LOA Category G 'Fuel oils' - 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**

The **'fuel oils'** category covers hydrocarbon streams typically produced by the distillation of products from a steam cracking process, by the distillation of products from an ethylene manufacturing process, obtained as the residual fraction from the distillation of the products of a steam cracking process, or produced by pyrolysis. Imported streams will need to confirm that they meet the chemical description and are in domain. Category members contain predominantly higher-boiling hydrocarbons, mostly cyclic olefins and aromatics, but at varying concentrations. These hydrocarbon streams have a carbon number distribution that is predominantly C8 and higher. Companies importing streams will need to confirm that such streams meet the chemical description and are in domain.

By definition, from the category, these streams have overlapping hydrocarbon compositions, within a defined range, and hence, will have similar properties. It is therefore reasonable to assume that the components of fuel oils will behave in a reasonably predictable manner, and with respect to phys-chem and environmental fate and effect properties read-across is valid.

With regard to mammalian endpoints, category members are viscous liquids with skin the primary route of exposure. The short term toxicity is driven by skin contact and potential irritation. The longer term health effects will be driven by inhalation as a route of exposure and effects and the classification of these streams will be driven by the content of benzene (when present at more than 0.1%) and toluene (when present at more than 5%) while their boiling range (130-400°C) indicates the probable presence of 3-7 ring PAH and supports overall classification Carc Cat 2/R45. Naphthalene (and other PAHs/PNAs) is regulated as a Category 3 carcinogen in the EU and is harmful by ingestion.

1.1.b.	**Applicability domain (AD) of the category**

The category applies to streams with the following PIONA* analysis: predominantly olefins, naphthenics and aromatics, and with a carbon number distribution predominantly C8 and higher.

Boiling Point –the streams in this category will boil predominantly in the range of 130 - 500ºC

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).

Benzene: up to 30%

Toluene: up to 20%

Ethylbenzene: up to 10%

Styrene: up to 15%

Naphthalene/Methyl-naphthalene: up to 60%

Biphenyl: up to 15%

Anthracene – up to 5% (streams with this component at >0.1% are candidates for authorisation as anthracene is a confirmed PBT)

PIONA* :

(iso)Paraffins – up to 20% : C# starting at 8

Olefins – up to 35% : C# starting at 8

Naphthenics – up to 85% : C# starting at 8

Aromatics – up to 100% : C# starting at 6

**: 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.*

1.2. Category Members

CAS Number	CAS Description	Registered Substance Name
101631-14-5	Distillates (petroleum), heavy steam-cracked	Quench oil
64742-90-1	Residues (petroleum), steam-cracked	Heavy Fuel oil (CBFS)
		residues (petroleum), steam-cracked
		Steam-cracked residue
		SC Tar
		Residues (petroleum) steam-cracked
		Residues (petroleum) steam-cracked (Pyrolysis Fuel Oil)
		ECR - Ethylene Cracker residue
64742-94-5	Solvent naphtha (petroleum), heavy arom.	Solvent naphtha (petroleum), heavy arom.
68475-80-9	Distillates (petroleum), light steam-cracked naphtha	Distillates (petroleum), light steam-cracked naphtha
68477-38-3	Distillates (petroleum), cracked steam-cracked petroleum distillates	Distillates (petroleum), cracked steam-cracked petroleum distillates
		Cracked Gasoil (chemcracker)
68513-69-9	Residues (petroleum), steam-cracked light	Residues, petroleum, steam-cracked light
68527-18-4	Gas oils (petroleum), steam-cracked	Gas oils (petroleum), steam-cracked
68987-42-8	Benzene, ethylenated, residues	Benzene, ethylenated, residues
69013-21-4	Fuel oil, pyrolysis	Fuel oil, pyrolysis.
85117-10-8	Naphtha, thermal cracked, residues, naphthalene cut	Naphtha, thermal cracked, residues, naphthalene cut
86290-83-7	Hydrocarbons, steam-cracking tar middle	Hydrocarbons, steam-cracking, tar middle
98072-36-7	Aromatic hydrocarbons, distn. residues, naphthalene-rich	Aromatic hydrocarbons, distn. Residues, naphthalene-rich
98219-64-8	Residues, steam cracked, thermally treated	Heavy Fuel oil (Polymer Oil)

1.3. Purity / Impurities

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:

- Known 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).

2.	Category justification

The **'fuel oils'** category covers hydrocarbon streams typically produced by the distillation of products from a steam cracking process, by the distillation of products from an ethylene manufacturing process, obtained as the residual fraction from the distillation of the products of a steam cracking process, or produced by pyrolysis. The physico-chemical properties associated with these types of UVCBs indicated that they comprise a category based on the range of boiling points (from 130°C to 500°C) and will have similar behaviour in the environment. The log Kow ranges from >3 to <6.5 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

'Fuel oils' 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 measured boiling point of streams in this category ranged from 114°C to 390°C (agreed category boiling point range of 130°C to 500°C).

- **Partition coefficient** - The streams in this category have partition coefficients ranges from log Kow >3.0 to <6.5.

- **Flash point** - The flash point of streams in this category is 57°C to 80°C. Some streams will have the following classification.

  Flashpoint of ≥ 23 °C and initial boiling point ≤ 60 °C.

  Flam. Liquid 3 (Hazard statement: H226: Flammable liquid and vapour.

Human Health Hazard Assessment

- **Toxicokinetics –** Toxicokinetic behaviour of some of the stream components has been extensively studied and reported. For this 'Fuel Oils' category the marker substances (benzene, toluene, ethylbenzene, styrene, naphthalene, anthracene and biphenyl) in their pure form, have well-defined toxicokinetic parameters that have been taken into account during the derivation of their respective DNEL's. The overall DNEL of this category is driven by the DNELs for benzene and naphthalene.

- **Acute toxicity –** Available data for specific streams within this category and on marker substances indicate that acute toxicity is expected to be low. Naphthalene has been shown to be acutely toxic (producing haemolytic anaemia) in humans following oral exposure and ethylbenzene is hazardous following acute inhalation exposure. Therefore, classification will be required for streams containing a high proportion of naphthalene (≥25%) but the highest concentration of ethylbenzene (10%) is too low to trigger classification. Following acute inhalation exposures to toluene in humans a number of subjective sensations such as headache, dizziness, feeling of intoxication, irritation and

sleepiness and decreases in acute neurobehavioural performance are seen. The NOAEC for acute neurobehavioural effects in humans is 50 ppm (188 mg/m3) and classification (R67/H336) will be required for streams containing ≥20% toluene.

- **Irritation –**Fuel Oils should be considered to be skin irritants. There is some evidence of eye irritation with controlled exposures to liquid test substances although the severity varies widely. Ethylbenzene and biphenyl are also considered to be respiratory irritants. The need for labelling with respect to eye and respiratory irritation is dependent upon available data for the specific stream or the concentration of benzene, ethylbenzene or biphenyl in the stream.

- **Sensitisation –** Not sensitising.

- **Repeat dose toxicity –** There are limited repeat dose toxicity data on any of the specific streams identified for this category. However, there are substantial data on the repeated dose toxicity of a number of specific components present in some streams i.e. benzene, toluene, ethylbenzene and styrene which demonstrate significant target organ toxicity and when present at concentrations greater than or equal to 1%, 10%, 10% or 10% respectively will drive the mammalian toxicity effects.

- **Genetic toxicity –** Genotoxicity data on streams within this category are limited and variable with both positive and negative in vivo and in vitro study results. However, there are substantial data on the genotoxicity of a number of specific components present in some streams. Of these, benzene has been shown to be mutagenic and when present in streams at concentrations equal or greater than 0.1% labelling for mutagenicity will be required.

- **Carcinogenicity –** There are no robust GLP carcinogenicity data on any of the streams within this category although Pyrolysis Fuel Oil was shown to be carcinogenic following skin painting in mice. Specific components present in some streams, benzene and naphthalene, have been shown to be carcinogenic and the boiling range of Fuel Oils (130-400°C) indicates the probable presence of 3-7 ring PAH and supports overall classification as carcinogenic.

- **Toxic to reproduction –** It is recognised that there are data gaps for developmental toxicity and multi-generation studies (REACH reference 8.7.2 and 8.7.3). However, the need for reproduction toxicity studies is waived as it is proposed that Fuel Oils streams are classified as mutagenic and carcinogenic. There are limited reproduction toxicity data available for streams within this category. However, there are sufficient data on component substances to indicate that no further testing is warranted and no classification is required with respect to effects on fertility. Data on the developmental toxicity of marker substances indicate that toluene possesses specific effects which warrant labelling. Therefore classification with respect to developmental toxicity is only required for streams containing ≥5% (EU/DPD) or ≥3% (GHS/CLP) toluene.

Environmental Hazard Assessment

- **Biodegradation** - Information is available for 3 streams in this Category. Results indicated that none of the streams could be considered readily biodegradable. Biodegradation range was 7.3% (no timeframe) - 29% after 28 days.

- **Bioaccumulation** - BCF have been calculated for various representative components of these streams. The calculated values ranged from 39-18220. (USEPA 2008).

- **Ecotoxicity** – There were short term ecotoxicity studies available for five streams. Similar sensitivity was seen over the three trophic levels. Fish had LL50 range of 1.1 to 32 mg/l; Invertebrates had EL50 range of 3.3 – 13 mg/l; Algae had ErL50 range 2.3-8.95mg/l.

  Based on the available experimental data streams in this category should have the classification

R51/53 under the DSD and Aquatic Chronic 2 under the CLP regulations.

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 >C8 carbon atoms and with a boiling point range of 100°C to 307.9 °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:

Worker

Risk characterization will be 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.

The most hazardous marker substances present are highlighted in the following table (details of DN(M)EL calculations follow the table):

Marker substance	**Indicative concentration** (%)	**Inhalation**		**Dermal**	
		DN(M)EL mg/m^3	**Relative hazard potential** (max % ÷ DN(M)EL)	**DN(M)EL** mg/kg bw/d	**Relative hazard potential** (max % ÷ DN(M)EL)
benzene	Up to 30	3.25	9.23	23.4	1.28
toluene	Up to 20	192	0.10	384	0.05
ethylbenzene	Up to 10	77	0.13	180	0.06
styrene	Up to 15	85	0.18	406	0.04
naphthalene	Up to 70	50	1.4	72	0.97
anthracene	Up to 5	*low systemic toxicity, no DNELs required*			
biphenyl	Up to 15	*low systemic toxicity, no DNELs required*			

Based on this analysis, demonstration of "safe use" for hazards associated with inhalation and dermal exposure to benzene will also provide adequate protection for workers against hazards arising from other marker substances present.

General population

Marker substance	**Indicative concentration** (%)	**Inhalation**		**Dermal**		**Oral**	
		DN(M)EL mg/m^3	**Relative hazard potential** (max % ÷ DN(M)EL)	**DN(M)EL** mg/kg bw/d	**Relative hazard potential** (max % ÷ DN(M)EL)	**DN(M)EL** mg/kg bw/d	**Relative hazard potential** (max % ÷ DN(M)EL)
benzene	Up to 30	*supply of streams containing ≥0.1% benzene prohibited*					
toluene	Up to 20	56.5	0.35	226	0.09	8.13	2.46
ethylbenzene	Up to 10	14.8	0.68	108	0.09	1.60	6.25
styrene	Up to 15	10.2	1.47	343	0.04	2.1	7.1
naphthalene	Up to 70	14.7	4.8	42.4	1.6	4.23	16.5
anthracene	Up to 5	*low systemic toxicity, no DNELs required*					
biphenyl	Up to 15	*low systemic toxicity, no DNELs required*					

For the general population the long term inhalation, dermal and oral DNELs for naphthalene will be used for risk characterization.