5

DATA

PVC handling, processing, and use of manufactured products require various types of data. This chapter contains data on PVC available in open literature.

The data included are divided between the following sections:

- General data and nomenclature
- Chemical composition and properties
- Physical properties
- Mechanical properties
- Health and safety
- Environmental information
- Use and application information

5.1 GENERAL DATA AND NOMENCLATURE

Table 5.1. General data and nomenclature

Property	Unit	Value
IUPAC name		poly(chloroethanediyl)
CAS number		9002-86-2
CAS name		ethene, chloro-, homopolymer
EC number		208-750-2
RTECS number		KV0350000
Empirical formula		$H(CH_2CHCl)_nH$
Monomer structure		$H_2C=CHCl$
Molecular weight of monomer	dalton g mol^{-1}	62.498820
Monomer CAS number		75-01-4
Monomer purity	%	99.9
Number of monomer units per polymer chain		600-3400
Method of synthesis	suspension, microsuspension, emulsion, bulk, living radical polymerization	

Table 5.1. General data and nomenclature

Property	Unit	Value
Formulation example	suspension: water, suspending agent, initiator; emulsion: water, emulsifier, water-soluble initiator; microsuspension: water, emulsifier, oil-soluble initiator; bulk: initiator	
Temperature of polymerization	°C	55-73
Yield	%	80-90
Activation energy of polymerization	J g^{-1}	398.4-1077.8
Concentration of residual monomer	ppm	<1
Mass average molecular weight	g/mol, amu	37,000-214,000
Inventor	Henri Victor Regnault (accidental polymerization), Fritz Klatte (technological developments), Waldo Semon (commercial applications)	
Dates of invention	1835, beginning of 20^{th} century, 1926	

5.2 CHEMICAL COMPOSITION AND PROPERTIES

Table 5.2. Chemical composition and properties

Property	Data
Bond length, pm	
C–C	154
C–H	109
C–Cl	177
Bond radius, pm	
C–C	77
C–H	3
C–Cl	99
Bond dipole moment, Debye	
C–C	0
C–H	0.4
C–Cl	1.46
Polydispersity, M_w/M_n	
suspension	1.90–2.59
emulsion	2.14–2.65
mass	2.00–2.06

Table 5.2. Chemical composition and properties

Property	Data
K number	
suspension	50-95
emulsion	60-80
mass	58-69
Branches, number/1000 VC	
chloromethyl branch	3.3-4.8
short branch from back-biting	0.8
long branch	0.1-0.2
tertiary chlorine	0.9
Unsaturations, number/1000 VC	
internal allylic chlorine	0.1-0.3
internal	0.1-0.6
end-group	0.75-0.8
total	0.95-1.7
Head-to-head, number/1000 VC	6-8
Initiator rests, number/1000 VC	0.1-0.4
Polymerization temperature, K	Tacticity index
318	1.75
233	2.40
183	3.30
Additives used in polymerization	
suspension	water, suspending agent, initiator
emulsion	water, emulsifier, water-soluble initiator
microsuspension	water, emulsifier, oil-soluble initiator
bulk (mass)	initiator
Common initiators	tert-octyl peroxyneodecanoate, dicyclohexyl peroxydicarbonate, tert-butyl peroxyneodecanoate, benzoyl peroxide, 2,2'-azobisbutylnitrile, tert-amyl peroxypivalate, dilauroyl peroxide
Half-life temperature of common initiators, ^{o}C	56-80
Heat of polymerization, kJ mol^{-1}	–96 to –109
Products of thermal degradation:	metal chlorides produced from thermal stabilizers, products of degradation of some antioxidants, hydrogen chloride (autocatalytic product of PVC degradation)
Products of photolysis:	free radicals, unsaturations, crosslinks

Table 5.2. Chemical composition and properties

Property	Data
Products of photooxidation:	free radicals, unsaturations, carbonyl groups, hydroperoxides, chain scissions
Important initiators and accelerators of photodegradation:	carbonyl groups, unsaturations, solvents forming hydroperoxides, sensitizing impurities (e.g., benzophenones), metaloorganics (copper-containing compounds, cadmium acetate, ferrocene, iron salts), some pigments and fillers (containing cobalt, zinc, manganese, and lead), metal oxides (of titanium, zinc, and aluminum),

5.3 PHYSICAL PROPERTIES

Table 5.3. Physical properties

Property	Unit	Value
Density amorphous fraction crystalline fraction typical commercial	g cm^{-3}	 1.373 1.530 1.381-1.389
Bulk density	g cm^{-3}	0.39-0.59
Molar volume at 298K crystalline amorphous	cm^3 mol^{-1}	 41.0 (calc.) 45.1-58.4
Van der Waals volume crystalline amorphous	cm^3 mol^{-1}	 29.2 (calc.) 29.2-39.0
Molecular cross-sectional area, calculated	10^{-16} cm^2	18.5
Radius of gyration	nm	5-28.2
Surface tension	mN m^{-1}	32-46
Specific volume	10^{-4} m^3 kg^{-1}	6.90-7.41
Thermal expansion coefficient	10^{-5} C^{-1} (K^{-1})	3.5-7.1
Thermal conductivity at 20°C without conductive fillers with 29.6 vol% graphite	W m^{-1} K^{-1}	 0.130-0.291 1.88
Thermal diffusivity at 20°C	10^{-4} cm^2 s^{-1}	11.92
Heat of crystallite melting	kJ kg^{-1}	74

Table 5.3. Physical properties

Property	Unit	Value
Melting temperature of perfectly syndiotactic PVC (estimate)	°C	400
Melting temperature of PVC	°C	103-230
Fusion temperature	°C	185-196
Vicat temperature rigid with HDT enhancer (ASA)	°C	 62-84 105
Heat distortion temperature	°C	60-88
Heat of combustion	MJ kg^{-1}	14.6-20.9
Specific heat	J K^{-1} kg^{-1}	2100-2600
Heat of fusion	kJ mol^{-1}	3.3-3.6
Heat capacity at 100°C	kJ K^{-1} mol^{-1}	0.0268
Glass transition temperature (commercial grades) rigid 5 phr plasticizer 30 phr plasticizer 100 phr plasticizer	°C	 82-87 66 13-52 −52 to −82
Dielectric constant at 1 kHz 25°C 40°C 60°C 80°C		 3.39 3.34 3.45 3.89
Dielectric loss factor at 1 kHz (25-60°C)		0.8
Electrical conductivity	Ω^{-1} m^{-1}	$1.1\text{-}93 \times 10^{-12}$
Work function of tribocharging	eV	4.86
Surface resistivity flexible flexible containing carbon black	Ω/sq	 10^{11} to 10^{12} 10^{4} to 10^{9}
Refractive index		1.532-1.548
Compressibility 100°C 120°C 140°C	bar^{-1}	 1.352 1.338 1.332
Cell type	orthorhombic	
Cell dimensions a, b, and c, respectively	nm	1.06, 0.54, 0.51
Unit cell angles	degree	α:β:γ=90:90:90

Table 5.3. Physical properties

Property	Unit	Value
Degree of crystallinity (commercial grades)	%	4-10
Crystallite size	nm	0.7-15
Crystalline structure	lamellar, fringed micelles	
Spacing between crystallites	nm	0.26-20
Diffraction peaks in amorphous trace	degree	0.36, 0.5
Diffraction peaks in crystalline area	degree	16-18, 25
Mean particle size suspension general purpose emulsion paste forming	µm	 100-150 40-50 2-25
Tacticity	55-68% (syndiotactic dyads); typical: 27.6-44.0% (syndiotactic), 4.8-21.8% (isotactic), 30.5-52.0% (heterotactic)	
Chain conformation		planar zigzag
Entanglement molecular weight	dalton g mol^{-1}	6,250
Lamellae thickness	nm	2.5-6
Chain thickness (calculated from Privalko's eq.)	nm	2.718
Critical molecular weight, M_c, correlating with the critical end-to-end-distance for entanglements, R_c		6250
X-ray long spacing	nm	6.16
Permeability coefficient at 25°C (rigid film) hydrogen nitrogen oxygen carbon dioxide water vapor ammonia	$m^3\ s^{-1}\ m^2\ Pa^{-1}\ 10^{-9}$	 1.3 0.0089 0.034 0.15 0.12 3.7
Activation energy of diffusion at 25°C hydrogen nitrogen oxygen carbon dioxide water vapor helium	kJ mol^{-1}	 34.5 62.0 54.4 64.5 41.8 20.7

Table 5.3. Physical properties

Property	Unit	Value
Oxygen diffusion coefficient	10^{12} m^2 s^{-1}	
40°C		3.5
55°C		9.0
70°C		21.0
Diffusion coefficient of DOP above and below T_g	cm^2 s^{-1} x 10^{10}	
60°C		1.68
65°C		3.44
70°C		5.29
75°C		8.21
78°C		10.00
80°C		12.9
83°C		16.5
85°C		21.9
90°C		39.5
95°C		68.4
100°C		110.00
Diffusion coefficients of plasticizers into unplasticized PVC at 80°C	cm^2 s^{-1} x 10^{10}	
di-n-hexyl phthalate		153
di-n-octyl phthalate		21.3
di-n-nonyl phthalate		13.7
di-n-decyl phthalate		1.98
di-(2-ethylhexyl) phthalate		12.9-13.2
Plasticizer sorption	phr	50-225
Plasticized PVC dry flow	s l^{-1}	5-25
Mark-Houwink parameters K and a, respectively	ml g^{-1}, –	
cyclohexanone	at 20°C	13,700 1.0
tetrahydrofurane		3,630 0.92
Activation energy of initiation of PVC dehydrochlorination	kJ mol^{-1}	118-170
Activation energy of propagation (zipping)	kJ mol^{-1}	52
Energy of formation of *trans*-polyene (activation energy of termination)	kJ mol^{-1}	78
Energy of formation of *cis*-polyene (activation energy of propagation)	kJ mol^{-1}	52

Table 5.3. Physical properties

Property	Unit	Value
Activation enthalpy of dehydrochlorination of	kcal mol^{-1} K^{-1}	
secondary chloroalkanes		42.7-51.2
trans-allyl chloroalkanes		32.9-47.9
cis-allyl chloroalkanes		27.6-37.7
initiation		32.2-33.4
propagation		12.4
termination		18.6
Activation entropy of dehydrochlorination of	cal mol^{-1} K^{-1}	
secondary chloroalkanes		−11.5 to −4.0
trans-allyl chloroalkanes		−19.8 to −3.0
cis-allyl chloroalkanes		−20.9 to −5.5
initiation		−19.2 to −16.1
propagation		−40.7
termination		−29.1
Enthalpy of polyene segment condensation to form benzene	kJ mol^{-1}	30
Maximum polyene length	number of double bonds	16-20
Time to 1% loss of Cl at	years	
105°C		3.6-20.7
40°C		$4x10^7$ to $2x10^9$
Plasticizer loss at 150°C during 1 h (concentration range from 10 to 40 wt%)	wt%	
epoxidized soybean oil		0.17-0.25
diisononyl phthalate		0.74-1.49
di-(2ethylhexyl) phthalate		1.48-2.05
di(2-ethylhexyl) adipate		2.21-6.01
benzyl butyl phthalate		1.38-3.91
Activation energy of photodehydrochlorination	kJ mol^{-1}	
nitrogen		32.1
air		19.6
Activation energy of photooxidation	kJ mol^{-1}	50-63
Spectral sensitivity	nm	310-370
Activation wavelength	nm	310-325, 327, 364
Excitation wavelength	nm	284, 290
Emission wavelength	nm	350,440

Table 5.3. Physical properties

Property	Unit	Value
Important initiators and accelerators	carbonyl groups, unsaturations, solvents forming hydroperoxides, sensitizing impurities (e.g., benzophenones), metaloorganics (copper-containing compounds, cadmium acetate, ferrocene, iron salts), metal chlorides produced from thermal stabilizers, products of degradation of some antioxidants, some pigments and fillers (containing cobalt, zinc, manganese, and lead), metal oxides (of titanium, zinc, and aluminum), hydrogen chloride (autocatalytic product of PVC degradation)	
Products of degradation	free radicals, unsaturations, carbonyl groups, hydroperoxides, chain scissions, crosslinks	
Photobleaching wavelength	nm	>350
Depth of UV radiation penetration	μm	200
Quantum energy of UV radiation (290-380 nm)	eV	4.3-3.3
Quantum energy of γ-radiation from ^{60}Co	MeV	1.25
Effect of EtOH sterilization (tensile strength retention)	%	113-115
Chemical resistance	dilute acids – very good dilute alkalis – very good oils & greases – good aliphatic hydrocarbons – very good aromatic hydrocarbons – poor halogen. hydrocarbons – moderate alcohols – good	
Hansen solubility parameters (two sets of values are in use in most research) dispersion component polar component hydrogen bonding component radius of interaction	$MPa^{1/2}$	 18.2 (8.94) 7.5 (4.12) 8.3 (1.45) 21.4
Hildebrand solubility parameter calculated from Hansen solubility parameters found in many available sources	$MPa^{1/2}$	 21.36 (9.95) 18.4-23.3

Table 5.3. Physical properties

Property	Unit	Value
Interaction parameter, χ		
carbon tetrachloride		1.14
chloroform		0.91
dichloromethane		1.63
Θ temperature	K	
cyclohexanone		324
dimethylformamide		309
benzyl alcohol		428
Solubility	g/100 ml	
cyclohexanone		8-15
dioxane		>4
dimethylformamide		soluble
dimethyl sulfoxide (90-100ºC)		10
MEK/THF industrial solvent		18
mesityl oxide		soluble
methyl ethyl ketone, MEK		22
methyl isobutyl ketone		soluble
N-methyl-2-pyrrolidone		partially soluble
nitrobenzene		soluble
tetrahydrofurane, THF		>15
Critical solvation temperatures with different plasticizers	ºC	
dibutyl phthalate		56
dioctyl phthalate		88
dioctyl adipate		105
diundecyl phthalate		129
Plastisol viscosity (Brookfield, 20 rpm) after 72 h	Pas	
30 phr of various plasticizers		1.8
50 phr of various plasticizers		1.8-9.8
70 phr of various plasticizers		2.6-7.7

Table 5.3. Physical properties

Property	Unit	Value
Typical absorption in infrared, wavenumber	cm^{-1}	
carbonyl		1714,1718,1720 1730,1679,1715
acid chloride		1785
carboxylate stabilizer		1510
β-chlorocarboxylic acid		1718
hydroperoxide		3476-3420
hydroxyl		3460
$–CH_2COOH$		1718
–CHCl–CO–CHCl		1745
–HC=CH– (isolated)		1650
–HC=CH– (conjugated)		1580
–HC=CH–CO (isolated)		1695
–HC=CH–CO (conjugated)		1605

5.4 MECHANICAL PROPERTIES

Table 5.4. Mechanical properties

Property	Unit	Value
Tensile strength	MPa	
rigid		35-39
20 phr plasticizer		34
30 phr of various plasticizers		14-25
50 phr of various plasticizers		12-23.1
70 phr of various plasticizers		16-18
75 phr of various plasticizers		15.6-17
80 phr of various plasticizers		9.5-12.6
Tensile modulus	MPa	2,430-4,000
Tensile stress at yield	MPa	39.2-88.3
Elongation	%	
rigid		18-80
20 phr plasticizer		190
30 phr of various plasticizers		270-300
50 phr of various plasticizers		290-410
70 phr of various plasticizers		390-460
75 phr of various plasticizers		460-500
80 phr of various plasticizers		360-450

Table 5.4. Mechanical properties

Property	Unit	Value
100% modulus	MPa	
30 phr plasticizer		9.0
50 phr of various plasticizers		7.0-14.6
70 phr of various plasticizers		5.0-6.8
75 phr of various plasticizers		4.5-5.2
Young modulus	MPa	
rigid (no impact modifier)		3270
rigid (10% impact modifier)		2470
80 phr plasticizer		4.5
Flexural strength	MPa	67-107
Flexural modulus	MPa	2,580-3,310
Tear strength	MPa	2.1-7.9
Tenacity (fiber) (standard atmosphere)	$cN\ tex^{-1}$	10-30
Tenacity (wet fiber, as % of dry strength)	%	100
Low temperature flexibility	°C	
30 phr plasticizer		−22
50 phr of various plasticizers		−25 to −31
70 phr of various plasticizers		−18 to −31
Clash and Berg temperature	°C	
50 phr of various plasticizers		−15.9 to −55.3
Brittle temperature	°C	
50 phr of various plasticizers		−28.6 to −68.5
80 phr of various plasticizers		−44 to −60
Izod impact, no impact modifier	$J\ m^{-1}$	100-160
Izod notched	$J\ m^{-1}$	
rigid (no reinforcement)		25-150
rigid (impact modified)		600-1300
Shore A hardness		
30 phr of various plasticizers		74-90
50 phr of various plasticizers		72-87
60 phr of various plasticizers		68-83
75 phr of various plasticizers		62-65
90 phr of various plasticizers		58-65
Shore D hardness, rigid		75
Wear resistance (volume loss), 80 phr plasticizer	mm^3	239.4
Adhesion to steel	$N\ m^{-1}$	3012-4209

Table 5.4. Mechanical properties

Property	Unit	Value
Poisson ratio		0.38
Mold shrinkage	m m^{-1}	0.005-0.025
Compression set (24 h at 70°C)	%	
DIDP 40 phr		70.0
DIDP 60 phr		69.7
DIDP 80 phr		70.3
DIDP 100 phr		68.2
DIDP 120 phr		67.3

5.5 HEALTH AND SAFETY

Table 5.5. Health and safety data

Property	Unit	Value
Permissible exposure limits:		
Cd and its compounds	mg m^{-3}	0.005
Pb and its compounds	mg m^{-3}	0.05
Sn compounds, tri-o-cresyl phosphate	mg m^{-3}	0.1
$Al(OH)_3$ As compounds	mg m^{-3}	0.5
vinyl chloride	ppm	1
triphenyl phosphate	mg m^{-3}	3
carbon black	mg m^{-3}	3.5
particulates, some phosphates & phthalates	mg m^{-3}	5
HCl	mg m^{-3}	7
TiO_2	mg m^{-3}	15
Carcinogen list (monomer & additives)	antimony trioxide, cadmium and cadmium compounds, carbon black, chlorinated paraffins, di-(2-ethylhexyl) phthalate, lead and lead compounds, silica (crystalline, respirable size), talc (containing asbestiform fibers), vinyl chloride, and wood dust	
PVC – evidence of carcinogenicity	inadequate evidence of carcinogenicity in humans. Inadequate evidence of carcinogenicity in animals. Overall evaluation: Group 3: The agent is not classifiable as to its carcinogenicity to humans. [IARC]	

Table 5.5. Health and safety data

Property	Unit	Value
Acceptable daily intake diisononyl phthalate diiso-n-octyl phthalate di-(2-ethylhexyl) phthalate diisodecyl phthalate butyl benzyl phthalate dibutyl phthalate	µg kg^{-1} body weight day^{-1}	 120-150 370 37 250 200 100
Di-(2-ethylhexyl) phthalate: tolerable daily intake by children (EU) newborn (EU) infants (3-12 months old) (EU) reference dose (EPA)	µg per kg body weight	 50 20 25 20
DOT class	not regulated for transportation	
ICAO/IATA class	not regulated for transportation	
UN/NA hazard class	none	
Autoignition temperature	ºC	435-454
Flash point	ºC	391
Limiting oxygen index	% O_2	37-49
Heat release	kW m^{-2}	176
NBS smoke chamber	Ds	349-500
Char at 500ºC	%	10.9-18.0
Heat of combustion	J g^{-1}	17,950
Volatile products of combustion	CO, CO_2, H_2O, HCl; traces of benzene and phosgene	
CO yield	%	8 (with flame retardant)
Explosive limits LEL UEL	%	not applicable
Acute toxicity, LD_{50}, oral, rat	mg kg^{-1}	10,000

Table 5.5. Health and safety data

Property	Unit	Value
Irritation		
skin	experience shows no unusual dermatitis hazard from routine handling	
eye	resin particles, like other inert materials, can be mechanically irritating. At process temperatures, product emissions may cause irritation.	
ingestion	no adverse health effects are anticipated	
inhalation	resin particles, like other inert materials, can be mechanically irritating. At process temperatures, product emissions may cause irritation	
Chronic effects	there are no known hazardous components above regulatory thresholds	
Route of entry	inhalation, ingestion	
First aid		
eyes	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. If eye irritation persists, seek medical attention.	
skin	Wash off with soap and plenty of water. If skin irritation persists, seek medical attention.	
inhalation	Move to fresh air in case of accidental inhalation of dust or fumes from overheating or combustion. When symptoms persist or in all cases of doubt seek medical advice	
ingestion	Not an anticipated hazard	
Flammability temperature	°C	
no fire retardants		180
with fire retardants		350-370
Self-ignition temperature	°C	
no fire retardants		385
with fire retardants		410
Flammability propagation temperature	°C	
no fire retardants		180
with fire retardants		350

Table 5.5. Health and safety data

Property	Unit	Value
Limiting oxygen index no flame retardants or phosphates with flame retardants	% oxygen	 21.4-26.3 27.9-49.4
NBS smoke no flame retardants with flame retardants	g^{-1}	 349-450 58-378
Char no flame retardants with flame retardants	%	 10.9-18.0 12.5-38.5
Toxic combustion products:	benzene, carbon monoxide, ethylene, hydrogen chloride, naphthalene, toluene, 1,3,5-trichlorobenzene	

5.6 ENVIRONMENTAL DATA

Table 5.6. Environmental information

Property	Unit	Value
Biodegradation probability	not readily biodegradable	
Environmental toxicity	adverse ecological impact is not known or expected under normal use	
Bioaccumulation potential	does not bioaccumulate	
Aquatic toxicity, *Daphnia magna*, LC_{50}, 48 h	mg l^{-1}	800-8,000
Cradle to grave non-renewable energy use	MJ kg^{-1}	53-55
Cradle to pellet greenhouse gasses	kg CO_2 kg^{-1} resin	2.0-2.1

5.7 USE AND APPLICATION DATA

Table 5.7. Use and application information

Property	Unit	Value
Typical processing methods	blow molding, calendering, extrusion, injection molding, plastisol coating, rotational molding, thermoforming	

Table 5.7. Use and application information

Property	Unit	Value
Extrusion (process parameters)		
screw temperature	°C	130-182
barrel temperature	°C	165-186
die temperature	°C	190-205
screw speed	rpm	50
die resistance		medium
Injection molding (process parameters)		
barrel temperature	°C	150-187
nozzle temperature	°C	171-185
mold temperature	°C	25-50
screw speed	rpm	80-400
cycle time	s	42
injection pressure	MPa	1380-2750
back pressure	kPa	345-690
Rotational molding (process parameters)		
oven temperature	°C	364-391
processing time	min	6
water cooling temperature	°C	60-70
cooling time	s	35-40
Drying temperature	°C	77-82
Outstanding properties	wide range of properties, products, and processing methods; large number of additives which can tailor-modify properties demanded in application; good chemical resistance; durability in outdoor and indoor use; inherent flame retarding properties; electrical insulating properties; hygienic properties; resource efficiency (only 43% of its mass is derived from petroleum)	

Table 5.7. Use and application information

Property	Unit	Value
Major products	*building industry*: benches, corrugated pipes, door profiles, drain pipes, fencing, floor coverings, frames, fascia boards, geomembranes, grating covers, gutter pipes, hoses, roofing membranes and sheets, sanitary installations, sealants, siding, swimming pool linings, tiles, utility buildings, vent pipes, waste water fittings, wallpaper, waste water pipes, water pipes, window profiles, wire coverings *electrical engineering*: acoustic panels, battery casing, battery terminals, cable & wire insulation, cable heads and distributors, cable jackets, electricity distribution boxes, insulation pipes, plug housings, plugs, semiconducting coverings, sockets, sound carrier sheet, telephone housings, transparent distributor box housings *mechanical engineering*: claddings, coatings, fittings, gaskets, hoses, pipe connections, pipes, pressure pipes, protective caps for pipes, stuffing boxes, thermostat housings, ventilation ducts, ventilators	
Major products	*packaging*: ball point pen cases, cling film, containers, crates, disposable pots, films and foils, letter trays, oil and beverage bottles, spice and cream containers *other*: artificial leather, balls, blinds, book covers, boots, car underbody seals, coated fabrics, composites, conveyor belts, divers masks, gloves, handbags, inflatable dinghies, inflatable warehouses and sport venues, irrigation pipes, membranes, office equipment, shoe soles, ski sunglasses, tablecloths, tarpaulins, toys, upholstery, water stop seal	