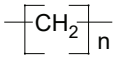
PE polyethylene

PARAMETER	UNIT	VALUE	REFERENCES
GENERAL			
Common name	-	polyethylene	
IUPAC name	-	polyethylene	
Acronym	-	PE	
CAS number	-	9002-88-4	
Formula			
RTECS number	-	TQ3325000	
HISTORY			
Person to discover	-	Hans von Pechmann (first synthesis); Eric Fawcett, Reginald Gibson, Michael Perrin (industrial synthesis)	
Date	-	1898; 1933	
SYNTHESIS			
Monomer(s) structure	-	$CH_2=CH_2$	
Monomer(s) CAS number(s)	-	74-85-1	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	28.05	
Comonomers		butene, hexene, octene	
Monomer ratio	-	100% (some polymers)	
Catalyst	-	Ziegler-Natta, single-site	
Heat of polymerization	kJ mol^{-1}	93.6	Kaminsky, W, Adv. Catalysis, 46, 89-159, 2001.
Mass average molecular weight, M_w	dalton, g/mol, amu	28,000-6,300,000	
Polydispersity, M_w/M_n	-	1.9-14.1	
Polymerization degree (number of monomer units)	-	30,121	
Xylene extractables	%	1.15-9.63	Auger, J; Duff, A; Weber, M; Bellehumeur, C, Antec, 456-60, 2004.
Hexene extractables	%	0.87-4.49	Auger, J; Duff, A; Weber, M; Bellehumeur, C, Antec, 456-60, 2004.
Molar volume at 298K	cm^3 mol^{-1}	calc.=28.1-32.8; exp.=33.1	
Van der Waals volume	cm^3 mol^{-1}	calc.=20.46; 20.50 (amorphous)	
Degree of branching	#/1000C	C_2 – 1; C_4 – 5-36; C_5 – 2-8; C_6 or more – 2	Mieda, N; Okamoto, K; Yamaguchi, M, Antec, 1-3, 2009.
STRUCTURE			
Crystallinity	%	35-94; 41-35 (dicumyl peroxide crosslinking 1-7%)	Nilsson, S; Hjertberg, T; Smedberg, A, Eur. Polym. J., 46, 1759-69, 2010.
Cell type (lattice)	-	orthorhombic (stable form); monoclinic (metastable form), and hexagonal (high pressure form)	
Cell dimensions	nm	a:b:c=0.736-0.742:0.493-0.495:0.253-0.255 (orthorhombic)	Kavesh, S; Schultz, J M, J. Polym. Sci., A-2, 8, 243, 1970.
Number of chains per unit cell	-	2	
Crystallite size	nm	5.1-23.9 (thickness); 7,000-1,000 (dicumyl peroxide crosslinking 1-7%)	Nilsson, S; Hjertberg, T; Smedberg, A, Eur. Polym. J., 46, 1759-69, 2010.

PE polyethylene

PARAMETER	UNIT	VALUE	REFERENCES
Spacing between crystallites	nm	22-42	
Chain conformation	-	helix 1*1/1	Androsch, R; Di Lorenzo, M L; Schick, C; Wunderlich, B, Polymer, 51, 4639-62, 2010.
Entanglement molecular weight	dalton, g/mol, amu	calc.=1422, 1854	
Degree of branching	CH_3/100C	0.05-6.94	
Lamellae thickness	nm	9.25-35.5 (HDPE); 12.6-20.6 (LDPE); 6.7-9.8 (low crystallization temperature); 26.3 (PE); 27.1 (XPE)	Bistolfi, A; Bellare, A, Acta Biomaterialia, in press, 2011.
COMMERCIAL POLYMERS			
Some manufacturers	-	Equistar; Formosa; Nova	
Trade names	-	Petrothene; Formolene: Sclair	
PHYSICAL PROPERTIES			
Density at 20°C	g cm^{-3}	0.90-0.98	
Color	-	milky transparency	
Refractive index, 20°C	-	calc.=1.4648-1.4939; exp.=1.4728-1.52	
Clarity	%	7-98	
Odor	-	odorless	
Melting temperature, DSC	°C	99-138	
Decomposition temperature	°C	335	Patel, P; Hull, T R; McCabe, R W; Flath, D; Grasmeder, J; Percy, M, Polym. Deg. Stab., 95, 709-18, 2010.
Thermal expansion coefficient, 23-80°C	$°C^{-1}$	1E-4 to 5.1E-4	
Thermal conductivity, melt	W m^{-1} K^{-1}	calc.=0.1721	
Glass transition temperature	°C	calc.=-59 to -133; exp.=-20 to -128	
Vicat temperature VST/A/50	°C	88-132	
Hansen solubility parameters, δ_D, δ_P, δ_H	$MPa^{0.5}$	16.8, 3.8, 3.8	
Interaction radius		6.6	
Hildebrand solubility parameter	$MPa^{0.5}$	calc.=16.2-19.93; exp.=15.76-17.6	
Surface tension	mN m^{-1}	calc.=35.1-37.6; exp.=31.0-35.7	
Dielectric constant at 100 Hz/1 MHz	-	2.28-2.32	
Electric strength K20/P50, d=0.60.8 mm	kV mm^{-1}	39	
Coefficient of friction	-	0.6	
Contact angle of water, 20°C	degree	94.9-97.2	
Surface free energy	mJ m^{-2}	33.5	
Speed of sound	m s^{-1}	32.5	
Acoustic impedance		1.73	
MECHANICAL & RHEOLOGICAL PROPERTIES			
Tensile strength	MPa	48.6	
Tensile modulus	MPa	190-240	
Tensile stress at yield	MPa	10.6-20.7	

PE polyethylene

PARAMETER	UNIT	VALUE	REFERENCES
Elongation	%	180-1000	
Tensile yield strain	%	19-24	
Young's modulus	MPa	498	Bistolfi, A; Bellare, A, Acta Biomaterialia, in press, 2011.
Tenacity (fiber) (standard atmosphere)	cN tex^{-1} (daN mm-2)	32-70	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Tenacity (wet fiber, as % of dry strength)	%	100	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Fineness of fiber (titer)	dtex	10-25	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Length (elemental fiber)	mm	38-200, filament	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Poisson's ratio	-	exp.=0.47-0.49	
Shrinkage	%	1.7-1.85	
Residual stress	MPa	2-5 (extruded pipes)	
Melt viscosity, shear rate=1000 s^{-1}	Pa s	150-400	
Melt index, 230°C/3.8 kg	g/10 min	3.2-9	
CHEMICAL RESISTANCE			
Acid dilute/concentrated	-	very good	
Alcohols	-	good	
Alkalis	-	very good	
Aliphatic hydrocarbons	-	poor	
Aromatic hydrocarbons	-	poor	
Esters	-	poor	
Greases & oils	-	good to poor	
Halogenated hydrocarbons	-	poor	
Ketones	-	poor	
Θ solvent, Θ-temp.=192.2, -73, 173.9, 133.3°C	-	amyl alcohol, carbon disulfide, n-heptane, n-hexane	
Good solvent	-	1,2,4-trichlorobenzene, decalin, halogenated hydrocarbons, aliphatic ketones, xylene (all above 60°C)	
Non-solvent	-	most common solvents	
FLAMMABILITY			
Ignition temperature	°C	340-343	
Autoignition temperature	°C	440	
Limiting oxygen index	% O_2	17.4-18.5	
Minimum ignition energy	J	0.01	
Heat of combustion	J g^{-1}	47,740	Walters, R N; Hacket, S M; Lyon, R E, Fire Mater., 24, 5, 245-52, 2000.
Volatile products of combustion	-	CO, CO_2, aldehydes, acrolein, oligomers, waxes, oxygenated hydrocarbons	

PARAMETER	UNIT	VALUE	REFERENCES
WEATHER STABILITY			
Spectral sensitivity	nm	<300	
Activation wavelengths	nm	300, 330-360	
Important initiators and accelerators	-	unsaturations, aromatic carbonyl compounds (deoxyanisoin, dibenzocycloheptadienone, flavone, 4-methoxybenzophenone, 10-thioxanthone), hydrogen bound to tertiary carbon at branching points, aromatic amines, groups formed on oxidation (hydroperoxides, carbonyl, carboxyl, hydroxyl) substituted benzophenones, complexes with ground-state oxygen, quinones (anthraquinone, 2-chloroanthraquinone, 2-tert-butylathraquinone, 1-methoxyanthraquinone, 2-ethylanthraquinone, 2-methylanthraquinone), transition metal compounds (Ni < Zn < Fe < Co), ferrocene derivatives, titanium dioxide (anatase), ferric stearate, polynuclear aromatic compounds (anthracene, phenanthrene, pyrene, naphthalene	
Products of degradation	-	free radicals, hydroperoxides, carbonyl groups, chain scission, crosslinking	
Stabilizers	-	UVA: 2-hydroxy-4-octyloxybenzophenone; phenol, 2-(5-chloro-2H-benzotriazole-2-yl)-6-(1,1-dimethylethyl)-4-methyl-; 2,2'-methylenebis(6-(2H-benzotriazol-2-yl)-4-1,1,3,3-tetramethylbutyl)phenol; 2,4-di-tert-butyl-6-(5-chloro-2H-benzotriazole-2-yl)-phenol; reaction product of methyl 3(3-(2H-benzotriazole-2-yl)-5-t-butyl-4-hydroxyphenyl propionate/ PEG 300; 2-[4,6-bis(2,4-dimethylphenyl)-1,3,5-triazin-2-yl]-5-(octyloxy) phenol; Screener: titanium dioxide; zinc oxide; carbon black; Acid scavenger: hydrotalcite; Fiber: carbon nanotube; HAS: 1,3,5-triazine-2,4,6-triamine, N,N'''[1,2-ethane-diyl-bis[[[4,6-bis[butyl(1,2,6,6-pentamethyl-4-piperidinyl) amino]-1,3,5-triazine-2-yl]imino]-3,1-propanediyl]bis[N',N''-dibutyl-N',N''-bis(1,2,2,6,6-pentamethyl-4-piperidinyl)-; bis(1,2,2,6,6-pentamethyl-4-piperidyl)sebacate + methyl-1,2,2,6,6-pentamethyl-4-piperidyl sebacate; 2,2,6,6-tetramethyl-4-piperidinyl stearate; reaction products of N,N'-ethane-1,2-diylbis(1,3-propanediamine), cyclohexane, peroxidized 4-butylamino-2,2,6,6-tetramethylpiperidine and trichloro-1,3,5-triazine; poly[[(6-[1,1,3,3-tetramethylbutyl)amino]-1,3,5-triazine-2,4-diyl][2,2,6,6-tetramethyl-4-piperidinyl)imino]-1,6-hexanediyl[2,2,6,6-tetramethyl-4-piperidinyl)imino]]; Phenolic antioxidant: 2,6,-di-tert-butyl-4-(4,6-bis(octylthio)-1,3,5,-triazine-2-ylamino) phenol; 3,3',3',5,5',5'-hexa-tert-butyl-a,a',a'-(mesitylene-2,4,6-triyl)tri-p-cresol; ,4,6(1H,3H,5H)-trione; 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol; 2',3-bis[[3-[3,5-di-tert-butyl-4-hydroxyphenyl]propionyl]]propionohydrazide; isotridecyl-3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate; 2,2'-ethylidenebis (4,6-di-tert-butylphenol); ethylene bis[3,3-bis[3-(1,1-dimethylethyl)-4-hydroxyphenyl]butanoate];1,3,5-tris(4-tert-butyl-3-hydroxy-2,6-dimethylbenzyl)-1,3,5-triazine-2,4,6-(1H,3H,5H)-trione; 2,2'-methylenebis(4-methyl-6-tertbutylphenol); 3,5-bis(1,1-dimethyethyl)-4-hydroxy-benzenepropanoic acid, C13-15 alkyl esters; 2,2'-isobutylidenebis(2,4-dimethylphenol); 1,1,3-tris(2'methyl-4'-hydroxy-5'tert-butylphenyl)butane; Phosphite: bis-(2,4-di-t-butylphenol) pentaerythritol diphosphite; tris (2,4-di-tert-butylphenyl)phosphite; trinonylphenol phosphite; distearyl pentaerythritol diphosphite; trilauryl trithiophosphite; Thiosynergist: didodecyl-3,3'-thiodipropionate; dioctadecyl 3,3'-thiodipropionate; 2,2'-thiodiethylene bis[3-(3,5-ditert-butyl-4-hydroxyphenyl)propionate]; 4,4'-thiobis(2-t-butyl-5-methylphenol); 2,2'-thiobis(6-tert-butyl-4-methylphenol); pentaerythritol tetrakis(b-laurylthiopropionate); Quencher: (2,2'-thiobis(4-tert-octyl-phenolato))-N-butylamine-nickel(II); Optical brightener: 2,2'-(2,5-thiophenediyl)bis(5-tert-butylbenzoxazole); Vitamin E in medical applications	Micheli, B R; Wannomae, K K; Lozynski, A J; Christensen, S D; Muratoglu, O K, J. Arthroplasty, in press, 2011.

PE polyethylene

PARAMETER	UNIT	VALUE	REFERENCES
Low earth orbit erosion yield	cm^3 $atom^{-1}$ x 10^{-24}	3.97	Waters, D L; Banks, B A; De Groh, K K; Miller, S K R; Thorson, S D, High Performance Polym., 20, 512-22, 2008.
BIODEGRADATION			
Colonized products		bags for oranges, food films, oxidized materials from LDPE, pipe wrap, polyethylene containing starch, shrink-wrap film, wood flower containg films	
Stabilizers	-	1-(2-(2,4-dichlorophenyl)-2-(2-propenyloxy)ethyl)-1H-imidazole, 2,4,4'-trichloro-2'-hydroxydiphenyl ether, benzoic anhydride, nisin, silver, zinc	
TOXICITY			
NFPA: Health, Flammability, Reactivity rating	-	0/1/0	
Carcinogenic effect	-	not listed by ACGIH, NIOSH, NTP	
Reproductive toxicity	-	not expected to occur	
TLV, ACGIH	mg m^{-3}	3 (respirable) 10 (inhalable)	
OSHA	mg m^{-3}	5 (respirable), 15 (total)	
Oral rat, LD_{50}	mg kg^{-1}	>2,000; 4,000	
Skin rabbit, LD_{50}	mg kg^{-1}	non-irritant	
ENVIRONMENTAL IMPACT			
Aquatic toxicity, *Daphnia magna*, LC_{50}, 48 h	mg l^{-1}	75,000	Lithner, Ph D Thesis, Univrsity of Gothenburg, 2011.
Cradle to grave non-renewable energy use	MJ/kg	73.7-81.8	Harding, K G; Dennis, J S; von Blottnitz, H; Harrison, S T L, J. Biotechnol., 130, 57-66, 2007.
PROCESSING			
Typical processing methods	-	blown film extrusion, cast film extrusion, extrusion, injection molding, molding, rotational molding, thin wall injection molding	
Processing pressure	MPa	5-6 (injection)	
Additives used in final products	-	Fillers: aluminum, barium sulfate, calcium carbonate, calcium sulfate whiskers, carbon black, diatomaceous earth, ferromagnetic powder, glass fiber, glass spheres, ground tire rubber, hollow silicates, hydrotalcite, kaolin, lignin, magnesium hydroxide, marble, mica, nickel fibers, red mud, sand, silica, soot, starch, superconductor ($YBa_2Cu_3O_{7-x}$), talc, wollastonite, wood flour, zirconium silicate; Plasticizers: dioctyl phthalate, EPDM, EVA, glycerin, glyceryl tribenzoate, mineral oil, paraffin oil, polyethylene glycol, sunflower oil; Antistatics: carbon black, copper complex of polyacrylic acid, ethoxylated amines, fatty diethanol amines, glycerol monostearate, graphite, ionomer, lauric diethanolamide, polyethylene glycol, quaternary ammonium compound, trineoalkoxy zirconate; Antiblocking: diatomaceous earth, natural silica, siloxane spheres, synthetic silica, talc, zeolite; Release: stearyl erucamide; Slip: erucamide, ethylene bisoleamide, oleamide	
Applications	-	packaging and film are the major applications, many other applications are part of normal industrial production, such as medical (artificial tendons, orthopaedic implants, wound dressing)	

PE polyethylene

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ANALYSIS			
FTIR (wavenumber-assignment)	cm^{-1}/-	CH_2 – 2916, 2848, 1463, 719; C=C – 1640	Shi, L-S; Wang, L-Y; Wang, Y-N, Eur. Polym. J., 42, 1625-33, 2006.
Raman (wavenumber-assignment)	cm^{-1}/-	CH_2 – 1464, 1443, 1420, 1372; C-C – 1138, 1070	Kim, J; Kim, Y; Chung, H, Talanta, 83, 879-84, 2011.
NMR (chemical shifts)	ppm	all-trans – 33.3; amorphous – 30.5, and more	Chaiyut, N; Amornsakchai, T; Kaji, H; Horii, F, Polym., 2470-81, 2006.