Human & Environmental Risk Assessment on ingredients of household cleaning products

Propylene Glycol n-Butyl Ether
CAS Number 5131-66-8 , 29387-86-8

Edition 1.0

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Abstract

Propylene glycol n-butyl ether (PnB; CAS# 5131-66-8 or 29387-86-8) has been used as a coupling agent and solvent in domestic and commercial cleaning solutions such as degreasers and hard surface cleaners. Within the scope of HERA applications, PnB finds use in various hard surface cleaners.

The HERA risk assessment has shown that the use of PnB in HERA applications results in environmental risk characterization ratios well below one, indicating no concern, for all environmental compartments. For human health, a margin of exposure of more than 300,000 has been calculated for the total aggregate consumer exposure. This MOE has been considered very large, large enough to account for the inherent uncertainty and variability of the database and inter and intra-species extrapolations.

The outcome of this HERA risk assessment which focuses on the specific uses of PnB in household cleaning products is fully consistent with that of the OECD high production volume chemical review which looked at all global uses of the category of propylene glycol ethers in general and PnB in particular. The SIDS initial assessment report (SIAR) concluded that propylene glycol ethers are considered of low priority for further work. The available data for all category members including PnB indicate that their aquatic and mammalian toxicity is low.

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1. Introduction

Propylene glycol n-butyl ether or Butoxypropan-1-ol (PnB, CAS# 5131-66-8 or 29387-86-8) is a chemical which is used as a coupling agent and solvent due to the high solvency, oil solubility, high formulating flexibility and low viscosity of this compound. Moreover, PnB is used as a degreaser and coupling agent in domestic and commercial cleaning solutions. Within the scope of HERA, PnB is only used in various hard surface cleaners.

This HERA report therefore covers the human and environmental risk assessment of the use of PnB in household cleaning applications building on the physico-chemical and hazard information provided in the OECD SIDS Initial Assessment Report (SIAR; OECD, 2003). The SIAR has been developed on the basis of a Screening Information Data Set (SIDS) for PnB, which contains an internationally agreed and harmonized data set providing general substance information and summarizing data on:

- exposure and use;
- physico chemical properties;
- environmental fate and pathways;
- ecotoxicity data; *and*
- human health data.

To characterise and assess the risks associated with the use of PnB in household cleaning products to human health and the environment according to the HERA methodology, the information provided in existing SIAR was supplemented by data from the various HERA teams on habits and practices of uses of detergents and PnB volumes used in the various household cleaning applications in Western Europe. Respective hazard summaries and calculations of PEC/PNEC ratio and Margin of Exposures (MOE) and their underlying data which form the basis for this risk assessment are annexed to this report.

2. Substance Characterization and Uses in Household Cleaning Applications

PnB is a propylene glycol ether which is used as components of coatings, (*e.g.*, paints and varnishes), cleaning fluids, inks, resins, cosmetics, and as inert carrier solvent in pesticide formulations (CEH, 2000). Because of its high solvency, oil solubility, surfactant, and coupling properties, and due to a good evaporation rate control, high formulating flexibility, low viscosity, as well as low toxicity, PnB may be used as a coupling agent and solvent in domestic and commercial cleaning solutions such as degreasers, paint removers, metal cleaners, and hard surface cleaners. PnB is also used as a coalescent for lowering minimum film formulation temperature (MFFT) in water-borne latex coatings and as a chemical intermediate for the production of epoxides, acid ester derivatives, solvents, and plasticizers.

Members of the propylene glycol ethers category are manufactured in closed, continuous equipment by the reaction of propylene oxide with methyl alcohol or n-butyl alcohol (CEH, 2000). This reaction can produce glycol ethers of varying chain length depending on the molar ratio of reactants and the temperatures and pressures used in the

reaction. Milder conditions and lower molar ratios of propylene oxide to alcohol will produce the mono-propylene glycol ethers, while using more propylene oxide and higher temperatures and pressures produce the di- and tri-propylene glycol mono-alkyl ethers. The products are purified by distillation.

In line with the objectives of the HERA initiative, this assessment will focus on the use of PnB in household cleaning products. Currently it is only used in hard surface cleaners at levels varying from 0 – 6.7%. In spray cleaners and surface wipes, PnB is typically used at concentrations from 0.5 – 2.5% with a maximum of 4%.

3. Environmental Assessment

Environmental Exposure

Tonnage Scenarios

The total use of propylene glycol ethers (PnB, DPnB, DPMA, TPM) in Western Europe has been estimated at 214,550 tonnes per annum (CEH, 2000), however it has been indicated that less then 5% of the total usage (to include both HERA and non HERA uses) can be attributed to PnB. It has been estimated that in HERA applications an annual tonnage of 3,400 of PnB has been used. The latter estimate is based on data received from a survey conducted among the detergent formulator companies and is representative for the volume being consumed in the European Union 15+3 countries (being Iceland, Switzerland and Norway). This volume has been adjusted to cover 100% of the tonnage used within the HERA applications, based on the assumption that the survey response covers 80% of the usage within the European Union. The calculations to of the predicted environmental concentration (PEC) have been based on the estimated tonnage used in the HERA applications.

Physico-Chemical Properties

The most important physico-chemical properties required to estimate a PEC value are aqueous solubility, vapour pressure, and the octanol/water partition coefficient. The physico-chemical properties that have been used in this assessment for PnB are presented in Annex 1.

Environmental Fate

PnB has been shown to be readily biodegradable within a 10 day window (OECD, 2003). Aerobic biodegradation of PnB occurred rapidly in different OECD and GLP compliant studies. Aerobic biodegradation data developed using standardised test methods have shown that PnB mineralization from the test medium has been 60% to 90% within 28 days. The OECD study 301E giving more than 90% DOC removal after 28 days, and with the removal satisfying the 10 day window criteria.

Using the EPIWN model, the photo-degradation of PnB has been estimated to be moderately rapid. Assuming a 12-hour day of sunlight and average hydroxyl radical concentration of 1.5×10^6 OH/cm^3, the atmospheric photo-degradation half-life has been estimated to be 4.6 hours (OECD, 2003).

PnB has been predicted to be stable in the presence of water at neutral pH and at ambient temperatures (OECD, 2003). Monitoring data for PnB in European surface waters is not available. Because of the low octanol-water partition coefficient (*i.e.*, log K_{ow} of 1.15 at 25ºC; Annex 1), PnB is likely to have no significant bioaccumulation potential (OECD, 2003).

Predicted Environmental Concentrations (PEC) Calculations

Using the European Union System for the Evaluation of Substances (EUSES; version 2.03), the degradation of PnB in a waste water treatment model has been calculated to be 87.1%, the remainder of PnB partitioned between air (0.2%), water (12.6%) and sludge (0.1%). The EUSES report file has been included in Annex 2.

The HERA environmental risk assessment for PnB has been based on the technical guidance document for new and existing substances (TGD, 2003). At the screening level it makes use of the EUSES programme (version 2.03, 2005) to calculate the local and regional exposure to PnB (Table 1). The total PnB tonnage produced for, and used in, detergents was assumed to follow the down-the-drain pathway to the environment. The production and formulation releases at local level were not considered because they fall outside the scope of HERA. For the calculation, the HERA exposure scenario (to assign 7% of the EU tonnage to the standard EU region, instead of the TGD default 10%, and to increase the emissions at local level by a factor of 1.5, instead of the TGD default factor of 4) has not been used, as the revised TGD has updated the default values for the regional emissions and the local input of substances used in household detergents, based on the experimental data submitted during the TGD revision process (Fox, 2001). More details and justification of these default values is presented in chapter 2.2.3 of the revised HERA methodology document (HERA, 2005).

The volume of PnB used in HERA applications was used to calculate the PECs. Therefore the subscript HERA has been added to the calculated PECs to indicate that the HERA volume of 3,400 tonnes per annum has been used. It should be stated that other releases of PnB to the environment are outside the scope of this assessment.

Table 1: PEC_{HERA}[1] estimates for PnB using EUSES

		Local			**Regional**
PEC_{HERA} Air	PEC_{HERA} Surface Water	PEC_{HERA} Freshwater Sediment	PEC_{HERA} Soil	PEC_{HERA} WWTP[2]	PEC_{HERA} Surface Water
(mg/m^3)	(mg/L)	(mg/kg WW^3)	(mg/kg WW^3)	(mg/L)	(mg/L)
1.97 E-6	3.9 E-3	3.96 E-3	1.71 E-4	0.0293	9.71 E-4

[1] The calculated PECs calculated are based on PnB volume used in HERA household applications (3,400 tonnes/year) and are as such denoted by the subscript HERA
[2] Micro organisms in waste water treatment plant
[3] WW (wet weight)

Environmental Effects

Ecotoxicological data for PnB mixture have been summarised in the IUCLID Dataset (ECB, 2000). Moreover, the SIDS on propylene glycol ethers gives an extensive summary of the ecotoxicological hazard data of PnB (OECD, 2003). A summary of those toxicological endpoints and considerations most relevant for the assessment of PnB in context of HERA have been attached in Annex 3.

Available data illustrate that PnB is of low acute aquatic toxicity (OECD, 2003). In a 96 hour study with freshwater fish (*i.e.*, *Poecilia reticulata*) an EC_{50} value for PnB has been determined as 560 mg/L based increased pigmentation and reduced swimming ability. In a 48 hour test with *Daphnia magna* the highest tested concentration of 1,000 mg/L did not cause any adverse effects on mobility. Hence, the acute no effect concentration (EC_0) was determined to be 1,000 mg/L. In a static 96 hour algal growth inhibition assay with *S. capricornutum* the growth has been shown to be inhibited by 42% at 1,000 mg/L, the highest tested concentration. Therefore it can be conservatively assumed that the algal EC_{50} is 1,000 mg/L and a NOAEC of 560 mg/L has been determined by the authors.

No chronic aquatic toxicity studies with marine or freshwater species have been reported. In the absence of any chronic toxicity data, the TGD recommends to apply an assessment factor of 1,000 if only acute toxicity data are available for fish, daphnia and algae (EC, 2003). The $PNEC_{aquatic}$ was calculated to be 0.56 mg/L on the basis of the LC_{50} of 560 mg/L determined in the fish study.

Information about the toxicity of PnB to micro-organisms has been derived from several biodegradation studies (OECD 301b,d,e). No toxicity to the test inoculum was observed at PnB concentrations ranging from 10-20 mg/L. The $NOEC_{micro\text{-}organism}$ has therefore been established to be 1 mg/L. This value has been derived from the ready biodegradability test by applying an assessment factor of 10 to the NOEC value as recommended by the TGD.

Data on aquatic toxicity of PnB in the sediment compartment were not available. The $PNEC_{aquatic}$ has been used to derive a $PNEC_{sediment}$ using equilibrium partitioning. The $PNEC_{sediment}$ has been calculated as 0.57 mg/kg wet weight (WW) using EUSES.

Similarly, data on toxicity to soil dwelling organisms are lacking. In the absence of soil toxicity data the TGD recommends that a $PNEC_{soil}$ be derived from equilibrium partitioning data from the $PNEC_{aquatic}$ as an initial screen. The partition coefficient soil water ($K_{soil\text{-}water}$) has been determined by EUSES and the $PNEC_{soil}$ of 0.17 mg/kg WW has been reported.

Environmental Risk Characterisation

The environmental risks associated with the use of PnB in HERA applications have been characterised by comparing the ratio of PEC_{HERA} derived from the EUSES calculation for the local worst case scenario based on the household HERA tonnage with the PNEC values for the different environmental compartments (Annex 4). The use of PnB in HERA applications results in risk characterisation ratios (RCR) well below 1 for

all relevant environmental compartments (Table 2). It can therefore be concluded that the use of PnB in HERA applications is of low environmental concern.

Table 2: Risk characterisation ratios in the relevant environmental compartments for PnB

	Local Water	WWTP	Local Sediment	Local Soil
PEC	0.0039 mg/L	0.0293 mg/L	0.00396 mg/kg WW	0.002 mg/kg WW
PNEC	0.56 mg/L	10 mg/L	0.57 mg/kg WW	0.17 mg/kg WW
RCR[1]	**0.007**	**0.029**	**0.0069**	**0.011**

[1] Differences in the risk characterisation ratios reported in this table and those calculated in the EUSES output file are related to rounding of the reported numbers.

4. Human Health Assessment

Consumers may be exposed to PnB through its presence in hard surface cleaners mainly via the dermal route through skin contact with the cleaning solution during hard surface cleaning, and to some extent also via the inhalation route. Since PnB is also used in spray cleaners, the consumer can also be exposed to PnB containing aerosols, which are generated by the sprayer.

Annex 5 provides the detailed consumer exposure assessment according to the HERA exposure assessment guidelines. These exposure estimates take into account maximum finished product concentrations of PnB in liquid household (*i.e.*, 6.7%) and in spray cleaners (*i.e.*, 4%). They further take account of habits and practice data, reflecting consumers' use of detergents in terms of gram per task, tasks per week and duration of task. The underlying data have been collated by the HERA Formulator team and the European Soap and Detergent Industry Association (AISE). The aggregate consumer exposure to PnB via its use in household cleaning products is estimated to be 2.9 µg/kg bw/d.

A thorough review of the available toxicological information and potential human health effects of PnB has been conducted as part of the OECD HPV review on the category of propylene glycol ethers (OECD, 2003). A summary of those toxicological endpoints and considerations relevant for the assessment of PnB in context of its use household cleaning applications has been attached in Annex 3.

A substantial amount of toxicological data and information is available on PnB. The existing data demonstrate that PnB is of low acute oral, dermal or inhalatory toxicity with LD_{50} values of greater than 2 g/kg body weight and LC_{50} values greater than 651 ppm (approximately 3.5 g/m^3). According to OECD eye irritation criteria, PnB is considered to be moderately irritating to eyes and skin when tested undiluted. PnB did not show any evidence for causing skin sensitization in experimental animals. Neither are any reports available that discuss skin sensitisation potential in humans. Moreover, there has been no evidence for PnB being genotoxic, mutagenic or carcinogenic.

To evaluate its repeated dose toxicity, PnB has been tested in a 13 week drinking water study in rats, in 13 week dermal application studies in rats and rabbits and in 2- and 4week inhalation studies with rats.

In the drinking water study, PnB showed only at the highest dose level of 1,000 mg/kg bw/d signs of toxicity as indicated by increased liver weights in males and increased kidney weights in females. Both effects were without associated histopathology. Moreover, slight alterations in clinical chemistries, electrolytes and haematology were noted in both sexes at the highest dose level. When tested specifically for possible haematological toxicity in male and female rats in an oral gavage study, a toxicological endpoint of concern for lower molecular weight ethylene glycol ethers, PnB did not show any signs of haemolysis. On the basis of the subchronic drinking water study, the SIAR established a NOAEL of 350 mg/kg bw/d and a LOAEL of 1,000 mg/kg bw/d.

The finding that high dose exposure to PnB may lead to increase in liver weights was also confirmed in three inhalation studies. In a 6-week inhalation study, female rates exhibited increased liver weights without accompanying histopathology at the highest dose level of 600 ppm. The NOAEL was established to be 300 ppm. When tested dermally for 91 days at doses up to 880 mg/kg bw/d, except for some local skin reactions, PnB did not show any signs of systemic toxicity. The NOAEL was established at 880 mg/kg bw/d, the highest dose tested.

There is no data to suggest that exposure to PnB causes reproductive or developmental toxicity. Although specific reproductive toxicity studies are not available for PnB, the results from the subchronic toxicity studies indicate that PnB does not cause toxicity to the testes or female reproductive organs. In all available studies, at a minimum testes and ovaries were examined histopathologically for potential chemically induced injury. In the 13 week studies, prostate, epididymides, seminal vesicles in males, and uterus and vagina in females were examined histopathologically in addition. No treatment related damages were reported.

The developmental toxicity of PnB has been examined by daily application of PnB at two different doses on gestation days 6 through 15 to the shaved skin of pregnant rats. In this study PnB did neither cause embryo- or fetotoxicity nor developmental toxicity in skeletal of soft tissues of the embryos. An observed slight increase in the incidence of supernumerary rudimentary thoracic ribs in the high dose group was not considered to be significant by the investigators since the incidence was within normal limits for these species. It was concluded that PnB was not maternally toxic, embryo- or fetotoxic, or teratogenic in rats. Hence, the NOAEL was established to be greater than 880 mg/kg bw/d. Similar results were obtained in a dermal developmental toxicity study with pregnant rabbits for which the NOAEL for maternal toxicity, embryo- or foetal toxicity, or developmental toxicity was established to be greater than 100 mg/kg bw/d, the highest tested dose.

Under the OECD review, NOAELs for PnB have been established and discussed for subchronic, reproductive and developmental toxicity. The NOAEL for oral exposure to PnB has been established at 350 mg/kg bw/d and that for dermal exposure at 880 mg/kg bw/d. Considering that PnB exposure via the use of hard surface cleaners predominantly occurs via the dermal route (*i.e.*, more than 99%), it is most appropriate to compare the aggregate exposure to PnB of 2.93 µg/kg bw/d to the NOAEL that has been derived

from dermal toxicity studies (*i.e.*, 880 mg/kg/d). This results in a Margin of Exposure (MOE) of greater than 300,000 (see Annex 6). This MOE is considered to be large enough to account for the inherent uncertainty of the database and potential inter- and intra species variability.

In summary, the human health risk assessment demonstrates that the use of PnB in household cleaning applications can be considered to be safe and does not raise any health concerns.

5. Contributions to the Report

This risk assessment was developed by the HERA Secretariat and THE WEINBERG GROUP, supported by DOW Europe. The HERA Human Health and Environmental Task Forces gave additional input.

Annex 1. Physical/Chemical Properties of PnB for EUSES

Property	Results	Reference
EINECS name	Butoxypropan-1-ol	
CAS numbers	29387-86-8 (mixture), 5131-66-8 (alpha isomer)	
EINECS number	249-598-7	
Smiles code	$C_4H_9OCH_2CH(CH_3)OH$	
Molecular weight	132.2 g/Mol	
Melting point	-85 ºC	Staples and Davies, 2002
Boiling point	171 ºC (at 1013 hPa)	Dow chemical company MSDS
Vapour pressure	1.63 hPa at 20 ºC	Staples and Davies, 2002
Log Octanol-Water partition coefficient (Log Kow)	1.15 at 25 ºC	Staples and Davies, 2002
Water solubility	55,000 mg/L	Staples and Davies, 2002
Henry's law constant	ND	
Transport and distribution	In air 2.3% In water 50.1% In sediment 0.1% In soil 47.5%	Calculated (fugacity level 1 type)

Annex 2. EUSES 2.03 Output Report

DEFAULT IDENTIFICATION

General name	Standard Euses 2.0	D	
Description	According to TGDs	D	

RELEASE ESTIMATION

Fraction of EU production volume for region	0	[%]	S
Fraction of EU tonnage for region (private use)	10	[%]	D
Fraction connected to sewer systems	80	[%]	D

SEWAGE TREATMENT

GENERAL

Number of inhabitants feeding one STP	1E+04	[eq]	D
Sewage flow	200	[l.eq-1.d-1]	D
Effluent discharge rate of local STP	2E+06	[l.d-1]	O
Temperature dependency correction	No		D
Temperature of air above aeration tank	15	[oC]	D
Temperature of water in aeration tank	15	[oC]	D
Height of air column above STP	10	[m]	D
Number of inhabitants of region	2E+07	[eq]	D
Number of inhabitants of continental system	3.5E+08	[eq]	O
Wind speed in the system	3	[m.s-1]	D

AREAS

REGIONAL

Area (land + rivers) of regional system	4E+04	[km2]	D
Area fraction of fresh water, region (excl. sea)	0.03	[-]	D
Area fraction of natural soil, region (excl. sea)	0.27	[-]	D
Area fraction of agricultural soil, region (excl. sea)	0.6	[-]	D
Area fraction of industrial/urban soil, region (excl. sea)	0.1	[-]	D
Length of regional sea water	40	[km]	D
Width of regional sea water	10	[km]	D
Area of regional sea water	400	[km2]	O
Area (land + rivers + sea) of regional system	4.04E+04	[km2]	O
Area fraction of fresh water, region (total)	0.0297	[-]	O
Area fraction of sea water, region (total)	9.9E-03	[-]	O
Area fraction of natural soil, region (total)	0.267	[-]	O
Area fraction of agricultural soil, region (total)	0.594	[-]	O
Area fraction of industrial/urban soil, region (total)	0.099	[-]	O

SUBSTANCE

SUBSTANCE IDENTIFICATION

General name	PnB		S
Description			D
CAS-No			D
EC-notification no.			D
EINECS no.			D

PHYSICO-CHEMICAL PROPERTIES

Molecular weight	132.2	[g.mol-1]	S
Melting point	-85	[oC]	S
Boiling point	171	[oC]	S
Vapour pressure at test temperature	1.63	[hPa]	S
Temperature at which vapour pressure was measured	20	[oC]	S
Vapour pressure at 25 [oC]	230	[Pa]	O
Octanol-water partition coefficient	1.15	[log10]	S
Water solubility at test temperature	5.5E+04	[mg.l-1]	S
Temperature at which solubility was measured	20	[oC]	S
Water solubility at 25 [oC]	5.89E+04	[mg.l-1]	O

PARTITION COEFFICIENTS AND BIOCONCENTRATION FACTORS

SOLIDS-WATER

Chemical class for Koc-QSAR	Predominantly hydrophobics (default QSAR)	D	
Organic carbon-water partition coefficient	10.8	[l.kg-1]	O
Solids-water partition coefficient in soil	0.215	[l.kg-1]	O
Solids-water partition coefficient in sediment	0.538	[l.kg-1]	O
Solids-water partition coefficient suspended matter	1.08	[l.kg-1]	O
Solids-water partition coefficient in raw sewage sludge	3.23	[l.kg-1]	O
Solids-water partition coefficient in settled sewage sludge	3.23	[l.kg-1]	O
Solids-water partition coefficient in effluent sewage sludge	3.98	[l.kg-1]	O
Soil-water partition coefficient	0.523	[m3.m-3]	O
Suspended matter-water partition coefficient	1.17	[m3.m-3]	O
Sediment-water partition coefficient	1.07	[m3.m-3]	O

AIR-WATER

Sub-cooled liquid vapour pressure	230	[Pa]	O
Fraction of chemical associated with aerosol particles	4.35E-07	[-]	O
Henry's law constant	0.516	[Pa.m3.mol-1]	O
Air-water partitioning coefficient	2.18E-04	[m3.m-3]	O

BIOCONCENTRATION FACTORS

PREDATOR EXPOSURE

Bioconcentration factor for earthworms	1.01	[l.kgwwt-1]	O

HUMAN AND PREDATOR EXPOSURE

Bioconcentration factor for fish	1.89	[l.kgwwt-1]	O
QSAR valid for calculation of BCF-Fish	Yes		O
Biomagnification factor in fish	1	[-]	O
Biomagnification factor in predator	1	[-]	O

BIOTA-WATER

FOR REGIONAL/CONTINENTAL DISTRIBUTION

Bioconcentration factor for aquatic biota	1.89	[l.kgwwt-1]	O

DEGRADATION AND TRANSFORMATION RATES

CHARACTARIZATION

Characterization of biodegradability	Readily biodegradable		S

STP

Degradation calculation method in STP	First order, standard OECD/EU tests		S
Rate constant for biodegradation in STP	24	[d-1]	O
Total rate constant for degradation in STP	24	[d-1]	O
Maximum growth rate of specific microorganisms	2	[d-1]	D
Half saturation concentration	0.5	[g.m-3]	D

RELEASE ESTIMATION

CHARACTERIZATION AND TONNAGE

High Production Volume Chemical	Yes		S
Production volume of chemical in EU	3.4E+03	[tonnes.yr-1]	S
Fraction of EU production volume for region	0	[%]	S
Regional production volume of substance	0	[tonnes.yr-1]	O
Continental production volume of substance	3.4E+03	[tonnes.yr-1]	O
Volume of chemical imported to EU	0	[tonnes.yr-1]	D
Volume of chemical exported from EU	0	[tonnes.yr-1]	D
Tonnage of substance in Europe	3.4E+03	[tonnes.yr-1]	O

USE PATTERNS

PRODUCTION STEPS

EMISSION INPUT DATA [1 ‘’]

Usage/production title			D
Industry category	15/0 Others		D
Use category	55/0 Others		D
Extra details on use category	No extra details necessary		D
Extra details on use category	No extra details necessary		D
Main category production	III Multi-purpose equipment		D
Use specific emission scenario	No		D
Emission scenario	no special scenario selected/available	S	
Fraction of tonnage for application	1	[-]	O
Total of fractions for all production steps	1	[-]	O
Relevant production volume for usage	3.4E+03	[tonnes.yr-1]	O
Regional production volume of substance	0	[tonnes.yr-1]	O
Regional production volume for usage	0	[tonnes.yr-1]	O

OTHER LIFE CYCLE STEPS

EMISSION INPUT DATA [2 ‘HERA HOME’]

Usage/production title	HERA Home		S

USE PATTERN

Industry category	5 Personal / domestic use		S
Use category	9 Cleaning/washing agents and additives		S
Extra details on use category	Unknown type		S
Extra details on use category	No extra details necessary		D

PRIVATE USE

Use specific emission scenario	Yes		S
Emission scenario	Emission fractions, fraction-main-source		S

TONNAGE

Fraction of tonnage for application	1	[-]	O
Fraction of chemical in formulation	1	[-]	D
Tonnage of formulated product	0	[tonnes.yr-1]	O
Relevant tonnage for application	3.4E+03	[tonnes.yr-1]	O
Regional tonnage of substance	0	[tonnes.yr-1]	O
Tonnage of formulated product	0	[tonnes.yr-1]	O
Regional tonnage of substance (private use step)	340	[tonnes.yr-1]	O
Continental tonnage of substance (private use step)	3.06E+03	[tonnes.yr-1]	O
Total of fractions for all applications	1	[-]	O

USE PATTERN 2

RELEASE FRACTIONS AND EMISSION DAYS [2 'HERA HOME']

PRIVATE USE

Emission scenario	Emission fractions, fraction-main-source	S	
Emission tables	A4.1 (specific uses), B4.1 (general table)	S	
Number of inhabitants feeding one STP	1E+04	[eq]	D
Number of inhabitants of region	2E+07	[eq]	D

RELEASE FRACTIONS

Fraction of tonnage released to air	0	[-]	O
Fraction of tonnage released to waste water	1	[-]	O
Fraction of tonnage released to surface water	0	[-]	O
Fraction of tonnage released to industrial soil	0	[-]	O
Fraction of tonnage released to agricultural soil	0	[-]	O
Emission fractions determined by special scenario	Yes		O

EMISSION DAYS

Fraction of the main local source	5E-04	[-]	O
Number of emission days per year	365	[-]	O
Emission day determined by special scenario	No		O

REGIONAL AND CONTINENTAL RELEASES [2 'HERA HOME']

PRIVATE USE

REGIONAL

Regional release to air	0	[kg.d-1]	O
Regional release to waste water	932	[kg.d-1]	O
Regional release to surface water	0	[kg.d-1]	O
Regional release to industrial soil	0	[kg.d-1]	O
Regional release to agricultural soil	0	[kg.d-1]	O

[2 'HERA HOME'] [PRIVATE USE]

Local emission to air during episode	0	[kg.d-1]	O
Emission to air calculated by special scenario	No		O
Local emission to wastewater during episode	0.466	[kg.d-1]	O
Emission to water calculated by special scenario	No		O
Show this step in further calculations	Yes		O
Intermittent release	No		D

[2 'HERA HOME'] [PRIVATE USE]

INPUT AND CONFIGURATION [2 'HERA HOME'] [PRIVATE USE]

Use or bypass STP	Use STP		D
Local emission to wastewater during episode	0.466	[kg.d-1]	O
Concentration in untreated wastewater	0.233	[mg.l-1]	O
Local emission entering the STP	0.466	[kg.d-1]	O

CONFIGURATION

Type of local STP	With primary settler (9-box)		D
Number of inhabitants feeding this STP	1E+04	[eq]	O
Effluent discharge rate of this STP	2E+06	[l.d-1]	O
Calculate dilution from river flow rate	No		O
Flow rate of the river	1.8E+04	[m3.d-1]	O
Dilution factor (rivers)	10	[-]	O
Dilution factor (coastal areas)	100	[-]	O

OUTPUT [2 'HERA HOME'] [PRIVATE USE]

Fraction of emission directed to air by STP	0.22	[%]	O
Fraction of emission directed to water by STP	12.6	[%]	O
Fraction of emission directed to sludge by STP	0.101	[%]	O
Fraction of the emission degraded in STP	87.1	[%]	O
Total of fractions	100	[%]	O
Local indirect emission to air from STP during episode	1.03E-03	[kg.d-1]	O
Concentration in untreated wastewater	0.233	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	0.0293	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	0.598	[mg.kg-1]	O
PEC for micro-organisms in the STP	0.0293	[mg.l-1]	O

REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION

PECS

REGIONAL

Regional PEC in surface water (total)	9.71E-04	[mg.l-1]	O
Regional PEC in sea water (total)	7.8E-05	[mg.l-1]	O
Regional PEC in surface water (dissolved)	9.71E-04	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in sea water (dissolved)	7.8E-05	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.08E-06	[mg.m-3]	O
Regional PEC in agricultural soil (total)	4.43E-06	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	1.44E-05	[mg.l-1]	O
Regional PEC in natural soil (total)	3.69E-06	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	3.69E-06	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	8.62E-04	[mg.kgwwt-1]	O
Regional PEC in sea water sediment (total)	6.99E-05	[mg.kgwwt-1]	O

CONTINENTAL

Continental PEC in surface water (total)	1.27E-04	[mg.l-1]	O
Continental PEC in sea water (total)	2.13E-08	[mg.l-1]	O
Continental PEC in surface water (dissolved)	1.27E-04	[mg.l-1]	O
Continental PEC in sea water (dissolved)	2.13E-08	[mg.l-1]	O
Continental PEC in air (total)	3.02E-07	[mg.m-3]	O
Continental PEC in agricultural soil (total)	8.23E-07	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	2.68E-06	[mg.l-1]	O
Continental PEC in natural soil (total)	1.03E-06	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	1.4E-06	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	1.13E-04	[mg.kgwwt-1]	O
Continental PEC in sea water sediment (total)	1.91E-08	[mg.kgwwt-1]	O

[2 'HERA HOME'] [PRIVATE USE]

LOCAL CONCENTRATIONS AND DEPOSITIONS [PRIVATE USE]

Concentration in air during emission episode	2.85E-07	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	2.85E-07 [mg.m-3]		O
Total deposition flux during emission episode	4.11E-07	[mg.m-2.d-1]	O
Annual average total deposition flux	4.11E-07	[mg.m-2.d-1]	O
Concentration in surface water during emission episode (dissolved)	2.93E-03 [mg.l-1]		O
Annual average concentration in surface water (dissolved)	2.93E-03	[mg.l-1]	O
Concentration in sea water during emission episode (dissolved)	2.33E-03 [mg.l-1]		O
Annual average concentration in sea water (dissolved)	2.33E-03	[mg.l-1]	O
Concentration in agric. soil averaged over 30 days	5.87E-04	[mg.kgwwt-1]	O
Concentration in agric. soil averaged over 180 days	1.67E-04	[mg.kgwwt-1]	O
Concentration in grassland averaged over 180 days	5.56E-05	[mg.kgwwt-1]	O
Fraction of steady-state (agricultural soil)	1	[-]	O
Fraction of steady-state (grassland soil)	1	[-]	O

LOCAL PECS [PRIVATE USE]

Annual average local PEC in air (total)	1.37E-06	[mg.m-3]	O
Local PEC in surface water during emission episode (dissolved)	3.9E-03	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in surface water (dissolved)	3.9E-03	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	3.96E-03	[mg.kgwwt-1]	O
Local PEC in sea water during emission episode (dissolved)	2.41E-03	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in sea water (dissolved)	2.41E-03	[mg.l-1]	O
Local PEC in marine sediment during emission episode	2.45E-03	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	5.9E-04	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	1.71E-04	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	5.92E-05	[mg.kgwwt-1]	O
Local PEC in pore water of agricultural soil	5.55E-04	[mg.l-1]	O
Local PEC in pore water of grassland	1.93E-04	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	5.55E-04	[mg.l-1]	O

EFFECTS

INPUT OF EFFECTS DATA

MICRO-ORGANISMS

Test system	Inhibition control test in base set tests		
EC50 for micro-organisms in a STP	??	[mg.l-1]	D
EC10 for micro-organisms in a STP	??	[mg.l-1]	D
NOEC for micro-organisms in a STP	10	[mg.l-1]	S

AQUATIC ORGANISMS

FRESH WATER

L(E)C50 SHORT-TERM TESTS

LC50 for fish	560	[mg.l-1]	S
L(E)C50 for Daphnia	1000	[mg.l-1]	S
EC50 for algae	1000	[mg.l-1]	S
LC50 for additional taxonomic group	??	[mg.l-1]	D
Aquatic species	other		D

ENVIRONMENTAL EFFECTS ASSESSMENT

ENVIRONMENTAL PNECS

FRESH WATER

Toxicological data used for extrapolation to PNEC Aqua	560	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	1000	[-]	O
PNEC for aquatic organisms	0.56	[mg.l-1]	O

MARINE

Toxicological data used for extrapolation to PNEC Marine	560	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Marine		1E+04	[-] O
PNEC for marine organisms	0.056	[mg.l-1]	O

FRESH WATER SEDIMENT

PNEC for fresh-water sediment organisms (equilibrium partitioning)	0.569 [mg.kgwwt-1]
Equilibrium partitioning used for PNEC in fresh-water sediment?	Yes
PNEC for fresh-water sediment-dwelling organisms	0.569 [mg.kgwwt-1]

TERRESTRIAL

Toxicological data used for extrapolation to PNEC Terr	??	[mg.kgwwt-1]	O
Assessment factor applied in extrapolation to PNEC Terr	??	[-]	O
PNEC for terrestrial organisms (from toxicological data)	??	[mg.kgwwt-1]	O
PNEC for terrestrial organisms (equilibrium partitioning)	0.172	[mg.kgwwt-1]	O
Equilibrium partitioning used for PNEC in soil?	Yes		O
PNEC for terrestrial organisms	0.172	[mg.kgwwt-1]	O

STP

Toxicological data used for extrapolation to PNEC micro	10	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	10	[-]	O
PNEC for micro-organisms in a STP	1	[mg.l-1]	O

ENVIRONMENTAL EXPOSURE

RISK CHARACTERIZATION OF [2 'HERA HOME'] [PRIVATE USE]

WATER

RCR for the local fresh-water compartment	6.96E-03	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	0.043	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O

SEDIMENT

RCR for the local fresh-water sediment compartment	6.96E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local marine sediment compartment	0.043	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O

SOIL

RCR for the local soil compartment	3.43E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local soil compartment, statistical method	??	[-]	O

STP

RCR for the sewage treatment plant	0.0293	[-]	O

REGIONAL

WATER

RCR for the regional fresh-water compartment	1.73E-03	[-]	O
RCR for the regional marine compartment	1.39E-03	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O

SEDIMENT

RCR for the regional fresh-water sediment compartment	1.51E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional marine sediment compartment	1.23E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O

SOIL

RCR for the regional soil compartment	2.57E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional soil compartment, statistical method	??	[-]	O

Annex 3. Summary of Toxicological Data of Relevance in the HERA Assessment

Study Type	Species	Endpoint/ Methodology	Exposure	Result	Study Quality (GLP, Klimisch Criteria	Reference
BIODEGRADATION						
Aerobic biodegradation test	Activated sludge from STW	OECD 301B (CO_2 evolution)	28 days Concentration: 0, 10, 20 mg/L	PnB is biodegradable to 60% after 28 days but not within a 10 day window.	GLP, Klimisch level 1	(Cardinaals and De Crom, 1987a) SIDS Dossier
Aerobic biodegradation test	Domestic sewage	OECD 301D (Closed bottle test)	28 days Concentration: 0, 2, 10 mg/L.	PnB although reaching the biodegradation limit of 60% within 28 day window did not do so in the 10 day window.	GLP, Klimisch level 1	(Cardinaals and De Crom, 1987b) SIDS Dossier
Aerobic biodegradation test	Activated sludge from STW	OECD 301E (modified OECD test)	28 days, Concentration: 0, 17 mg/L.	PnB is degraded to 90% after 28 days and reaches 60% in the 10 d window. PnB is readily biodegradable.	GLP, Klimisch level 1	SIDS Dossier
ECOTOXICOLOGY						
Acute toxicity to fish	*Poecilia reticulata* (freshwater)	EC50 (static renewal), OECD 203	96 hours Concentrations: 0, 100, 180, 320, 560, 1,000 mg/L	560 mg/L Test result based on an inability to swim and increased pigmentation. **$PNEC_{aquatic}$ 0.56 mg/L.**	GLP, Klimisch level 1	(Van der Hoeven and Welboren, 1987) SIDS Dossier
	Onchorhynchus mykiss, Lepomis macrochirus, Carassius auratus (freshwater)	LC50 (static)	24 hours	> 5 mg/L, higher concentrations have not been studied	ND	SIDS Dossier

Study Type	Species	Endpoint/ Methodology	Exposure	Result	Study Quality (GLP, Klimisch Criteria	Reference
Acute toxicity to aquatic invertebrates	*Daphnia magna* (freshwater)	EC50 (static), OECD 202	48 hours, Concentrations of 100, 180, 320, 560, and 1,000 mg/L	No toxicity observed at the highest concentration, >1,000 mg/L	Klimisch level 1	(Borges and Welboren, 1987) SIDS Dossier
Toxicity to aquatic plants	Selenastrum capricornutum (freshwater)	EC50 (growth rate), OECD 201	96 hours Concentrations: 0, 100, 180, 320, 560, 1,000 mg/L	Growth inhibition 42% at 1,000 mg/L, NOAEC is 560 mg/L	Klimisch level 2	(Hughes, 1987) SIDS Dossier
HUMAN TOXICOLOGY						
Acute Toxicity						
Oral	Rat	LD50 OECD Guideline 401	1,800, 2,400, or 3,200 mg/kg bw	ca. 3,300 mg/kg	GLP, Klimisch level 1	(Reijnders *et al*., 1987a) SIDS Dossier
Inhalation	Rat	LC0 OECD Guideline 403	650 ppm	> 650 ppm	GLP, Klimisch level 1	(Corley *et al*., 1987) SIDS Dossier
Dermal	Rat	LD50 OECD Guideline 402	2,000 mg/kg bw	> 2,000 mg/kg bw	GLP, Klimisch level 1	(Reijnders *et al*., 1987b) SIDS Dossier

Study Type	Species	Endpoint/ Methodology	Exposure	Result	Study Quality (GLP, Klimisch Criteria	Reference
Skin Irritation	Rabbit	OECD Guideline 404	0.5 ml for 4 hours under semi-occlusive dressing	Moderately irritating The primary skin irritation index amounted to 4.0. Based on these results and the clinical judgement, the test substance should be considered as moderately irritating to skin (EC classification: irritant)	GLP, Klimisch level 1	(Weterings *et al.*, 1987a) SIDS Dossier
	Rabbit	OECD Guideline 404	0.5 ml of each of three solutions (25%, 50%, 75% w/w water) for 4 hours under semi-occlusive dressing	In all cases skin irritation disappeared within 7 days. The primary skin irritation indices amounted to 0, 0.8, and 2.5 for the 25%, 50% and 75% dilutions	GLP, Klimisch level 1	(Weterings *et al.*, 1987b) SIDS Dossier
Eye irritation	Rabbit	OECD Guideline 405	0.1 ml of neat test substance	Based on the estimated Draize score of 34 (1hour) the test substance should be classified as moderately irritating according to the scheme of Kay and Calandra (EC classification: Eye irritant)	GLP, Klimisch level 1	(Weterings *et al.*, 1987b) SIDS Dossier
Skin sensitisation	Guinea pig	OECD Guideline 406 (Buehler test)	0.3 ml PnB in propylene glycol applied on a patch once a week for three weeks; after induction animals were left untreated for 2 weeks before primary challenge with 40% solution of PnB	Negative	GLP, Klimisch level 1	(Vanderkom *et al.*, 1987) SIDS Dossier

Study Type	Species	Endpoint/ Methodology	Exposure	Result	Study Quality (GLP, Klimisch Criteria	Reference
Repeated Dose Mammalian Toxicity						
Oral	Rat	Subchronic toxicity OECD Guideline 408	13 week exposure 0, 100, 350, 1,000 mg/kg bw/d in drinking water	NOAEL = 350 mg/kg bw/d LOAEL = 1,000 mg/kg bw/d The primary effects of PnB administration were at 1,000 mg/kg bw/d in both males and females. Absolute and relative liver weights were higher in males and absolute and relative kidney weights were higher in females given 1,000 mg/kg bw/d. Minor alterations in clinical chemistries, electrolytes, haematology, and urinalysis were also noted. No gross or histopathological alterations were associated with PnB administration. No effects attributable to test material administration were evident in male and female rats administered 100 or 350 mg/kg bw.	GLP, Klimisch level 1	(Granjean *et al*., 1992) SIDS Dossier
Inhalation	Rat	Repeated inhalation toxicity	31 day exposure to 600 ppm 7 hours/day, 5 days/week	NOAEL = 600 ppm	ND	(Pozzani and Carpenter, 1965) SIDS Dossier

Study Type	Species	Endpoint/ Methodology	Exposure	Result	Study Quality (GLP, Klimisch Criteria	Reference
Dermal	Rat	Subchronic dermal toxicity OECD Guideline 411	13 week exposure once daily (5 days/week) to 0, 88, 264, 880 mg/kg bw/d	NOAEL = 880 mg/kg bw/d Skin reactions at the application site, consisting of erythema, oedema, scaliness, small wounds, incrustations and/or occasionally superficial scar tissue were observed in all groups. No substance-related clinical signs were observed. No compound related changes were observed in the ophthalmologic examination, in body weights, food intake, food gross and microscopic examination.	GLP, Klimisch level 1	(Jonker *et al*., 1988) SIDS Dossier
Reproductive toxicity (repeated dose toxicity studies only)	Rat	90 day drinking water	0, 100, 350, 1,000 mg/kg bw/d	No effects on reproductive organs NOAEL > 1,000 mg/kg bw/d	GLP, Klimisch level 1	(Granjean *et al*., 1992) SIDS Dossier
	Rat	90 day dermal	0, 88, 264, 880 mg/kg bw/d	No effects on reproductive organs NOAEL > 880 mg/kg bw/d	GLP, Klimisch level 1	(Jonker *et al*., 1988) SIDS Dossier
	Rabbit	90 day dermal	0, 10, 100, 1,000 mg/kg bw/d	No effects on reproductive organs NOAEL > 1,000 mg/kg bw/d		(Hazleton Labs, 1987) SIDS Dossier

Study Type	Species	Endpoint/ Methodology	Exposure	Result	Study Quality (GLP, Klimisch Criteria	Reference
Developmental toxicity/terato-genicity	Rat	OECD Guideline 414	Dermal exposure to 0, 264, 880 mg/kg bw/d during days 6 – 16 of gestation	No maternal toxicity at any dose level $NOAEL_{mat}$ > 880 mg/kg bw/d No effects in offspring at any dose level $NOAEL_{dev}$ > 880 mg/kg bw/d Dermal exposures up to 880 mg/kg bw/d did not induce embryo/fetotoxicity or teratogenic effects. No deaths and no abnormalities in condition and behaviour	GLP, Klimisch level 1	(Waalkens-Berendsen *et al.*, 1989) SIDS Dossier
Developmental toxicity/terato-genicity	Rabbit	OECD Guideline 414	Dermal exposure to 0, 10, 40, 100 mg/kg bw/d during days 7 – 18 of gestation	No maternal toxicity at any dose level $NOAEL_{mat}$ > 100 mg/kg bw/d No effects in offspring at any dose level $NOAEL_{dev}$ > 100 mg/kg bw/d There were no statistically significant differences between test and control groups for maternal body weight gain, food consumption, number of corpora lutea per ovary implantations, live foetuses, early and late resorptions, foetal body weights, gender, or gross external changes. No signs of maternal toxicity were observed; however, mild erythema occurred at the site of application at the 100 mg/kg bw/d dose level.	GLP, Klimisch level 1	(Gibson *et al.*, 1989) SIDS Dossier

Study Type	Species	Endpoint/ Methodology	Exposure	Result	Study Quality (GLP, Klimisch Criteria	Reference
In vitro genotoxicity	Ames test	OECD guideline 471 TA98, TA 100, TA 1535, TA 1537	5, 15.8, 50, 158, 500, 1,580, 5,000 µg/plate	Negative with and without metabolic activation	Klimisch level 1	(Bruce *et al*., 1987) SIDS Dossier
	Chromosomal aberration assay	OECD Guideline 473	500, 1,667, 5,000 µg/mL	Negative with and without metabolic activation	GLP, Klimisch level 1	(Bhaskar Gollapudi *et al*., 1988) SIDS Dossier
	Mouse Lymphoma	N/a	N/a	Negative with and without metabolic activation	Klimisch level 1	(Kirby *et al*., 1987) SIDS Dossier
	Unscheduled DNA Synthesis	N/a	N/a	Negative with and without metabolic activation	Klimisch level 1	(Thilagar *et al*., 1987) SIDS Dossier

Annex 4. PEC_{HERA}/PNEC Ratios for the Different Environmental Compartments

Compartment	PEC_{HERA}	PNEC	Ratio (RCR)	Comment
Local freshwater water	0.0039 mg/L	0.56 mg/L	0.007	To simulate a worst case scenario the local PEC_{HERA} for surface waters calculated using EUSES was divided by the $PNEC_{aquatic}$. The resulting ratio is well below 1 and therefore the use of PnB in household applications poses no concern in surface waters. However, it should be noted that it is possible that other sources of PnB could contribute to surface water load that where not considered here, especially considering that PnB has been determined as stable in neutral waters.
WWTP	0.029 mg/L	10.0 mg/L	0.029	The PEC in the influent to the sewage treatment is much lower than the $PNEC_{microorganism}$ and therefore the risk for sewage treatment organisms from PnB is of no concern.
Sediment	0.00396 mg/kg WW	0.57 mg/kg WW	0.0069	The RCR for this compartment is very low and well below 1.
Soil	0.002 mg/kg WW	0.17 mg/kg WW	0.011	The soil compartment is adequately protected considering the very low RCR.

Annex 5. Consumer Exposure Assessment

Product types and concentrations

In line with the objectives of the HERA initiative, this human exposure assessment will focus on the use of PnB in household cleaning products. Within this context, PnB is exclusively used in hard surface cleaners at levels from 0 to 6.7%. In spray cleaners and surface wipes PnB is typically used at concentrations from 0.5 to 2.5% and at maximum at 4%.

Consumer contact scenarios

For the use of PnB the following consumer exposure scenarios have been identified and assessed:

1. Direct skin contact with diluted consumer product during hard surface cleaning.
2. Inhalation of aerosols generated by spray cleaners.
3. Accidental or intentional overexposure.

Consumer exposure estimates

There is a consolidated overview concerning habits and practices of use of detergents and surface cleaners in Western Europe which has been tabulated and issued by the European Soap and Detergent Industry Association, AISE (AISE, 2002). This table reflects consumers' use of detergents in g/task, tasks/week, duration of task and other uses of products and has been largely the basis for the exposure estimates in the following paragraphs. In some instances (*e.g.*, habits & practices (H&P) of pre-treatment of laundry), additional H&P information for a targeted exposure assessment has been directly provided by the member companies of AISE. The calculations of the estimated consumer exposures have been based on the highest relevant concentrations that consumers can be exposed to.

Direct skin contact from surface cleaners

During this task, the PnB containing hard surface cleaning solution comes into direct contact with the skin of the hands. The dermal systemic exposure (Exp_{sys}) to PnB via hard surface cleaner applications can be estimated according to the following algorithm:

$$\mathbf{Exp_{sys} = F_1 \times C \times S_{der} \times T_{der} \times t_F \times n / BW} \qquad \mathbf{(1)}$$

The terms have been defined with following values for the calculation of a worst case exposure estimate:

F_1	weight fraction of substance in product	***6.7%*** (Liquid)
C	product concentration	***22 mg/cm^3*** (AISE, 2002)
S_{der}	surface area of exposed skin	***840 cm^2*** (TGD, 2003)
T_{der}	thickness of product layer in contact with skin	***0.01 cm*** (TGD, 2003)
t_F	daily exposure fraction	***0.014*** (equals daily exposure of 20 min; AISE 2002)
n	product use frequency (tasks per day)	***1*** (AISE, 2002)
BW	body weight	***60 kg*** (TGD, 2003)

$$\mathbf{Exp_{sys}} = [0.067 \times (22\ mg/cm^3) \times (840\ cm^2) \times 0.01cm \times 1 \times 0.014]/\ 60\ kg$$
$$= \mathbf{2.9\ \mu g/kg\ bw/day}$$

This exposure calculation can be considered as conservative as the percentage of PnB has been based on a concentrated formulation which has been diluted to the same extent as a regular liquid. Moreover, in the absence of human dermal absorption data, the exposure calculation assumes a daily absorption of 100%. Considering that a surface cleaning task takes at maximum 20 minutes, the total absorption of PnB in contact with skin is 1.4%.

Inhalation of aerosols from cleaning sprays

PnB has also been present in surface cleaning sprays. The HERA guidance document specifies the algorithm to be used for calculation of consumers' worst-case exposure to PnB containing aerosols generated by the spray cleaner:

$$\mathbf{Exp_{sys} = F_1 \times C` \times Q_{inh} \times t \times n \times F_7 \times F_8 / BW}$$

The terms used in this algorithm are defined as follows:

F_1	percentage weight fraction of substance in product	***4 %*** (Table 1; Cleaning spray)
C`	product concentration in air:	***0.35 mg/m³*** * (Procter and Gamble, 1996)
Q_{inh}	ventilation rate	***0.8 m³/h*** (TGD, 2003)
t	duration of exposure	***10 min*** (AISE, 2002)
n	product use frequency (tasks per day)	***1*** (AISE, 2002)
F_7	weight fraction of respirable particles	***100 %*** (worst case)
F_8	weight fraction absorbed or bioavailable	***75 %*** (TGD, 2003)
BW	body weight	***60 kg*** (TGD, 2003)

* this value has been obtained by experimental measurements of the concentration of aerosol particles smaller than 6.4 microns in size which have been generated upon spraying with typical surface cleaning spray products

$Exp_{(inhalation)}$ = [0.04 x (0.35 mg/m³) x (0.8 m³/h) x (0.17 h) x 1 x 1 x 0.75] / 60 kg
= **0.0238 µg/kg bw/day**

Accidental or intentional overexposure

Accidental or intentional over-exposure to PnB may occur via swallowing of hard surface cleaners. Typically, one would estimate that no more than 20 ml of hard surface cleaner (equals a maximum of 1.3 g of PnB) would be swallowed. Studies of acute oral toxicity in animals demonstrate that the toxic dose of PnB is higher than this, even for a toddler.

This assessment is confirmed by the absence of any reports on fatal accidents. For example, the German Federal Institute for Health Protection of Consumers and Veterinary Medicine (BgVV, 1999) published a report on products involved in poisoning cases. No fatal case of poisoning with household cleaning products has been reported. These products are not mentioned as dangerous products with a high incidence of poisoning.

Accidental contact with the eyes can be possible by splashes of hard surface cleaners. Also, spillage of undiluted cleaning products may lead to inadvertent skin contact. Therefore, the skin and eye irritation potential has to be considered when assessing the risks of accidental exposures.

Equally, in the UK, the Department of Trade and Industry (DTI) produced an annual report of the home accident surveillance system (HASS). The data in this report summarized the information recorded at accident and emergency (A&E) units at a sample of hospitals across the UK. It also includes death statistics produced by the Office for National Statistics for England and Wales. The figures for 1998 show that for the representative sample of hospitals surveyed, there were 33 reported accidents involving detergent washing powder (the national estimate being 644) with none of

these resulting in fatalities (DTI, 1998). In 1996 and 1997, despite their being 43 and 50 reported cases, respectively, no fatalities has been reported either.

Total Consumer Exposure

In the unlikely event of maximum worst case exposure from all sources, the total exposure to PnB from its use in cleaning products would be 2.92 µg/kg bw/day.

Annex 6. Calculation of the Margin of Exposure

The margin of exposure (MOE) is the ratio of the no observed adverse effect level (NOAEL) or an appropriate substitute (*e.g.*, NOEL) to the estimated or actual level of human exposure to a substance. In context of the OECD review of PnB, NOAELs have been discussed for chronic, reproductive and developmental toxicity. The NOAEL for oral exposure to PnB has been established at 350 mg/kg bw/d and that for dermal exposure at 880 mg/kg bw/d. It is most appropriate to compare the dermal exposure to PnB of 2.9 µg/kg bw/d to the NOAEL that has been derived from dermal toxicity studies (*i.e.*, 880 mg/kg/d). For assessing the inhalatory exposure to PnB (via its presence in spray cleaners), the exposure is compared to a systemic NOAEL of 315 mg/kg bw/d. This systemic NOAEL assumes that about 90% of an orally applied dose of PnB is systemically available and takes account of pharmacokinetic data reported in the SIAR for PnB (OECD, 2003).

Exposure scenario: direct skin contact from hard surface cleaning

The MOE has been calculated by dividing the NOAEL of 880 mg/kg bw/day by the estimated exposure from hard surface cleaning of 2.9 µg/kg bw/day.

$$\mathbf{MOE_{direct\ skin\ hard\ surface\ cleaning}} = 880{,}000/2.9\ [\mu g/kg\ bw/day] = \mathbf{303{,}448}$$

Exposure scenario: inhalation of aerosols from cleaning sprays

For calculation of the MOE, the NOAEL of 315 mg/kg bw/day has been divided by the daily systemic dose of 0.0238 µg/kg bw/d, which has been estimated for the inhalation of PnB containing aerosols in spray cleaning applications. This exposure results in a very large MOE (>> 1,000,000) and does not significantly add to the overall exposure. It will therefore not be considered in the risk assessment

Exposure scenario: oral route from accidental ingestion and eye contact

Accidental ingestion of a few milligrams of PnB as a consequence of accidental ingestion of cleaning products is not expected to result in any significant adverse health effects given the low toxicity profile of cleaning products in general, and PnB in particular. This view is supported not only by available toxicological information from animal studies, but also by the fact that national poison control centres have not reported a case of lethal poisoning or severe health effects with cleaning products containing PnB.

Accidental eye contact with undiluted cleaning products can be expected to cause mild to moderate irritation which is fully reversible shortly after the accidental exposure. Considering the generally low levels of PnB in cleaning products, this response can, however, only to a minor extent be related to PnB. Nevertheless, in the case of accidental eye contact, immediate rinsing with plenty of water has been recommended. This immediate action has been shown in animal experiments to minimize irritation effects.

Total Consumer Exposure

In a worst case scenario, the consumer exposure from direct skin contact of PnB containing cleaning products, and inhalation of PnB containing aerosols from spray cleaner applications, results in an estimated systemic PnB exposure of 2.93 µg/kg bw/day. The MOE can be calculated by dividing the NOAEL of 880,000 µg/kg bw/day by the total exposure. This takes account that the PnB exposure via the use of hard surface cleaners predominantly occurs via the dermal route (*i.e.*, more than 99%). Hence, it is most appropriate to compare the aggregate exposure to PnB of 2.93 µg/kg bw/d to the NOAEL that has been derived from dermal toxicity studies (*i.e.*, 880 mg/kg/d):

$$\mathbf{MOE_{total}} = 880{,}000/2.93\ [\mu g/kg\ bw/day] = \mathbf{300{,}341}$$

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