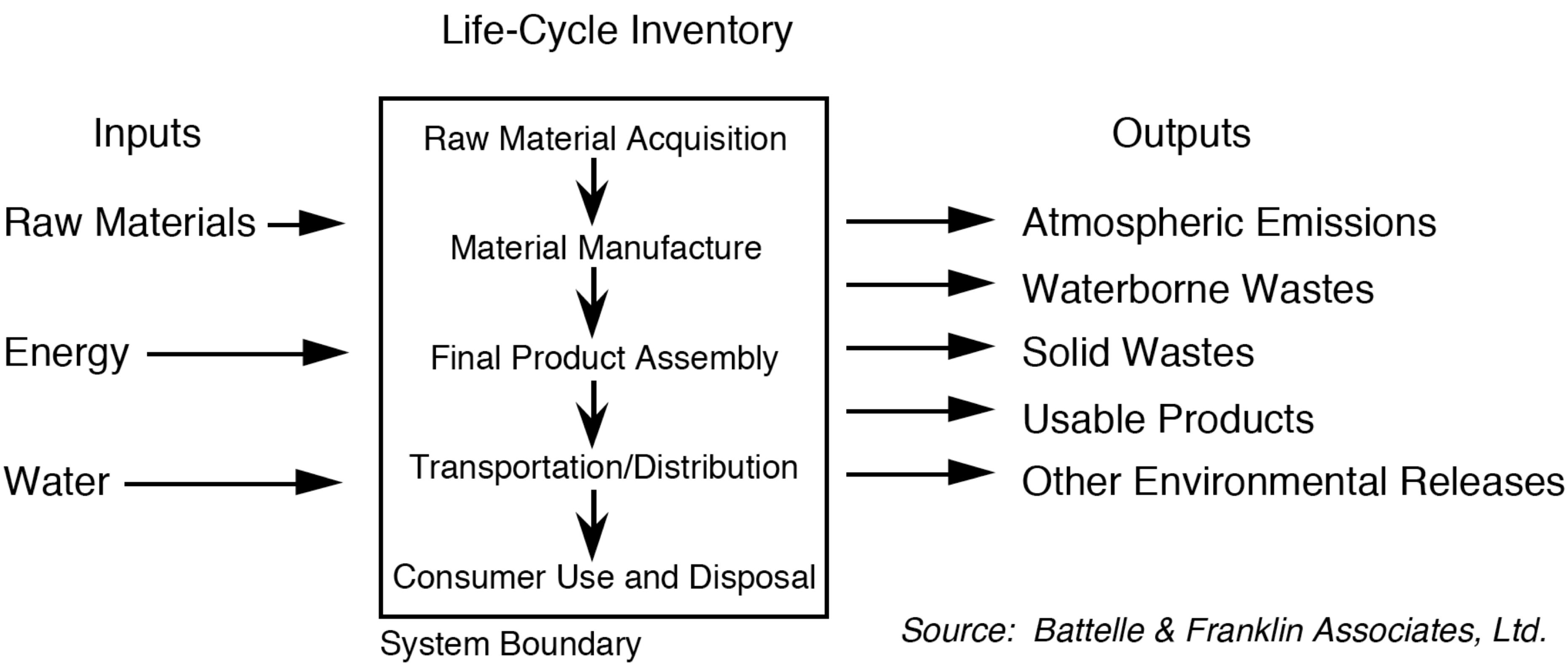
Entradas e Saídas de um Sistema:



http://www.umich.edu/~nppcpub/resources/compendia/CORPpdfs/CORPlca.pdf

Análise de Inventário

Definindo as Fronteiras do Sistema:



Source: Battelle & Franklin Associates, Ltd.

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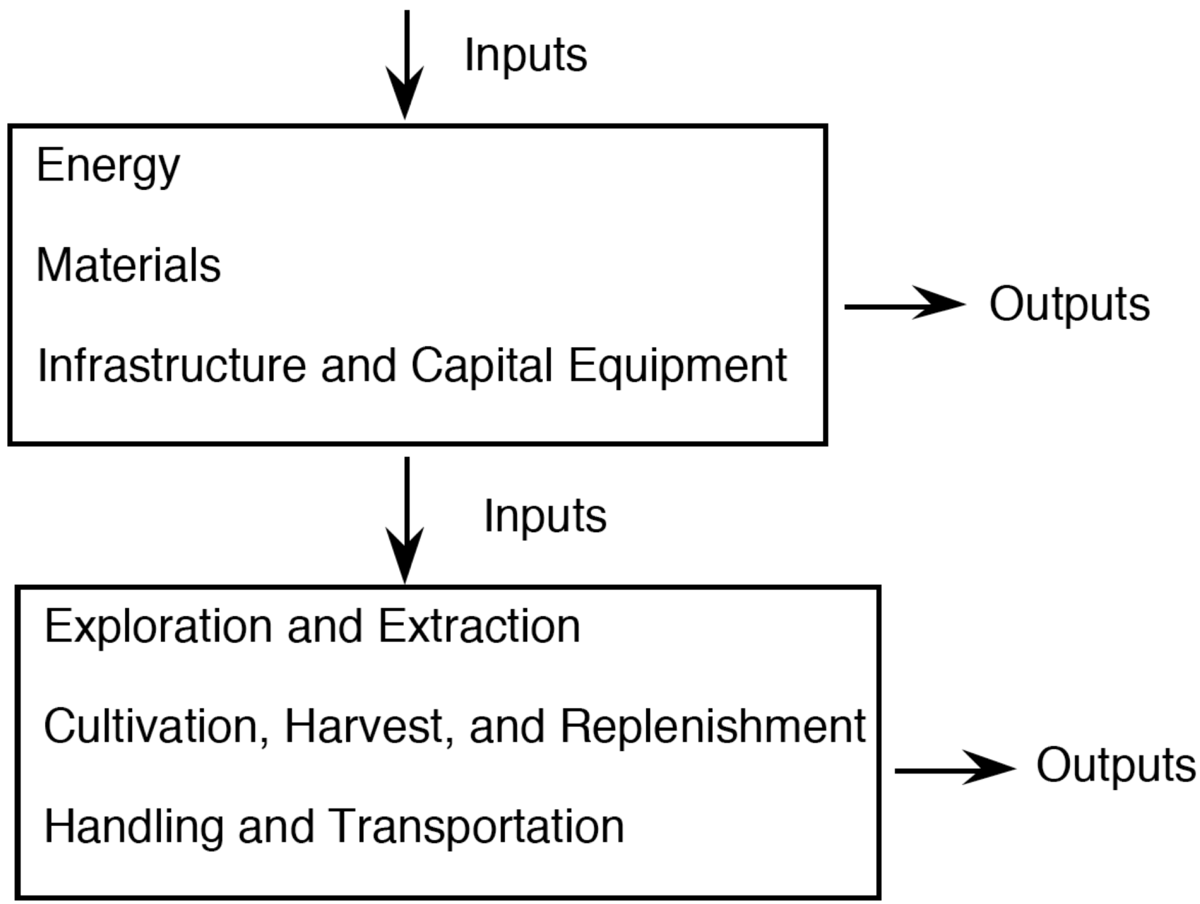
Análise de Inventário

Subsistema de Aquisição de Matéria-Prima:



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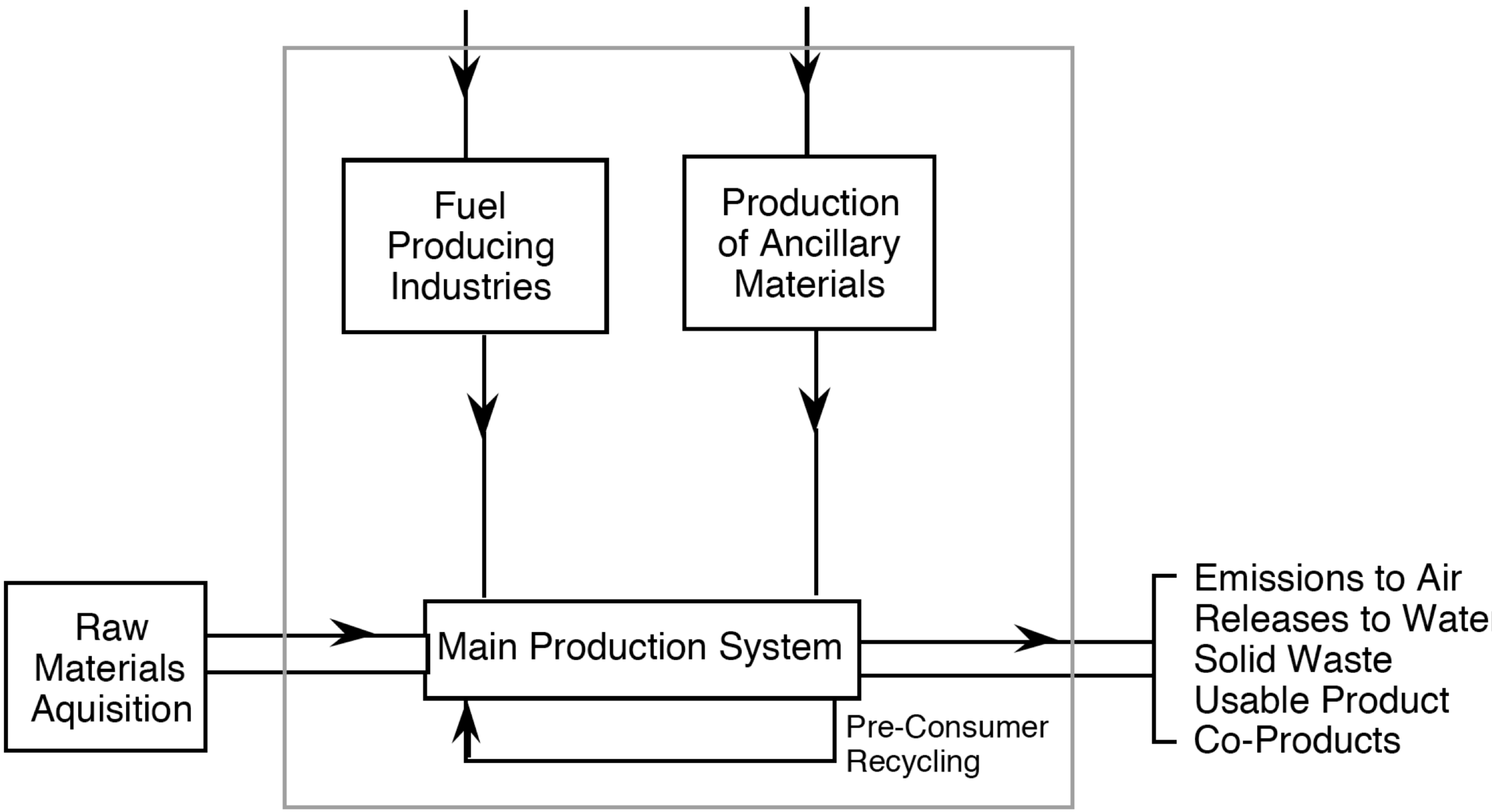

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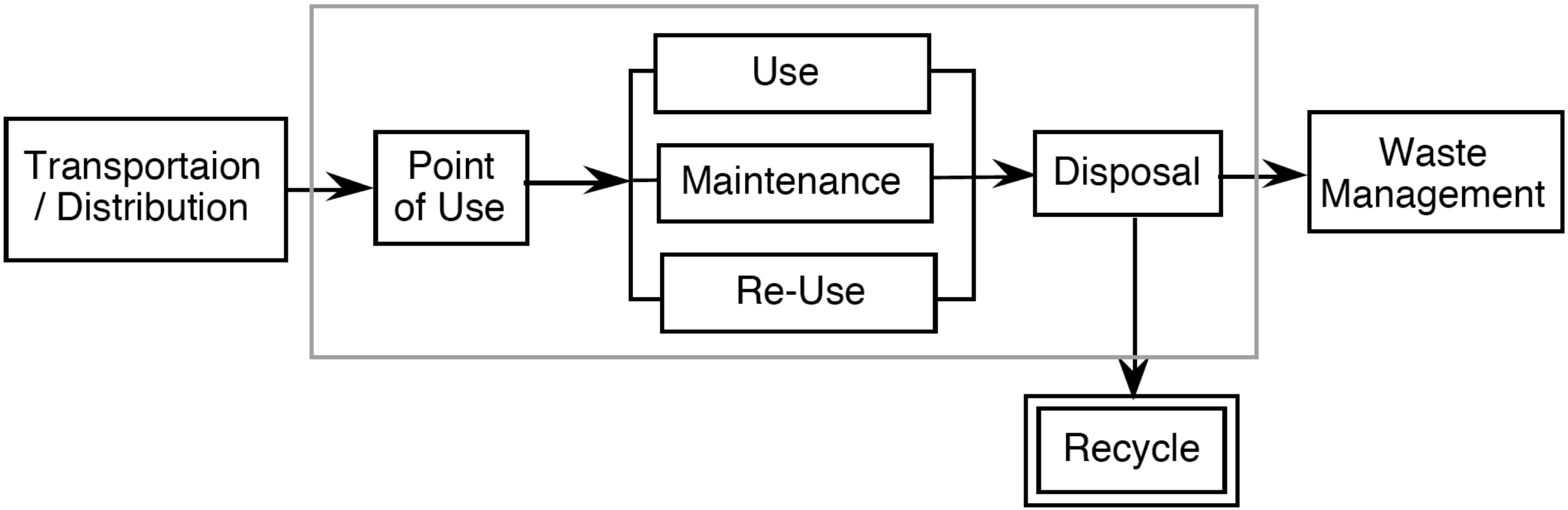
Análise de Inventário

Subsistema de Uso/Descarte pelo Consumidor:



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Análise de Inventário

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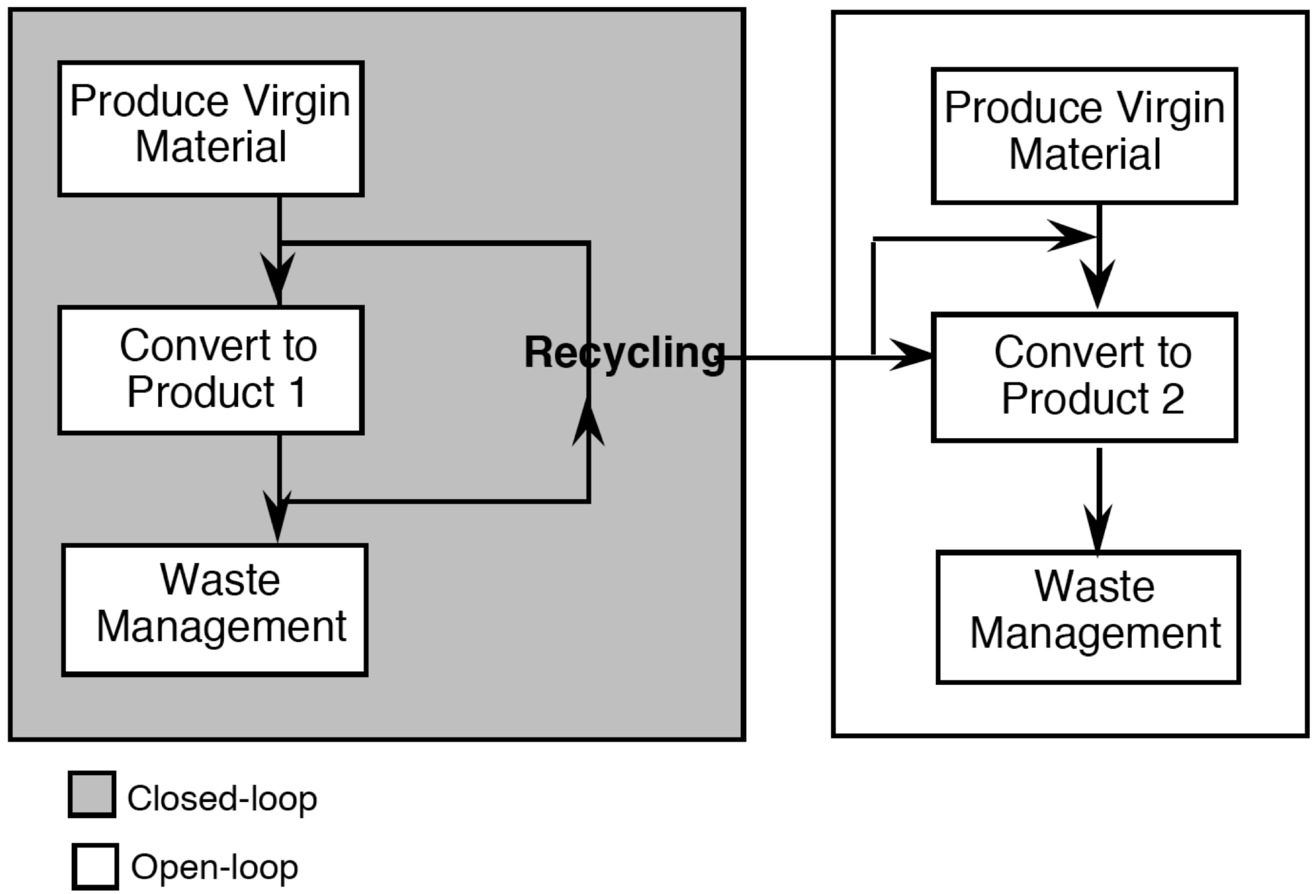

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ACV em Química

- Escopo e Definição das Fronteiras do Sistema
- Impactos da Produção e Utilização
- Quantificação das Entradas e Saídas de Produtos Químicos/Reações
- Propriedades das "Entradas e Saídas" de Produtos Químicos/Reações
- "Economia" da Reação
- Requerimentos Regulatórios

Incorporation of Pollution Prevention Principles Into Chemical Science Education
Jonathan W. Greene
Center for Sustainable Systems – Umich
http://www.umich.edu/~nppcpub/resources/compendia/CHEMpdfs/

ACV em Química

Propriedades:

TABLE 4: Physical and Chemical Properties of Chemicals and Chemical Reactions

CHEMICALS	*CHEMICAL REACTIONS*
Form (solid/liquid/gas)	Activation Energy (ΔH = exo/endothermic)
Density	Net Temperature
Deactivation Rate (catalysts)	Net Pressure
Melting Point	pH
Boiling Point	Reaction Time/Reactor Time
Vapor Pressure	Selectivity
Lower Explosive Limit (LEL)	Atom Economy
Upper Explosive Limit (UEL)	Percent Conversion of Reactants
Speciation (ions, compounds, radicals)	Reaction Yield
Partition Coefficient (Log K_{OW})	Batch/Continuous
Persistence ($T_{1/2}$)	
Water Solubility	
Bioaccumulation Factor (chem. concentraion in biota or water)	
Freezing Point	

ACV em Química

Propriedades:

TABLE 5: Health and Physical Hazards Associated with Chemicals (60)

PHYSICAL HAZARDS	*HEALTH HAZARDS*[3]
Fire Hazards	**Acute**
combustible liquid	irritantsG31
flammable aerosols	cutaneous hazards
flammable gases	toxic agents
flammable liquids	highly toxic agents
flammable solids	eye hazards
oxidizers	blood/hematopoietic agents
pyrophoric materials	
	Chronic
Other Physical Hazards	sensitizers
water reactive materials	carcinogens
compressed gases	reproductive toxins
explosives	hepatotoxins
shock- sensitive chemicals	nephrotoxins
heat-sensitive chemicals	neurotoxins
unstable materials	pulmonary toxins

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Propriedades:

TABLE 6: Statutory Terminology that Applies to Chemicals and Reaction Residuals

STATUTE	***TERMINOLOGY***
Resource Conservation and Recovery Act	**Hazardous Waste, Solid Waste**
Atomic Energy Act	**Nuclear Waste**
Comprehensive Environmental Response, Compensation, and Liability Act	**Hazardous Substance (reportable quantity chemicals, metals)**
Clean Air Act	**Hazardous Air Pollutants, Criteria Pollutants**
Clean Water Act	**Waste Water, Water Pollutants**

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Propriedades:

TABLE 7: Renewable and Non-renewable Reaction Feedstock and Energy Sources (10)

	RENEWABLE	NON-RENEWABLE
FEEDSTOCKS	Biomass (agriculture-based, forests)	Petroleum, Minerals, Ores, & Metals
ENERGY	Solar	Fossil Fuels
	Wind	Nuclear
	Geothermal	
	Hydroelectric	
	Biomass (e.g., wood, crop/animal wastes, or glucose-based ethanol / methanol fuels)	
	Combustion of landfill methane	
	Combustion of solid and hazardous wastes	

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Propriedades:

TABLE 8: Ecological Impacts Associated with Renewable Feedstock and Energy Sources (10, 16)

CONSTRUCTION OF HYDROELECTRIC DAMS
- Loss of critical habitats and endangered flora and fauna, alteration of aquatic habitats
- Alteration in sediment and ground/surface water flows
- Displacement of human populations and loss of historical artifacts

BIO-BASED FUEL/FEEDSTOCK SOURCES
- Deforestation and land-clearing , topsoil erosion, loss of critical habitats & species diversity
- Surface and groundwater contamination from excessive pesticide and fertilizer applications

SOLAR POWER
- Hazardous materials (metals) utilized in batteries for long-term energy storage

HAZARDOUS AND SOLID WASTE COMBUSTION
- Air pollution associated with combustion and processing of fuels
- Ash and other residual solid wastes have concentrated toxicity
- Combustion and processing of inert materials may result in conversion to highly toxic species (i.e., ,dioxin and derivatives)

ACV em Química

"Economia" da Reação:

TABLE 9: Reaction Costing Framework Based on ABC/M and TCA Principles (14)

USUAL PRODUCTION COSTS

Capitol Costs	*Production Costs*	*Production Revenue*
• Buildings	• Residual Mgmt. / Disposal	• Desired Rxn Product
• Production Equip.	• Utilities	• Rxn Co-products
• Pollution Control Equip.	• Raw Materials	• Recycled Residuals
	• Misc. Supplies	• Managed Residuals
	• Labor	

HIDDEN & LESS-TANGIBLE COSTS & BENEFITS

Capitol Costs	*Expenses*	*Benefits*
• Emission-monitoring equip.	• Closure/post-closure care	• Green marketing
• Safety/control technology	• Reporting & recordkeeping	• Corporate image
• Personal protective equip.	• Monitoring/Testing	• Consumer loyalty
	• Planning/studies/modeling	
	• Medical surveillance	
	• Worker Training	
	• Insurance and material use taxes	
	• Facility and product labeling	
	• Research and Development	

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"Economia" da Reação:

LIABILITY COSTS[7]

- Legal staff or consultants
- Penalties and fines
- Workplace injury
- Customer injury due to product malfunction (product liability lawsuits)
- Future liabilities from contamination of production and residual disposals
  - soil and waste removal , treatment
  - ground water removal and treatment
  - personal injury to surrounding community (health care, insurance ramifications)
  - economic loss, real property damage
  - natural resource damage
- Bans and taxes on chemicals and chemically based products
  - fines for non-compliance
  - capitol expenses for re-tooling of production equipment
  - research and development to identify alternatives

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Requerimentos Regulatórios:

TABLE 10: Federal Laws for Consideration in Chemical Production and Utilization (10, 14, 63)

STATUTE	*MEDIA/AREA OF REGULATION*
Clean Air Act[8]	Air pollution discharges(point/non-point source; mobile/stationary sources)
Clean Water Act	Water pollution discharges (industrial, agricultural, municipal sources; stationary/mobile sources)
Safe Drinking Water Act	Sets health based standards for levels of contaminants in water delivered to users of public water supplies
Comprehensive Environmental Response, Compensation, and Liability Act	Allocates federal and state authority to clean up industrial sites contaminated with chemicals
Federal Insecticide, Fungicide, and Rodenticide Act	Regulates sale, labeling, and testing of pesticides, herbicides, fungicides, and rodenticides
Occupational Safety and Health Act	Regulates safety and health of workers in the occupational environment
Resource Conservation and Recovery Act	Generation, storage and disposal of solid and hazardous waste
Toxic Substances Control Act	Production, use, distribution of new chemicals into industrial and consumer markets
Mining Safety and Health Act	Regulates all aspects of mining activities in U.S.
Pollution Prevention Act	Establishes a national policy for P2
National Environmental Policy Act	Requires all applicable federally funded projects to undergo an environmental impact assessment prior to initiation

Estudo de Caso

Anticongelantes: etilenoglicol vs. propilenoglicol

PG-BASED ANTIFREEZE	*% OF TOTAL*
Water	**3.20**
Propylene Glycol	**94.00**
Sodium Hydroxide	**0.20**
Sodium Nitrate	**0.30**
Sodium Silicate	**0.29**
Sodium Tetraborate	**2.01**

EG-BASED ANTIFREEZE	*% OF TOTAL*
Water	**2.20**
Ethylene Glycol	**96.20**
Sodium Hydroxide	**0.22**
Sodium Nitrate	**0.15**
Sodium Silicate	**0.23**
Sodium Tetraborate	**0.70**
Sodium Orthophosphate	**0.30**

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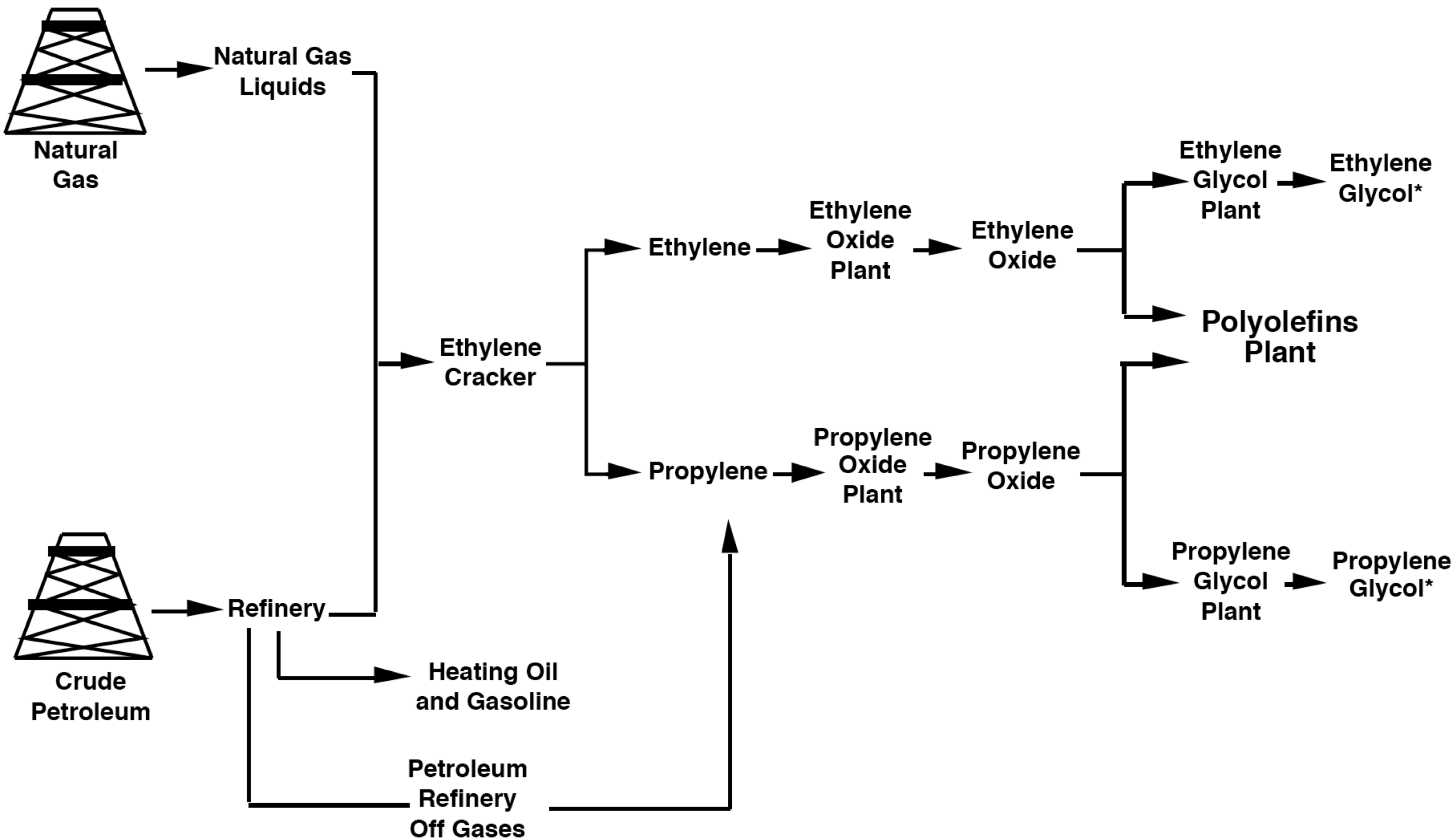
Escopo: EUA

PG PRODUCTION	Hydrolysis of Propylene Oxide (PO) in Water
EG PRODUCTION	Hydrolysis of Ethylene Oxide (EO) in Water
PO PRODUCTION	Weighted Average of Chlorohydrination, Isobutane Hydroperoxidation, and Ethylbenzene Hydroperoxidation
EO PRODUCTION	Catalytic Oxidation of Ethylene

Escopo: EUA

Figure 4: Summary of Production Processes of EG- and PG-Based Antifreeze Solutions



Quantificação de "Entradas e Saídas"

TABLE 11: Component Weights for EG- and PG-based Antifreeze Product and Packaging System (55)

	EG ($lbs/10^3 gallons$)	*PG ($lbs/10^3 gallons$)*
Feedstocks and other Reaction Inputs		
Ethylene	14,590.00 to 31,265.00	–
Ethylene Oxide	2,751.00	–
Silver Catalyst	n/a	–
Molydenum Catalyst	–	n/a
Isobutane	–	34,394.00
tert–butyl hydroperoxide	–	6,405.00
Propylene Oxide	–	3,241.00
Propylene	–	29,891.00
Methyl Tert–butyl Ether (co–product)	–	n/a
Antifreeze Product		
Ethylene Glycol	4,274.00	–
Propylene Glycol	–	4,316.00
Sodium Tetraborate	31.10	92.80
Sodium Silicate	10.20	13.30
Sodium Nitrate	6.70	13.80
Sodium Orthophosphate	13.30	–
Sodium Hydroxide	9.80	9.60
Water	95.90	147.00
Water Added by Consumer	4,442.00	4,072.00
Primary Packaging		
HDPE Containers	162.00	171.80
Polypropylene Cap	5.10	5.37
Bleached Paperboard Cap Liner	0.77	0.80
Aluminum Foil & HDPE Film Safety Seal	0.11	0.12
Tertiary Packaging		
Corrugated Cardboard	166.60	176.20
LDPE Stretchwrap	2.00	2.10

TABLE 12: Energy (Btu) Requirements for Production and Utilization of 1,000 gallons of EG- and PG-Based Antifreeze Solutions (55)

	Process	Transportation	Material Resource	WTE Credit	Total
EG	63.2	3.9	65.9	(4.6)	128.5
PG	119.6	5.7	69.0	(4.6)	189.7

TABLE 13: Energy (Btu) Requirements for Components of EG- and PG-Based Antifreeze Product and Packaging Systems (55)

	EG Energy	% Total	PG Energy	% Total
Glycol Production	114.6 Btu	86.1	175.2 Btu	90.2
Formulation Chemicals	0.5	0.3	0.8	0.4
Antifreeze Formulation	5.4	4.0	5.0	2.6
Primary Packaging	6.5	4.9	6.9	3.6
Tertiary Packaging	2.6	2.0	2.8	1.4
Disposition	3.5	2.7	3.6	1.8
Total	133.1 Btu		194.2 Btu	

Note:
- All numbers expressed in terms of 10^6 Btu
- Dilution ratios are 50% water / 50% EG product, 47% water / 53% PG product

TABLE 14: Energy Sources Associated with Production and Utilization of 1,000 Gallons of EG- and PG-Based Antifreeze Solutions (56)

	Natural Gas	Oil	Coal	Hydro	Nuclear	Wood	Other	*Total*
EG	86.6	29.8	10.8	0.61	4.3	0.96	0.074	133.1 Btu
PG	113.8	44.7	24.5	1.25	8.8	1.02	0.15	194.2 Btu

Note:
- All numbers expressed in terms of 10^6 Btu
- Dilution ratios are 50% water / 50% EG product, 47% water / 53% PG product
- Data account for portion of electricity generated at manufacturing facilities & sold to grid

TABLE 15: Solid Waste Associated with Production and Utilization of 1,000 Gallons of EG- and PG-Based Antifreeze Solutions (56)

	Industrial Solid Waste Process		Fuel		*Post-Consumer Solid Waste*		*Total Solid Waste*	
	(lbs)	(ft^3)	(lbs)	(ft^3)	(lbs)	(ft^3)	(lbs)	(ft^3)
EG	**95**	**1.9**	**388**	**7.8**	**232**	**13.9**	**715**	**23.6**
PG	**346**	**6.9**	**831**	**16.6**	**246**	**14.7**	**1424**	**38.3**

NOTE:
- Dilution ratios are 50% water / 50% EG product, 47% water / 53% PG product
- 55% of corrugated containers are recycled; 19% of unrecycled packaging materials are combusted and 81% landfilled
- 94% of combustion of unrecyclable solid waste occurs at WTE facilities
- Data accounts for hazardous waste production but does not identify quantities

TABLE 16: Industrial Atmospheric Emissions Associated with Production of 1,000 Gallons of EG- and PG-Based Antifreeze Solutions[8] (55)

	Process EG (lbs.)	*Process PG (lbs.)*	*Fuel EG (lbs.)*	*Fuel PG (lbs.)*	*Total EG (lbs.)*	*Total PG (lbs.)*
acid	–	0.2	–	–	–	0.2
aldehydes *	0.033	0.034	0.26	0.035	0.29	0.39
ammonia	0.015	0.23	0.035	0.068	0.05	0.3
carbon dioxide *	2186	739	9313	17,609	11,499	18,348
carbon monoxide *	1.04	1.09	17.4	26.9	18.5	28
chlorine * ^	8.7E-05	0.0052	–	–	8.7E–05	0.0052
ethylbenzene	–	4.2	–	–	–	4.2
ethylene glycol #	7.29	–	–	–	7.29	–
ethylene oxide #	1.31	–	–	–	1.31	–
hydrocarbons	73.8	92.5	38	66.2	112	159
hydrogen fluoride	1.5E-04	1.6E-04	–	–	1.5E-04	1.6E-04
isobutane	–	6.75	–	–	–	6.75
kerosene *	–	–	8.87E-04	0.0018	8.8E-04	0.0018
lead ^	0.0012	0.0013	2.7E-04	5.1E-04	0.0015	0.0018
mercury * ^	3.7E-06	0.0014	–	–	3.7E-06	0.0014
methane	2.09	–	0.11	0.19	2.19	0.19
nitrogen oxides *	3.42	3.59	37.8	69.7	41.2	73.3
odorous sulfur	0.0051	0.054	–	–	0.0051	0.0054
other organics *	0.072	0.073	3.09	3.25	3.16	3.33
particulates *	1.45	1.39	11.5	25.4	13.0	26.8
propylene $	–	0.92	–	–	–	0.92
propylene chlorohydrin$	–	0.034	–	–	–	0.034
propylene oxide $	–	2.07	–	–	–	2.07
sulfur oxides *	4.17	4.37	30.7	66.9	34.8	71.3

* Emission results from acquisition and fuel combustion; mat'ls w/o designation were process-related wastes

^ Emission results from production of sodium hydroxide and chlorine utilized in paper manufacturing

Emission results from EG process only

$ Emission results from PG process only

TABLE 17: Industrial Waterborne Emissions Associated with Production of 1,000 Gallons of EG- and PG-Based Antifreeze Solutions (55)

	Process EG (lbs.)	*Process PG (lbs.)*	*Fuel EG (lbs.)*	*Fuel PG (lbs.)*	*Total EG (lbs.)*	*Total PG (lbs.)*
acid*	0.37 lbs	44.2 lbs	2.03 lbs	4.53 lbs	2.40 lbs	48.7 lbs
ammonia	0.0015	0.0016	–	–	0.0015	0.0016
biological oxygen demand	0.56	0.59	0.035	0.068	0.60	0.66
chromium	1.4E-04	1.5E-04	–	–	1.4E-04	1.5E-04
chemical oxygen demand	0.63	0.66	0.098	0.19	0.73	0.85
cyanide	1.6E-06	1.6E-06	–	–	1.6E-06	1.6E-06
dissolved solids *	9.56	19.6	13.9	25	23.5	44.6
fluorides	8.5E-05	9.0E-05	–	–	8.5E-05	9.0E-05
herbicides !	1.7E05	1.8E-05	–	–	1.7E-05	1.8E-05
hydrocarbons ##	–	4.07	–	–	–	4.07
iron *	4.1E-06	4.4E-06	1.6	3.3	1.6	3.30
lead ^	5.5E-09	2.1E-06	–	–	5.5E-09	2.1E-06
mercury ^	1.0E-08	3.8E-06	–	–	1.0E-08	3.8E-06
metal ion *	3.5E-05	3.8E-05	0.51	1.14	0.51	1.14
nickel	5.5E-09	2.1E-06	–	–	5.5E-09	2.1E-06
nitrogen !	0.002	0.002	–	–	0.0020	0.0021
oil	0.23	0.024	0.018	0.034	0.25	0.27
pesticide !	8.6E-06	9.1E-06	–	–	8.6E-06	9.1E-06
phenol*	7.7E-05	5.87	0.0089	0.017	0.0089	5.89
phosphates	0.019	0.02	–	–	0.019	0.020
sodium hydroxide	–	6.27	–	–	–	6.27
sulfides	0.17	0.18	0.0089	0.017	0.18	0.19
sulfuric acid *	–	–	0.019	0.039	0.019	0.039
suspended solids	2.26	0.75	0.053	0.1	2.31	0.85
zinc	0.0031	0.0032	–	–	0.0031	0.0032

Figure 5: Post-Production End Use, Waste Management, and Recycling Scenarios for EG- and PG-Based Spent Antifreeze Solutions

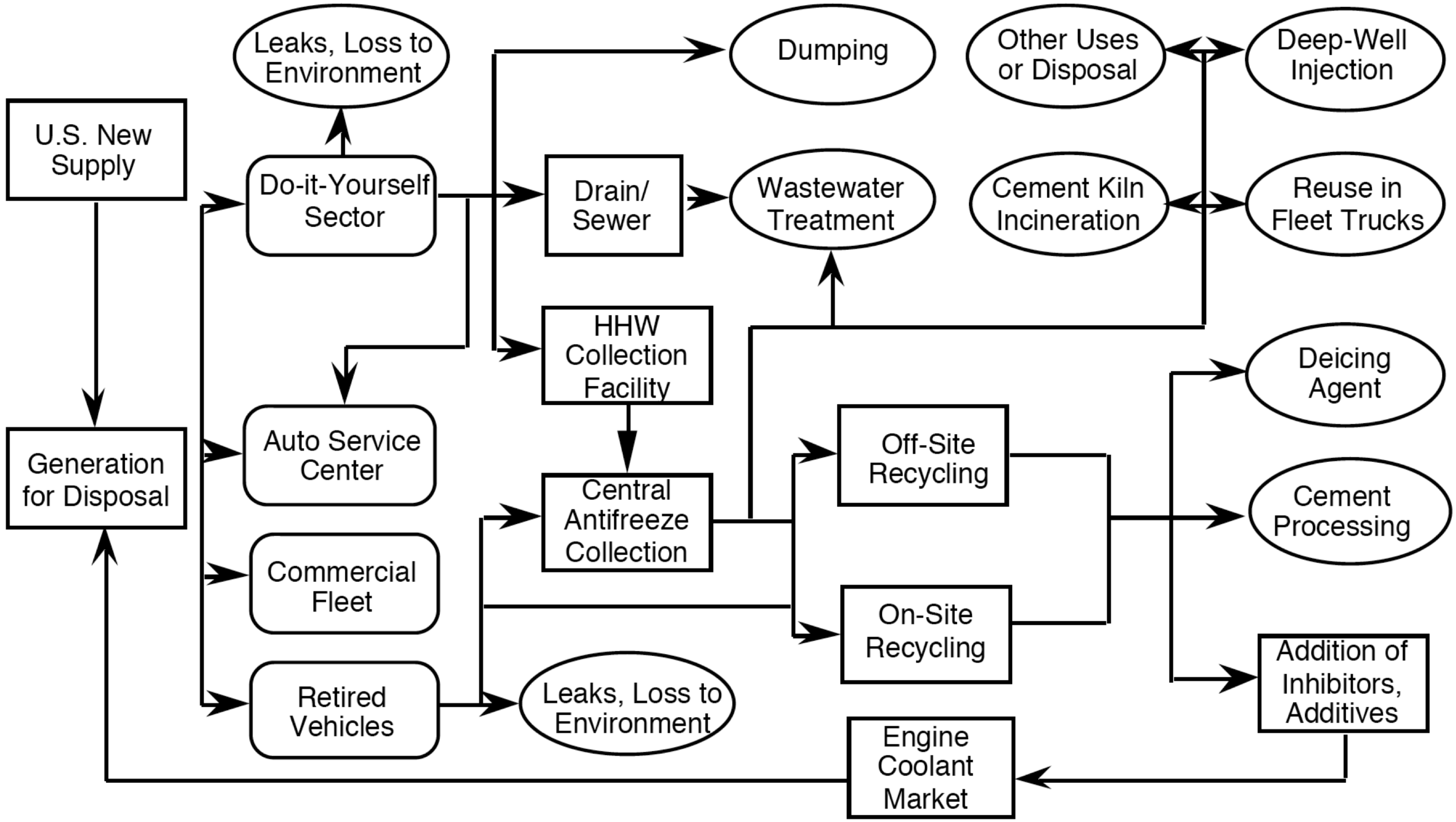


TABLE 18: Waterborne Wastes Generated by Improper Disposal of 1,000 gallons of EG- and PG-Based Antifreeze Solutions (55)

	lbs. EG*	lbs. PG*	lbs. PG**
Ethylene Glycol	1,665.000	0	0
Propylene Glycol	0	1,586.000	1,681.000
Sodium Hydroxide	3.810	3.540	3.710
Sodium Nitrate	2.420	5.060	5.400
Sodium Orthophosphate	5.190	0	0
Sodium Silicate	3.810	4.900	5.060
Sodium Tetraborate	12.100	34.100	36.100
Lead***	0.016	0.016	0.016
TOTAL	1692.340	1,633.620	1,731.270

Note: * Dilution ratio is 50% antifreeze product / 50% water

** Dilution ratio is 53% antifreeze product / 46% water

*** Lead is not present if antifreeze product is dumped in unused form

Propriedades

TABLE 19: Physical and Chemical Properties of Feedstock Chemicals Used in Production of EG- and PG-Based Antifreeze Products (66, 67, 68, 69, 71)

	EG	*PG*	*EO*	*PO*	*TBH*
REACTION PROPERTIES					
Rxn Temperature (°C)	200	125–200	220–275	110–120	120–140
Rxn Pressure (MPa)	n/a	2	1–2.2	4	3.63–5.0
% Feedstock Conversion	n/a	n/a	7–15	98 (9%/pass)	48
% Selectivity	90	~ 90	80	80	50
PRODUCT PROPERTIES					
Boiling Point@101.3 kPa (°C)	197.6, 107*	187.9, 104.5*	10.8	34.23	n/a
Freezing Point (°C)*	-36.67	-33.33	n/a	n/a	n/a
Vapor Pressure (Pa)	300@65°C	11@20°C	145.6@20°C	58.8@20°C	n/a
LEL (vol %)	3.20	2.6	2.6	2.3	n/a
UEL (vol %)	53	n/a	100	36	n/a
Ignition Temperature (°C)	410	410	429	430	n/a
Flash Point (°C)	111	103	n/a	-37	n/a

TABLE 20: Toxicity and Adverse Health Effects Associated With EG, PG, EO, and PO (66, 67, 68,69, 71)

	EG	PG	EO	PO
Acute Health Effects	narcosis, kidney damage	little to none	headaches, nausea, vomiting, numbness	headache, skin and respiratory irritation
Acute Oral Toxicity (LD_{50})	1.56 g/Kg (adult)	20 g/Kg	0.33 g/Kg (adult)	300–1000 g/Kg (rats) (rats)
Chronic Health Effects	kidney damage	none reported	sensory-motor neuropathy	CNS depression
Lethal Dose (Adult)	0.1 L	1 L	n/a	n/a
Evidence of Teratogenicity	yes (mice, rats)	none reported (mice, rats, rabbits)	none reported in rats	none reported
Evidence of Carcinogenicity	none reported	none reported	yes$	yes#

Detalhes - Reações

ETHYLENE GLYCOL

$$C_2H_4 + O_2 \text{ or Air} \xrightarrow{Ag} H_2COCH_2 + HO(CH_2CH_2O)_{n+1} + CO_2$$

Ethylene → Etheylene Oxide + EG mixture

220–277°C 1–3 MPa, where n=1, 2, 3

$$nEO + H_2O \longrightarrow HOCH_2CH_2OH + HO(CH_2CH_2O)_{n+1}H$$

EG + Higher EGs

200°C , where n=1, 2, 3

Detalhes - Reações

PROPYLENE GLYCOL

$C_3H_6 + Ca(OH)_2 + Cl_2 + H_2O$—$C_3H_6O + CaCl_2 + H_2O + C_3H_8O_2$ 45–90°C + 20–30°C, 1.1–1.9 bar

Propylene PO PG exothermic input

$C_6H_5CH_2CH_3 + O_2$———— $C_6H_5C_2H_4(OOH)$ 132–146°C, 2 bar

Ethylbenzene Ethylbenzene Hydroperoxide

Mb or Ti

$C_6H_5C_2H_4(OOH) + C_3H_6$————————PO + $C_6H_5CH_3CH0H$

a–phenylethanol

$C_6H_5CH_3CH0H$————$C_6H_5CHCH_2 + H_2O$

Co–product Styrene

$4\ C_3H_6 + 3O_2$————2 C_3H_9COOH + 2 C_3H_9COH 120–140°C, 25–35 bar

isobutane *tert*–butyl hydroperoxide *tert*–butyl alcohol

Mb

2 $C_3H_9COOH + C_3H_6$——————2 PO + 2 C_3H_9COH 110–120°C, 40bar

C_3H_9COH——metyl *tert*–butyl ether + H_2O

PO + 15 H_2O*——100 $HOCH_2CH(CH_3)OH$ + 10 $HO(CH_2CH_2O)_2$ + 1 $HO(CH_2CH_2O)_3$ 125°C, 2MPa

PG di–PG tri–PG

*15 molar excess of water produces mono, di–, and tri– PG in ratio of 100:10:1

ETHYLENE GLYCOL

(1) Assumptions:
- 3,877 g (62.53 mols) of EG is goal based on FAL data
- EG selectivity is 90%, 100% conversion of feedstocks

H_2COCH_2 + H_2O ——————— $HOCH_2CH_2OH$ + Mixture of higher EG hemalogues
ethylene oxide (EO) — ethylene glycol (EG)

62.53 mols PO x 44 g/mol = 2751 g PO

(2) Assumption:
- Oxidation with pure oxygen
- 7% to 15% conversion of ethylene
- 80% selectivity for PO

C_2H_4 = 1/2 O_2 ——— H_2COCH_2 + Other Products
ethylene — EO

62.53 mols ethylene x 1/0.80 x 1/0.07 x 28 g ethylene/mol = **31,265 g ethylene @ 7% conversion**
62.53 mols ethylene x 1/0.80 x 1/0.15 x 28 g ethylene/mol = 14,590 g ethylene @ 15% conversion

Detalhes – Reações - Estequiometria

PROPYLENE GLYCOL

(1) Assumptions:
- 3694 g of PG is goal based on FAL data
- isobutane hydroperoxidation is the production process
- 15 molar excess of water produces mono, di, and tri PGs in a ratio of 100:10:1

C_3H_6O + H_2O ———— $(HOCH_2CH(CH_3)OH)$ + $HO(CH_2CH_2O)_2$ + $HO(CH_2CH_2O)_3$
propylene oxide (PO) — propylene glycol (PG) — di–PG — tri–PG

346 total carbons = 100 (3 carbons in PG) + 10 (4 carbons in di–PG) + 1 (6 carbons in tri–PG)
346/3 = 115

115 C_3H_6O + 1,725 H_2O ——100 $(HOCH_2CH(CH_3)OH)$ + 10 $HO(CH_2CH_2O)_2$ + 1 $HO(CH_2CH_2O)_3$
PO — PG — Di–PG — Tri–PG

3,694 g PG x 1 mol/76 g x 115 mol PO/100 mol PG x 58 g PO/mol = **3241 g PO –or– 55.89 mols PO**

(2) Assumptions:
- Reactants dissolved in toluene
- Molybdenum catalyst
- Selectivity for PO is 80%
- Propylene conversion is 98% with ten–fold excess of propylene

$2C_3H_9COOH$ + $2C_3H_6$ ——Mb—— $2C_3H_6O$ + $2C_3H_9C0H$
tert–butyl hydroperoxide (TBH) — Propylene — PO — *tert*–butyl alcohol (TBA)

55.8 mols PO x 1/0.80 x 1/0.98 = 71.17 mols TBH x 90 g/mol = **6,405 g TBH**
711.7 mols propylene x 42 g/mol = **29,891 g propylene**

(3) Assumptions:
- Isobutane generated from mixed butane fraction
- 48% conversion of isobutane
- 50% selectivity for TBH, 48% selectivity for TBA, 4% residual selectivity

$4C_3H_9CH$ + $3O_2$ ———— $2C_3H_9COOH$ + $2C_3H_9COH$
isobutane — TBH — TBA

71.17 mols TBH x 1/0.48 x 1/0.5 x 4 mols isobutane/2 mols TBH = **593 mols Isobutane**
593 mols Isobutane x 90 g/mol = **34, 394 g Isobutane; 65.5 mols TBA or 4845 g TBA**