QFL5931/MPT6009 – Química Verde

Análise de Ciclo de Vida – Aula 3

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v.2018

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**

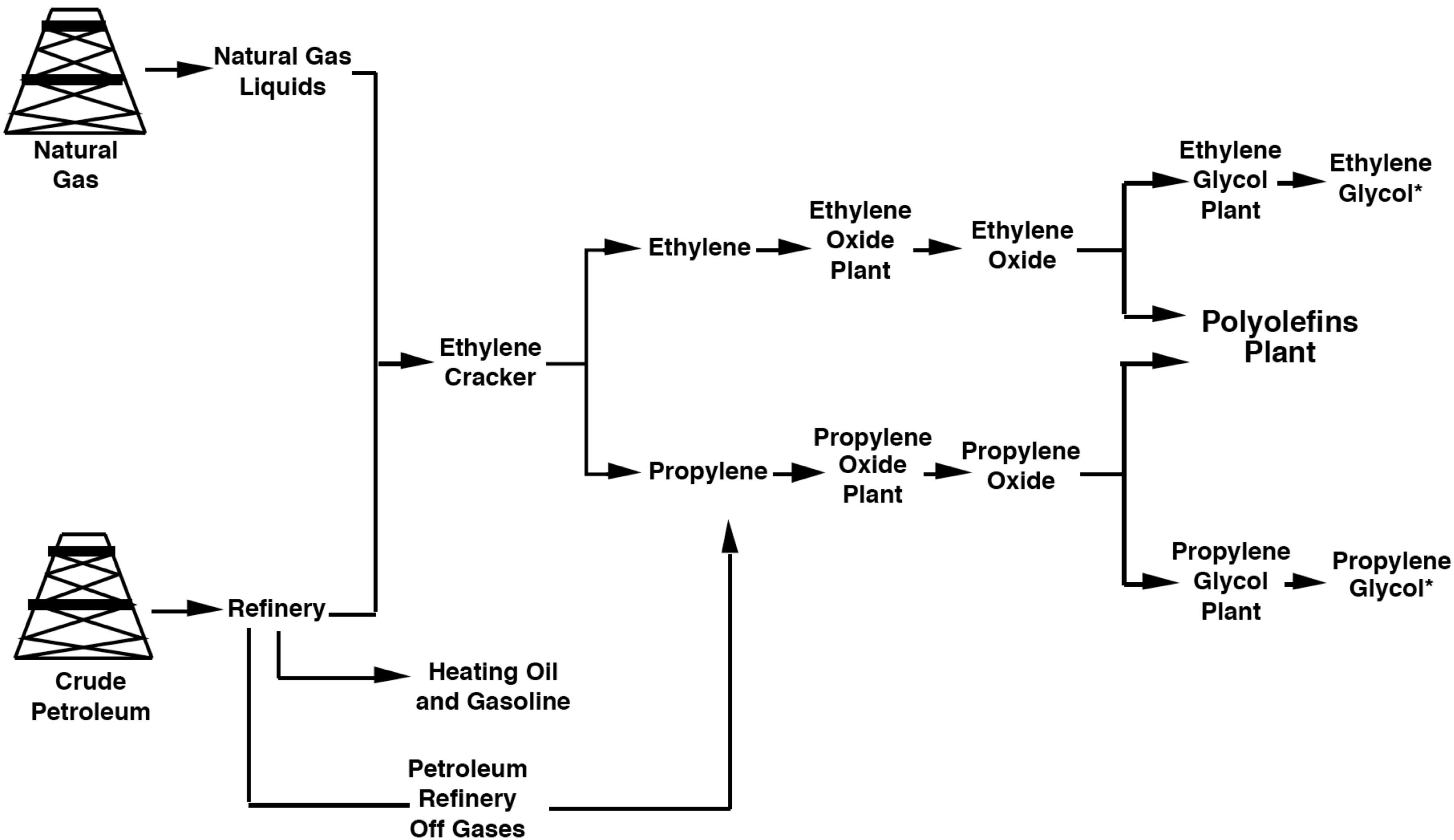
Incorporation of Pollution Prevention Principles Into Chemical Science Education
Jonathan W. Greene
Center for Sustainable Systems - UMich
http://www.umich.edu/~nppcpub/resources/compendia/CHEMpdfs/

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



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

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

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

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

$$C_3H_6O + H_2O \longrightarrow (HOCH_2CH(CH_3)OH) + HO(CH_2CH_2O)_2 + HO(CH_2CH_2O)_3$$

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

$$115\ C_3H_6O + 1{,}725\ H_2O \longrightarrow 100\ (HOCH_2CH(CH_3)OH) + 10\ HO(CH_2CH_2O)_2 + 1\ HO(CH_2CH_2O)_3$$

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

$$2C_3H_9COOH + 2C_3H_6 \xrightarrow{Mb} 2C_3H_6O + 2C_3H_9C0H$$

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

$$4C_3H_9CH + 3O_2 \longrightarrow 2C_3H_9COOH + 2C_3H_9COH$$

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**

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

Resíduos

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

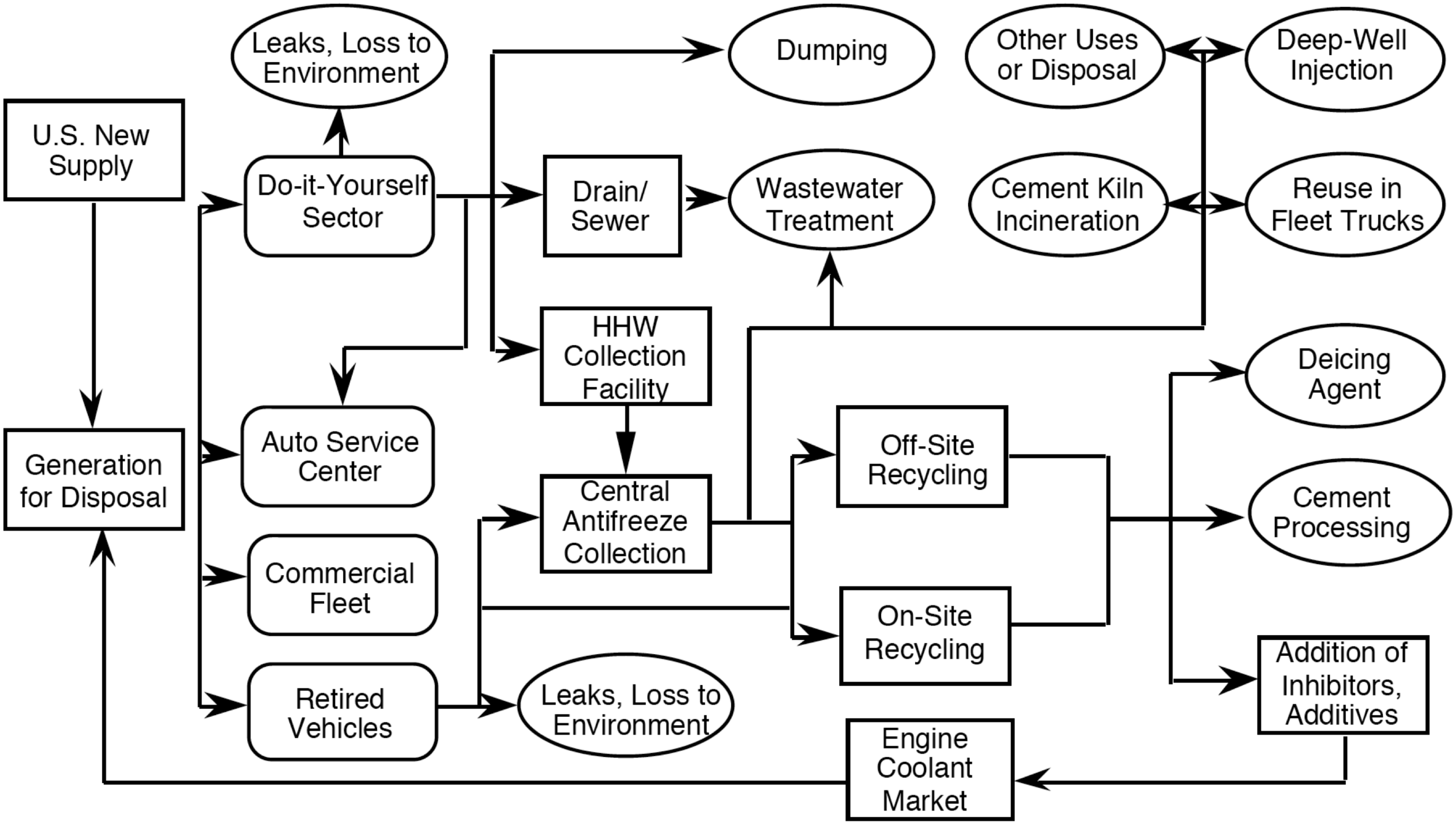


TABLE 18: Waterborne Wastes Generated by Improper Disposal of 1,000 gallons of EG- and PG-Based Antifreeze Solutions (55)

	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#

Estudo de Caso

LCA para polietileno e polipropileno (baseados em petróleo) e PHB – Poli(ácido beta-hidróxi-butírico) (baseado em processo biológico)

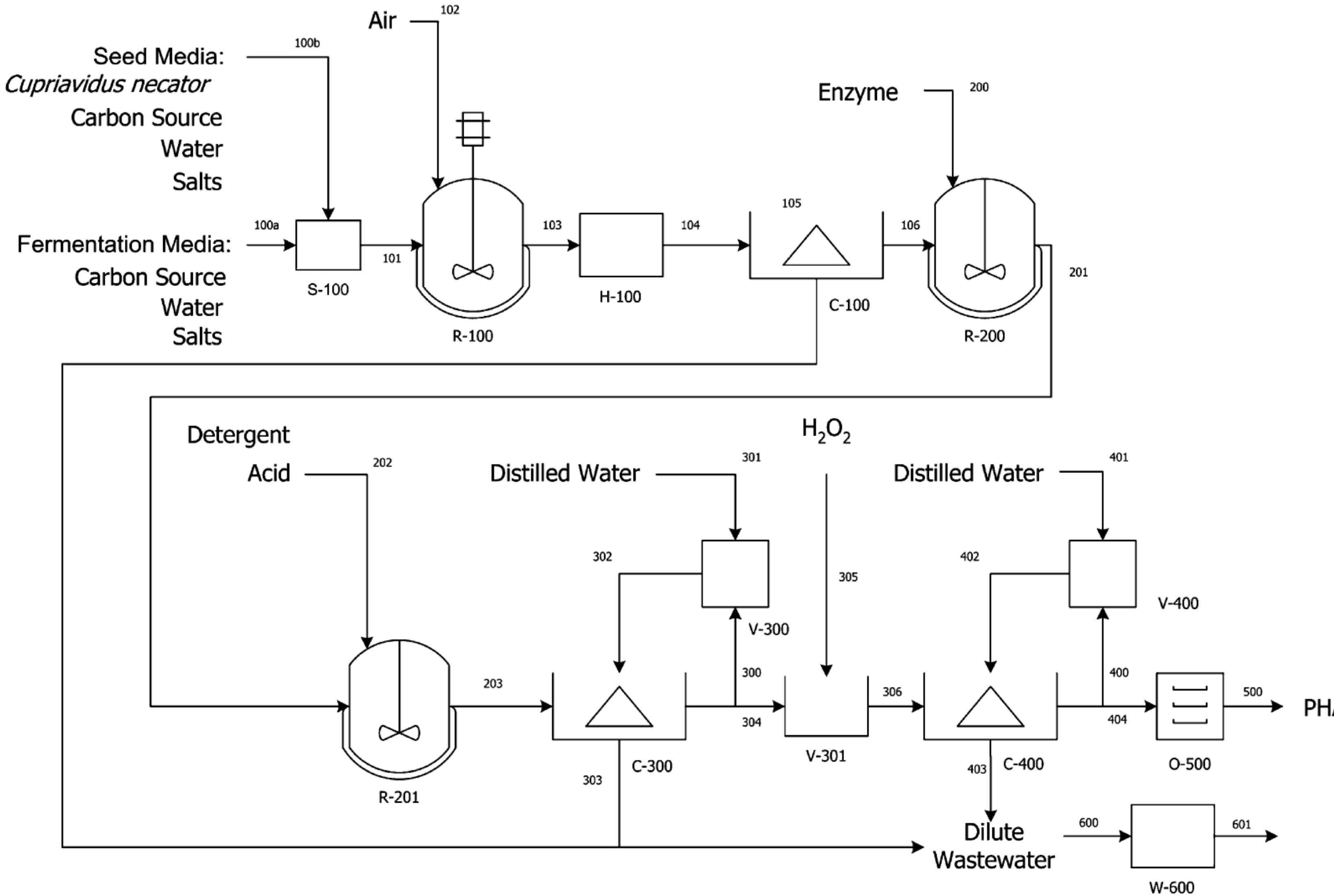
Environmental analysis of plastic production processes: Comparing petroleum-based polypropylene and polyethylene with biologically-based poly-β-hydroxybutyric acid using life cycle analysis
K.G. Harding[a], J.S. Dennis, H. von Blottnitz, S.T.L. Harrison
Journal of Biotechnology, Volume 130, Issue 1, 31 May 2007, Pages 57–66

Escopo: "craddle-to-gate" / berço-ao-portão

Propriedades dos Polímeros

	Units	Polypropylene	PHB
Density	kg/m^3	900–910[a]	1250[b]
Melting point	°C	176[c]	45–180[c] P(3HB) = 180[c]
Tensile strength	MPa	38[d]	13–40[b]
Shrinkage	%		1–3[b]
Elongation	%	400[d]	5–680[d]
Young's modulus	MPa	17000[d]	350–1000[b]
Glass-transition temperature	°C	−10[c]	15[a] P(3HB) = 4[c]
Service temperature	°C		−30 to 120[b]
Specific heat (20–80 °C)[d]	kJ/kgK	1.9	
Thermal conductivity (20–150 °C)[d]	kW/mK	0.42–0.61	

Produção de PHB



S-100	–	**Steam sterilisation**
R-100	–	**Microbial Growth Reactor**
H-100	–	**High Pressure Homogeniser**
C-100	–	**Centrifugation**
R-200	–	**Enzyme Washing Reactor**
R-201	–	**Detergent Washing Reactor**
C-300	–	**Centrigugation**
V-300	–	**PHB Re-suspension**
V-301	–	**Hydroxide Addition**
C-400	–	**Centrifugation**
V-400	–	**PHB Re-suspension**
O -500	–	**Spray Drying**
W-600	–	**Wastewater treatment**

Condições de Processo

Process conditions for the production of 1000 kg of PHB

	Unit	
Seed media		*Cupriavidus necator*, sucrose (10 kg/m^3), $(NH_4)_2SO_4$ (1.8 kg/m^3), K_2HPO_4 (1.9 kg/m^3), $NaHPO_4$ (1.56 kg/m^3), $MgSO_4.7H_2O$ (0.8 kg/m^3), $FeSO_4.7H_2O$ (0.008 kg/m^3), trace salts solution ($CuSO_4.5H_2O$, $ZnSO_4$.7H2O, $MnSO_4.H_2O$, $CaCl_2.2H_2O$)
Fermentation media		Sucrose (270 kg/m^3), H_3PO_4 (0.8 dm^3/m^3), $(NH_4)_2SO_4$ (1.1 kg/m^3), K_2SO_4 (1.4 kg/m^3), $MgSO_4.7H_2O$ (1.6 kg/m^3), trace salts (Na_2SO_4, $MnSO_4.H_2O$, $ZnSO_4$.7H2O, $CuSO_4.5H_2O$), PPG.EEA 142 antifoam (0.375 kg/m^3)
Sterilisation	S-100	139 °C (continuous sterilisation) – including heat integration
Microbial growth	R-100	Temperature: 30 °C; pH: 7
		Reactor volume: 9.4 m^3 (working)
		Total reaction time: 80 h
		Aeration: 0.6 vol/vol/min
		Agitation energy: 0.5 kW/m^3
		Biomass (PHB) concentration: 150 (106) g/l
		Polymer concentration: 71% PHB
Cell disruption	H-100	High pressure homogenisation
		3 passes; 70 MPa; 16 °C
		Energy efficiency of breakage: 1.25 J/mg biomass disrupted
Enzyme addition	R-200	Re-suspensions equivalent to 150 kg/m^3
		Optimase L660 (MKC) – alkaline serine protease enzyme
		Agitation energy: 0.8 kW/m^3
		Temperature: 70 °C; pH: 8
		Residence time: 2 h
(Non-ionic) detergent addition	R-201	Synperonic NP8
		Agitation energy: 0.8 kW/m^3
		Temperature: 70 °C; pH: 7
		Residence time: 2 h
Water washing (I)	V-300	Number of washes: 4
	C-300	Wash volume: 1/3 of reactor volume (3.1 m^3)
		Centrifugation: 20 min; 10,000 g
		Power required: 2.11 kW/m^3 (per wash)
H_2O_2 addition	V-301	Concentration: 1.20% v/v

Process conditions for the production of 1000 kg of PHB

	Unit	
Seed media		*Cupriavidus necator*, sucrose (10 kg/m^3), $(NH_4)_2SO_4$ (1.8 kg/m^3), K_2HPO_4 (1.9 kg/m^3), $NaHPO_4$ (1.56 kg/m^3), $MgSO_4.7H_2O$ (0.8 kg/m^3), $FeSO_4.7H_2O$ (0.008 kg/m^3), trace salts solution ($CuSO_4.5H_2O$, $ZnSO_4$.7H2O, $MnSO_4.H_2O$, $CaCl_2.2H_2O$)
Fermentation media		Sucrose (270 kg/m^3), H_3PO_4 (0.8 dm^3/m^3), $(NH_4)_2SO_4$ (1.1 kg/m^3), K_2SO_4 (1.4 kg/m^3), $MgSO_4.7H_2O$ (1.6 kg/m^3), trace salts (Na_2SO_4, $MnSO_4.H_2O$, ZnSO4.7H2O, $CuSO_4.5H_2O$), PPG.EEA 142 antifoam (0.375 kg/m^3)
Sterilisation	S-100	139 °C (continuous sterilisation) – including heat integration
Microbial growth	R-100	Temperature: 30 °C; pH: 7
		Reactor volume: 9.4 m^3 (working)
		Total reaction time: 80 h
		Aeration: 0.6 vol/vol/min
		Agitation energy: 0.5 kW/m^3
		Biomass (PHB) concentration: 150 (106) g/l
		Polymer concentration: 71% PHB
Cell disruption	H-100	High pressure homogenisation
		3 passes; 70 MPa; 16 °C
		Energy efficiency of breakage: 1.25 J/mg biomass disrupted
Enzyme addition	R-200	Re-suspensions equivalent to 150 kg/m^3
		Optimase L660 (MKC) – alkaline serine protease enzyme
		Agitation energy: 0.8 kW/m^3
		Temperature: 70 °C; pH: 8
		Residence time: 2 h
(Non-ionic) detergent addition	R-201	Synperonic NP8
		Agitation energy: 0.8 kW/m^3
		Temperature: 70 °C; pH: 7
		Residence time: 2 h
Water washing (I)	V-300	Number of washes: 4
	C-300	Wash volume: 1/3 of reactor volume (3.1 m^3)
		Centrifugation: 20 min; 10,000 g
		Power required: 2.11 kW/m^3 (per wash)
H_2O_2 addition	V-301	Concentration: 1.20% v/v
Water washing (II)	V-400	Number of washes: 2
	C-400	Wash volume: 1/3 of reactor volume (3.1 m^3)
		Centrifugation: 20 min; 10,000 g
		Power required: 2.11 kW/m^3 (per wash)
Spray drying	O-500	Initial moisture content: 11%
		Final moisture content: 0.1%
		Drying rate: 4.8 GJ/t

Downstream processing recovery: 95%

Energia

Breakdown of steam and electricity requirements for production of 1000 kg PHB

Steam (kg)		Electricity (MJ)		Natural gas (MJ)	
Medium sterilization	1065	Agitation:		Spray drying (Baker and McKenzie, 2005)	2123
Steam out vessel	9.6	Reactor R-100 (0.5 kW/m^3)	1360		
Backing steam	3819	Enzyme washing R-200 (0.8 kW/m^3)	18.1		
		Detergent washing R-201(0.8 kW/m^3)	18.1		
		Cell disruption, HPH, 1.25 J/mg biomass H-100 (Engler, 1985)	1770		
		Centrifuge energy, 8 kW/h/1000 gal (Perry et al., 1984)	263.5		
Total	4890	Energy for aeration (Aspen model)	512		
Energy equivalent; 2.6 MJ/kg (MJ)	12700	Electricity total	3942	Natural gas total	2123
Total energy for 1000 kg PHB (GJ)					18.8

Massa e Energia

Mass and energy values for PHB production used in the LCA study

Products			
PHB (kg)	1000		
Feed			
Electricity (MJ)	3942	Sulphates:	
Steam (2.6 MJ/kg) (kg)	4893	$MgSO_4.7H_2O$ (kg)	20.9
Energy equivalent (MJ)	12700	K_2SO_4 (kg)	18.6
Natural gas (MJ)	2123	$(NH_4)_2SO_4$ (kg)	14.8
Air (kg)	290	Na_2SO_4 (kg)	3.0
Process water (m^3)	65.2	$ZnSO4.7H_2O$ (kg)	1.16
Cooling water (m^3)	13.1	$MnSO_4.H_2O$ (kg)	0.92
Sucrose (from cane sugar) (kg)	1810	$FeSO_4.7H_2O$ (kg)	0.82
Acids:		$CuSO_4.5H_2O$ (kg)	0.12
H_2SO_4 (kg)	3.02	$CaCl_2$.2H2O (kg)	2.3
H_3PO_4 (conc.) (kg)	8.12	K_2HPO_4 (kg)	0.095
H_2O_2 (kg)	52.9	$NaHPO_4$ (kg)	0.078
Optimase L660 (MKC) (kg)	2.4	PPG.EEA 142 antifoam (m^3)	0.005
Synperonic NP8 (ICI Ltd.) (m^3)	0.033		
Waste			
Dilute wastewater (m^3)	65.2	Solid waste (biomass) (kg)	420
COD (te O_2)	0.80		

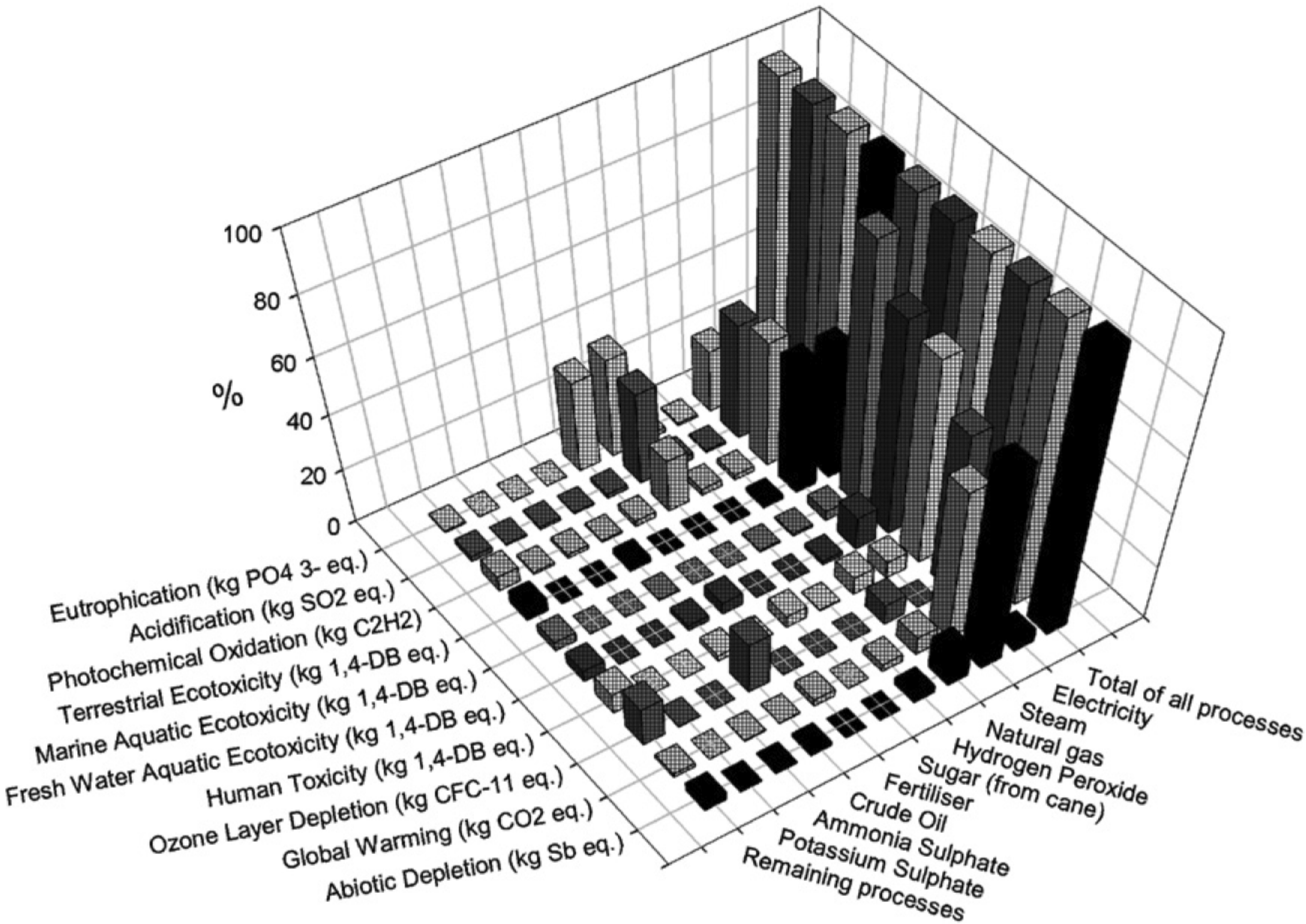
Categorias de Impactos

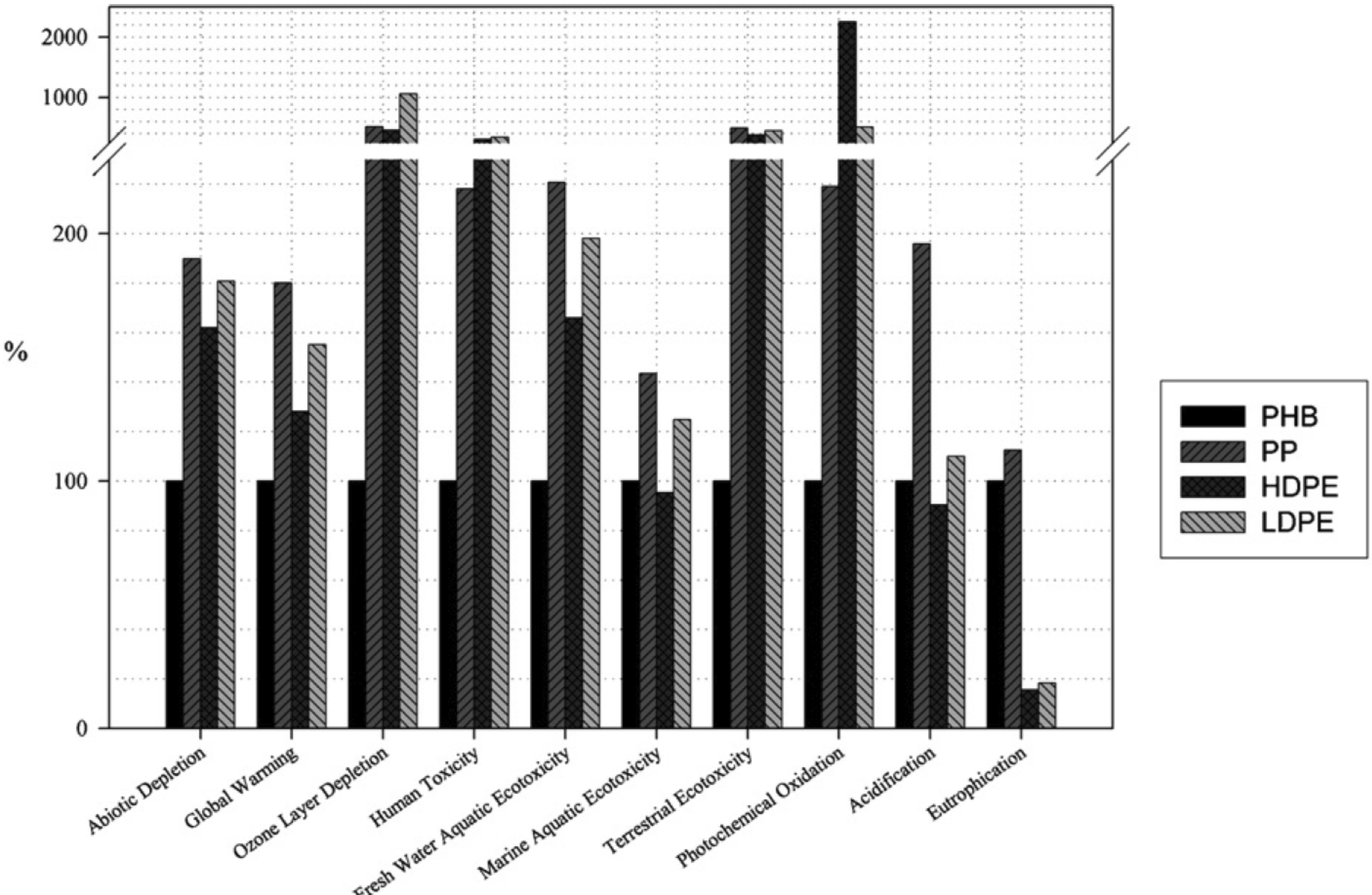
- Depleção abiótica;
- Aquecimento global;
- Redução camada de ozônio;
- Toxicidade humana;
- Ecotoxicidade em água doce;
- Ecotoxicidade em água do mar;
- Ecotoxicidade terrestre;
- Oxidação fotoquímica;
- Acidificação;
- Eutroficação

Impactos

LCIA of polymer production for 1000 kg of polymer product—CML 2 Baseline 2000 V2.03

		This study	Boustead (2000)		
Impact category	Unit	PHB	PP	HDPE	LDPE
Abiotic depletion	kg Sb_{eq}	**21.8**	41.4	35.3	39.4
Global warming (GWP100)	kg $CO_{2\ eq.}$	**1960**	3530	2510	3040
Ozone layer depletion (ODP)	kg CFC-11_{eq}	**0.00017**	0.000862	0.000766	0.0018
Human toxicity	kg 1,4-DB_{eq}	**857**	1870	2590	2890
Fresh water aquatic ecotoxicity	kg 1,4-DB_{eq}	**106**	234	176	210
Marine aquatic ecotoxicity	kg 1,4-DB_{eq}	**1,290,000**	1,850,000	**1,230,000**	**1,610,000**
Terrestrial ecotoxicity	kg 1,4-DB_{eq}	**8.98**	44	33.7	40.3
Photochemical oxidation	kg C_2H_2	**0.78**	1.7	17.5	3.92
Acidification	kg $SO_{2\ eq.}$	**24.9**	48.8	**22.5**	**27.4**
Eutrophication	kg $PO_4{}^{3-}{}_{eq.}$	5.19	5.84	**0.811**	**0.951**


100
80
60
40
20
0
%
Eutrophication (kg PO4 3- eq.)
Acidification (kg SO2 eq.)
Photochemical Oxidation (kg C2H2)
Terrestrial Ecotoxicity (kg 1,4-DB eq.)
Marine Aquatic Ecotoxicity (kg 1,4-DB eq.)
Fresh Water Aquatic Ecotoxicity (kg 1,4-DB eq.)
Human Toxicity (kg 1,4-DB eq.)
Ozone Layer Depletion (kg CFC-11 eq.)
Global Warming (kg CO2 eq.)
Abiotic Depletion (kg Sb eq.)
Total of all processes
Electricity
Steam
Natural gas
Hydrogen Peroxide
Sugar (from cane)
Fertiliser
Crude Oil
Ammonia Sulphate
Potassium Sulphate
Remaining processes


2000
1000
200
100
0
%
PHB
PP
HDPE
LDPE
Abiotic Depletion
Global Warming
Ozone Layer Depletion
Human Toxicity
Fresh Water Aquatic Ecotoxicity
Marine Aquatic Ecotoxicity
Terrestrial Ecotoxicity
Photochemical Oxidation
Acidification
Eutrophication

Breakdown of total energy for cradle-to-gate production of 1 kg PHB

Energy used in PHB production only	Energy (MJ)	Total energy used in cradle-to-gate production of PHB	Energy (MJ)
Electricity	3.9	Non-renewable, fossil	38.8
Steam	12.7	Non-renewable, nuclear	2.6
Natural gas	2.1	Renewable, biomass	1.03
		Renewable, wind, solar, geothermal	0.03
		Renewable, water	0.41
Total	18.8	Total	42.9
Energy used in processes prior to PHB production			24.1