

Category D 'C4, high 1,3-butadiene (>0.1%)' - Chemical Category Justification

(NB : all compositions are in w/w for liquids and v/v for gases)

Category definition and its members		
1.1.	Category Definition	
1.1.a.	Category Hypothesis	
<p>The 'C4, high 1,3-butadiene (>0.1%)' category covers hydrocarbon streams containing high purity hydrocarbons, hydrocarbon substances with impurities and complex hydrocarbon reaction products. These hydrocarbon streams have a carbon number distribution that is predominantly C4 but with a range of C3-C5 and more than 0.1% 1,3-butadiene. Category members are typically produced from the steam-cracking of naphtha as a C4-rich stream. Companies importing streams will need to confirm that such streams meet the chemical description and are in domain. The category contains streams that have claimed compositions of single substances up to over 80%. These are not considered as pure substances as the variability during manufacture is such that this is not always the case and usually the production processes are not designed to make substances at such a high purity.</p> <p>It is reasonable to assume that the phys-chem and environmental fate properties of the category members will be very similar due to the small spread of carbon numbers. The streams will have similar environmental effects as their constituents cover a narrow carbon range and all act in similar manner, via narcosis. With regard to mammalian endpoints, category members are very volatile low boiling liquids, liquefied gases or gases with inhalation representing the primary route of exposure. CNS depression (marker substance: butenes) "and irreversible effects (marker substance: 1,3-butadiene) are likely to drive health hazard assessment. It can therefore be assumed that streams meeting the applicability domain will behave in a similar manner and therefore the use of read-across is valid.</p> <p>For mammalian endpoints, the classification of these streams will be driven by the content of 1,3-butadiene as this is more than 0.1% w/w (or v/v for gases) for all category members.</p>		
1.1.b.	Applicability domain (AD) of the category	
<p>The category applies to streams with essentially the following PIONA* analysis: 100% (iso)paraffins and olefins with more than 0.1% 1,3-butadiene and a predominant carbon number distribution of 3 – 5.</p> <p><i>Boiling Point</i> – the streams in this category will boil predominantly in the range of -15 - +15°C</p> <p>Specific components (The range entered below is that currently based on received analytical data, it is not intended to be prescriptive. See section 1.3).</p> <p><i>1,3-butadiene: 0.1 – over 80%</i></p> <p>PIONA* :</p> <p>(Iso)Paraffins – up to 70% : C# 3 - 5</p> <p>Olefins – up to 99% : C# 3 - 5</p> <p>Naphthenics – typically <1%</p> <p>Aromatics – typically <1%</p> <p><i>*: PIONA refers to a description of the type of hydrocarbons present, paraffins, isoparaffins, olefins, naphthenics and aromatics. It does not refer to a specific type of analysis or determination.</i></p>		
1.2.	Category Members	
CAS Number	CAS Description	Registered Substance Name

68476-52-8	Hydrocarbons, C4, ethylene-manuf.-by-product	Hydrocarbons, C4, ethylene-manuf.-by-product
		Crude C4s (steam cracked)
		Hydrocarbons, C4, ethylene-manuf.-by-product. A complex combination of hydrocarbons produced by distillation of products from a cracking process in an ethylene plant. It consists predominantly of C4 hydrocarbons.
		C4 Mixture
68477-42-9	Gases (petroleum), extractive, C3-5, butene-isobutylene-rich	Raffinate 1, (iso) butylenes
		Gases (petroleum), extractive, C3-5, butene-isobutylene-rich
68955-28-2	Gases (petroleum), light steam-cracked, butadiene conc.	Gases (petroleum), light steam-cracked, butadiene conc.
		Gases (petroleum), light steam-cracked, butadiene conc. A complex combination of hydrocarbons produced by the distillation of products from a thermal cracking process. It consists of hydrocarbons having a carbon number predominantly of C4.
		Gases (petroleum) light steam-cracked. Butadiene conc. (C 4 Fraction)
87741-01-3	Hydrocarbons, C-4	Hydrocarbons, C4
92045-23-3	Hydrocarbons, C4, steam-cracker distillate	Hydrocarbons, C4, steam-cracker distillates
		C4 Steam cracker distillate
		Raffinate 1 C4
		Hydrocarbons, C4 steam-cracker distillate. Butenes (Raffinate-I)
1.3.	Purity / Impurities	
<p>The substances in this category are UVCBs and as such are considered to be 100% pure. The term impurity is not relevant for UVCBs, however, substances will be described using the following:</p> <ul style="list-style-type: none"> ○ <u>Known</u> constituents present at 10% or greater (if any), identified by IUPAC name and EC number/CAS number, indicating typical concentrations and/or concentration ranges; ○ Constituents relevant for hazard classification (if any); ○ Constituents relevant for PBT assessment (if any). <p>Primary marker</p> <p><u>1,3-Butadiene</u> (CAS# 106-99-0): tox classification: Carc Cat 1 R45, Mut Cat 2 R46</p> <p>Tox statements:</p> <p><u>1,3-Butadiene</u> is regulated in the EU as a germ cell mutagen and a non-threshold carcinogen. Humans occupationally exposed to 1,3-butadiene are at increased risk of developing lymphohaematopoietic cancer (leukemia).</p>		
2.	Category justification	

The '**C4, high 1,3-butadiene (>0.1%)**' category covers hydrocarbon streams containing high purity hydrocarbons, hydrocarbon substances with impurities and complex hydrocarbon reaction products. These hydrocarbon streams have a carbon number distribution that is predominantly C4 but with a range of C3-C5 and more than 0.1% 1,3-butadiene. Category members are typically produced from the steam-cracking of naphtha as a C4-rich stream. The physico-chemical properties associated with these types of UVCBs indicated that they comprise a category based on the range of boiling points (from -15°C to +15°C) and will have similar behaviour in the environment. The log Kow ranges from 2.09-2.31 and the streams in this category are not considered to be readily biodegradable. The mammalian toxicity information and environmental assessment also indicated that the streams in this category exert similar effects.

3. Data matrix

'**C4, high 1,3-butadiene (>0.1%)**' is a UCVB category and therefore identification of trends between category members is not appropriate and therefore, according to the ECHA Guidance on information requirements and chemical assessment Chapter R.6, it is not feasible to establish a full data matrix for this category. Consequently, a data set that applies to all members of this category has been developed.

4. Conclusions per endpoint for C&L, PBT/vPvB and dose descriptor

CLASSIFICATION AND LABELLING

Physico-chemical Hazard Assessment

- **Boiling point** - The boiling point of streams in this category was not required as they are all gases at room temperature.
- **Partition coefficient** - The streams in this category have partition coefficients ranges from log Kow 2.09-2.31.
- **Flash point** - The flash point of streams in this category is <-30.0°C to -18°C.

Flam. Gas 1 (Hazard statement: H220: Extremely flammable gas.)

Human Health Hazard Assessment

- **Toxicokinetics** – The component substances, have well-defined toxicokinetic parameters that have been taken into account during the derivation of the DN(M)ELs for this category. The overall DN(M)EL of this category is driven by the DMEL for 1,3-butadiene.
- **Acute toxicity** – Category members have low acute inhalational toxicity with LC50 values in excess of 10,000 ppm (22,948 mg/m³). Oral and dermal exposures are not relevant as category members are gases at room temperature.
- **Irritation** – Category members are not irritating. They may cause burns and frostbite due to the extreme cold of the liquid gases.
- **Sensitisation** – There are no indications that category members are sensitizers.
- **Repeat dose toxicity** – Category members have low sub-chronic inhalational toxicity. Nasal lesions were observed in 2 year studies on the component substance 2-methylpropene in rats (NOAEC 2000 ppm; 4589 mg/m³). The component substance 1,3-butadiene defines the repeat dose toxicity of the category. 1,3-Butadiene had low toxicity in rats (the most appropriate test species). The mouse was the most sensitive species where the target organs are bone marrow, ovary and testis. Species differences in metabolism are believed to be responsible for the species specific toxicity with humans being more similar to rats The NOAEL of 1000 ppm

(2212 mg/m³) was identified from the key study on 1,3-butadiene in rats.

- **Genetic toxicity** – All category members are contain at least 0.1% w/w 1,3-butadiene and this substance drives the mutagenicity classification for this category. 1,3-Butadiene is genotoxic in vitro and in vivo in both somatic and germ cells in the mouse but is not genotoxic in vivo in both somatic and germ cells in the rat. The available data on several groups of 1,3-butadiene-exposed workers did not show any association between 1,3-butadiene exposure and increased gene mutations. The results of genotoxicity studies on category members reflect the proportion of 1,3-butadiene in the stream at the time of testing. Negative, positive and weakly positive results were variously obtained.. The presence of 1,3-butadiene therefore indicates that members of this category are assumed to be mutagenic
- **Carcinogenicity** – All category members are contain at least 0.1% w/w 1,3-butadiene and this substance drives the carcinogenicity classification for this category. Humans occupationally exposed to 1,3-butadiene are at increased risk of developing lymphohaematopoietic cancer (leukemia). Various models have established a dose response-relationship for cumulative exposure to 1,3-butadiene, especially concentrations above 100 ppm. The available data therefore indicates that members of this category may be carcinogenic in humans.
- **Toxic to reproduction** – Category members have low reproductive toxicity, no significant treatment-related effects on reproduction or fertility occurred (NOAEC 3000 ppm, 7131 mg/m³) The potential for developmental toxicity is also low but the component substance 1,3-butadiene caused developmental toxicity in rats and mice, in the presence of maternal toxicity. The NOAEC for developmental toxicity is 40 ppm (88 mg/m³), based on the key study in mice.

Environmental Hazard Assessment

- **Biodegradation** - Based on two experimental studies the streams in this category have not been shown to be readily biodegradable and will not be considered readily biodegradable.
- **Bioaccumulation** - Log Kow values (log Kow = 2.09-2.31) indicate that streams in this category will have very low bioaccumulative potential.
- **Ecotoxicity** - The members of the category, 68955-28-2, 87741-01-3 and 92045-23-3 are listed in Annex I but are not classified for environmental hazards. Additionally the major constituent component- 1,3-butadiene is also listed but not classified for environmental hazards.

Based on the results of the hazard assessment the streams in this category are not classified.

CONCLUSION FOR PBT

The screening assessment of the available data indicates that the properties of the members of this category do not meet the specific criteria detailed in Annex XIII or do not allow a direct comparison with all the criteria in Annex XIII but nevertheless indicate that the substance would not have these properties and therefore are not considered PBT/vPvB.

CONCLUSION FOR DOSE DESCRIPTOR

Environment: Deriving PNECs for UVCB substances based on WAF information is inappropriate. As the substance is a hydrocarbon UVCB the hydrocarbon block method has been used for environmental risk assessment (see REACH guidance, R7, app.13-1). The Petrorisk model (Redman, A. (2010). PETRORISK Users Guide, HydroQual, Inc., for Conservation of Clean Air and Water in Europe (CONCAWE)), was used for the environmental assessment. Blocks of C3-C5 carbon atoms and with a boiling point range of 34.5 °C to 100.6 °C were used in the modelling exercise. The model assigns

individual structures from the library to the hydrocarbon blocks that the user enters. The input parameters are provided in Appendix B of the CSR. Details of the library structure mapping, some relevant physico-chemical properties and the mass fraction that is assigned to each chemical are also found in this appendix.

Human Health:

Risk characterization is based on the premise that a marker substance with a low DN(M)EL present at high concentration in a stream will possess a greater relative hazard potential than a marker substance with a higher DN(M)EL present at the same or lower concentration. It will also focus on the potential of the markers to cause serious long-term health effects rather than on short-term or irritation-related changes.

In the case of this stream, the hazardous marker substances present are ranked as follows:

Marker substance	Indicative concentration (%)	Inhalation	
		DN(M)EL mg/m ³	Relative hazard potential (max % ÷ DN(M)EL)
1,3-butadiene	0.1 to over 80%	2.21	36.2
Butene isomers	up to 99%	769	0.13

Based on this analysis, demonstration of “safe use” for hazards associated with the presence of 80% 1,3-butadiene will also provide adequate protection against hazards arising from butenes that are also present.

The long-term inhalation DMELs for 1,3-butadiene will therefore be used for worker risk characterization.