Dispersion Modelling – Basis of EAL

Vapour Composition

Since emission limits are required for all components emitted from the White Oil Docks vent stack, it is considered that assuming the vapour released is the same composition at the liquid is overly conservative as it is unlikely that the heavier components present in the liquid will be present in the same proportion in the vapour. Therefore, more detailed simulations have been carried out to determine the actual vapour composition released from the stack when loading MoGas.

The simulation was carried out using ProII software. The simulation used the typical compositions of MoGas under review from EOUK's REACH Chemical Safety Report (this compositions was used to ensure alignment with the EA's REACH methodology for the derivation of EALs).

To calculate vapour composition, a feed stream was created with the specified composition (based on the REACH Chemical Safety Report) and a flowrate of 1000 gallons per day. This was set to be at bubble point at 20 °C. The stream was then split in an isobaric flash with a specified vapour rate in lb per day equivalent to respective loading losses (shown in the table above), which gives a vapour flow matching the loss factor. The composition of the vapour stream was then reported.

The composition of the vapour is shown below:

REACH Constituent	Pro2 Representative Component	MOGAS_VAP
butane	n-butane	11.66
pentane	n-pentane	8.42
n-hexane	n-hexane	1.61
heptane	n-heptane	0.25
octane	n-octane	0.02
nonane	n-nonane	2.44E-03
decane	n-decane	8.06E-04
undecane	n-undecane	0
isobutane	isobutane	15.86
2-methylbutane	isopentane	19.28
Alkanes, C6, Branched	2-methylpentane	6.89
Alkanes, C7, Branched	2-methylhexane	1.61
Alkanes, C8, Branched	2-methylheptane	1.14
Alkanes, C9, Branched	2-methyloctane	0.02
Alkanes, C10, Branched	2-methylnonane	1.26E-03
Alkanes, C11, Branched	no iso C11 in ProII - iC11 added to nC1	
Alkanes, C12, Branched	2,2,4,6,6-pentamethylheptane	0.01
Alkenes, C4, Linear, Branched and Cyclic	1-butene	11.04
Alkenes, C5, Linear, Branched and Cyclic	1-pentene	14.53
Alkenes, C6, Linear, Branched and Cyclic	1-hexene	3.11
Alkenes, C7, Linear, Branched and Cyclic	1-heptene	0.65
Alkenes, C8, Linear, Branched and Cyclic	1-octene	0.07
cyclopentane	cyclopentane	0.32
Cycloalkanes, C6	cyclohexane	0.64
Cycloalkanes, C7	cycloheptane	0.19
Cycloalkanes, C8	cyclooctane	0.02
Cycloalkanes, C9	cyclononane	4.77E-04
Cycloalkanes, C10	cyclodecane	0
Cycloalkanes, C11	hexylcyclopentane	0
Cycloalkanes, C12	heptylcyclopentane	8.37E-05
C6 aromatics	benzene	0.44
C7 aromatics	toluene	1.40
Hydrocarbons, C8, Aromatic	ethylbenzene	0.67
Hydrocarbons, C9, Aromatic	cumene	0.15
Hydrocarbons, C10, Aromatic	naphthalene	1.48E-03
Hydrocarbons, C12, Aromatic	1-ethylnaphthalene	1.52E-04

EALs

The following table shows the vapour compositions for each of the substances from ProII. This table also shows the EALs that EOUK will use to assess the risk from all VOC emissions when loading at Tranmere. The following methodology was used:

1. Where possible, EALs were taken from the values shown in: https://www.gov.uk/guidance/air-emissions-risk-assessment-for-your-environmental-permit#environmental-standards-for-air-emissions

2. If no EALs were available, EALs were derived using Derived No-Effect Levels (DNELs), based on the REACH process described in Section 8 of: https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/914697/Derivation_of_new_EALs_to_air.pdf

    a. DNELs were taken from the toxicological data for each component from the European Chemicals Agency: https://echa.europa.eu/
    b. EOUK will adopt the DNELs as EALs.
    c. The long-term and short-term inhalation DNELs (for the general population) are assumed to be the annual and hourly EALs for that component, respectively.

3. If there was no available data from the European Chemicals Agency for DNELs for a component, then the EALs were assumed to be equivalent to that of the most similar component. The justification for each assumed value is shown in the table.

[4] Toxicological dat

REACH Constituent	Vapour Composition (wt%)		EALs [1]		Inhalation DNEL General Population [2]			Basis of EAL to be used if no data available [3]		
	Pro2 Representative Component	MOGAS_VAP	Annual	Hourly	Long-Term (annual)	Acute (hourly)	Source	Basis of EAL	Annual	Hourly
butane	n-butane	11.66	14500 µg/m3	181000 µg/m3						
pentane	n-pentane	8.42			643 mg/m3	No hazard identified [4]	https://echa.europa.eu/brief-profile/-/briefprofile/100.003.358			
n-hexane	n-hexane	1.61	720 µg/m3	21600 µg/m3						
heptane	n-heptane	0.25			447 mg/m3	No hazard identified	https://echa.europa.eu/brief-profile/-/briefprofile/100.005.058			
octane	n-octane	0.02			608 mg/m3	No hazard identified	https://echa.europa.eu/brief-profile/-/briefprofile/100.003.539			
nonane	n-nonane	2.44E-03			608 mg/m3	No hazard identified	https://echa.europa.eu/brief-profile/-/briefprofile/100.003.558			
decane	n-decane	8.06E-04			No hazard identified	No hazard identified	https://echa.europa.eu/brief-profile/-/briefprofile/100.004.262			
undecane	n-undecane	0			No hazard identified	No hazard identified	https://echa.europa.eu/brief-profile/-/briefprofile/100.013.001			
isobutane	isobutane	15.86			No Data	No Data	https://echa.europa.eu/brief-profile/-/briefprofile/100.000.780	Use butane EALs as representative - and model as butane in dispersion modelling	14500 µg/m3	181000 µg/m3
2-methylbutane	isopentane	19.28			643 mg/m3	No hazard identified	https://echa.europa.eu/brief-profile/-/briefprofile/100.001.039			
Alkanes, C6, Branched	2-methylpentane	6.89			No Data	No Data	https://echa.europa.eu/brief-profile/-/briefprofile/100.003.204	Use hexane EALs as representative - and model as hexane in dispersion modelling	720 µg/m3	21600 µg/m3
Alkanes, C7, Branched	2-methylhexane	1.61			No Data	No Data	https://echa.europa.eu/substance-information/-/substanceinfo/100.008.847	Use heptane EALs as representative - and model as heptane in dispersion modelling	447 mg/m3	No hazard identified
Alkanes, C8, Branched	2-methylheptane	1.14			No Data	No Data	https://echa.europa.eu/substance-information/-/substanceinfo/100.008.863	Use octane EALs as representative - and model as octane in dispersion modelling	608 mg/m3	No hazard identified
Alkanes, C9, Branched	2-methyloctane	0.02			No Data	No Data	https://echa.europa.eu/substance-information/-/substanceinfo/100.019.771	Use nonane EALs as representative - and model as nonane in dispersion modelling	608 mg/m3	No hazard identified
Alkanes, C10, Branched	2-methylnonane	1.26E-03			No Data	No Data	https://echa.europa.eu/substance-information/-/substanceinfo/100.011.649	Use decane EALs as representative - and model as decane in dispersion modelling	No hazard identified	No hazard identified
Alkanes, C11, Branched	no iso C11 in ProII - iC11 added to nC11									
Alkanes, C12, Branched	2,2,4,6,6-pentamethylheptane	0.01			No hazard identified	No hazard identified	https://echa.europa.eu/brief-profile/-/briefprofile/100.033.401			
Alkenes, C4, Linear, Branched and Cyclic	1-butene	11.04			229.4 mg/m3	No hazard identified	https://echa.europa.eu/brief-profile/-/briefprofile/100.003.137			
Alkenes, C5, Linear, Branched and Cyclic	1-pentene	14.53			No hazard identified	No hazard identified	https://echa.europa.eu/brief-profile/-/briefprofile/100.003.359			
Alkenes, C6, Linear, Branched and Cyclic	1-hexene	3.11			No hazard identified	No hazard identified	https://echa.europa.eu/brief-profile/-/briefprofile/100.008.868			
Alkenes, C7, Linear, Branched and Cyclic	1-heptene	0.65			No Data	No Data	https://echa.europa.eu/brief-profile/-/briefprofile/100.008.881	Use hexene EALs as representative - and model as hexene in dispersion modelling	No hazard identified	No hazard identified
Alkenes, C8, Linear, Branched and Cyclic	1-octene	0.07			No hazard identified	No hazard identified	https://echa.europa.eu/brief-profile/-/briefprofile/100.003.540			
cyclopentane	cyclopentane	0.32			643 mg/m3	No hazard identified	https://echa.europa.eu/brief-profile/-/briefprofile/100.005.470			
Cycloalkanes, C6	cyclohexane	0.64			206 mg/m3	412 mg/m3	https://echa.europa.eu/brief-profile/-/briefprofile/100.003.461			
Cycloalkanes, C7	cycloheptane	0.19			No Data	No Data	https://echa.europa.eu/substance-information/-/substanceinfo/100.005.483	Use heptane EALs as representative - and model as heptane in dispersion modelling	447 mg/m3	No hazard identified
Cycloalkanes, C8	cyclooctane	0.02			No Data	No Data	https://echa.europa.eu/substance-information/-/substanceinfo/100.005.484	Use octane EALs as representative - and model as octane in dispersion modelling	608 mg/m3	No hazard identified
Cycloalkanes, C9	cyclononane	4.77E-04			No Data	No Data	https://echa.europa.eu/substance-information/-/substanceinfo/100.063.432	Use nonane EALs as representative - and model as nonane in dispersion modelling	608 mg/m3	No hazard identified
Cycloalkanes, C10	cyclodecane	0			No Data	No Data	https://echa.europa.eu/substance-information/-/substanceinfo/100.005.485	Use decane EALs as representative - and model as decane in dispersion modelling	No hazard identified	No hazard identified
Cycloalkanes, C11	hexylcyclopentane	0			No Data	No Data	No data sheet available on echa.europa.eu	Use undecane EALs as representative - and model as undecane in dispersion modelling	No hazard identified	No hazard identified
Cycloalkanes, C12	heptylcyclopentane	8.37E-05			No Data	No Data	No data sheet available on echa.europa.eu	Use undecane EALs as representative - and model as undecane in dispersion modelling	No hazard identified	No hazard identified
C6 aromatics	benzene	0.44	5 µg/m3	30 µg/m3 (24 hour average)						
C7 aromatics	toluene	1.40	1910 µg/m3	8000 µg/m3						
Hydrocarbons, C8, Aromatic	ethylbenzene	0.67	4410 µg/m3	55200 µg/m3						
Hydrocarbons, C9, Aromatic	cumene	0.15			16.6 mg/m3	No hazard identified	https://echa.europa.eu/brief-profile/-/briefprofile/100.002.458			
Hydrocarbons, C10, Aromatic	naphthalene	1.48E-03	No limit	3 µg/m3 (24 hour average)						
Hydrocarbons, C12, Aromatic	1-ethylnaphthalene	1.52E-04			No Data	No Data	https://echa.europa.eu/substance-information/-/substanceinfo/100.013.121	Use C10 aromatics DNELs https://echa.europa.eu/brief-profile/-/briefprofile/100.122.986	32 mg/m3	No hazard identified

[1] EALs from https://www.gov.uk/guidance/air-emissions-risk-assessment-for-your-environmental-permit#environmental-standards-for-air-emissions
[2] DNELs from https://echa.europa.eu/
[3] No available data from the European Chemicals Agency for DNELs
[4] See example on next page

echa.europa.eu/brief-profile/-/briefprofile/100.003.358

Pentane

Substance description | Scientific properties

Brief Profile - Last updated: 14/10/2021 Print

Toxicological information

This section provides toxicological information compiled from all automatically processable data from REACH registration dossiers that is available to ECHA at the time of generation. The quality and correctness of the information remains the responsibility of the data submitter. The Agency thus cannot guarantee the correctness of the information displayed.

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Derived No- or Minimal Effect Level (DN(M)EL)

M/C **Summaries**

1 summary submitted
1 summary processed

The derived no- or minimum effect level (DN(M)EL) is the level of exposure above which a human should not be exposed to a substance. Please note that when more than one summary is provided, DN(M)EL values may refer to constituents of the substance and not to the substance as a whole. More detailed information is available in the dossiers.

Data for WORKERS

INHALATION Exposure	Threshold	Most sensitive study
Systemic Effects		
Long-term:	(DNEL) 3 000 mg/m³	repeated dose toxicity
Acute /short term:	No hazard identified	
Local Effects		
Long-term:	No hazard identified	
Acute /short term:	No hazard identified	

DERMAL Exposure	Threshold	Most sensitive study
Systemic Effects		
Long-term:	(DNEL) 432 mg/kg bw/day	repeated dose toxicity
Acute /short term:	No hazard identified	
Local Effects		
Long-term:	No hazard identified	
Acute /short term:	No hazard identified	

Data for the GENERAL POPULATION

INHALATION Exposure	Threshold	Most sensitive study
Systemic Effects		
Long-term:	(DNEL) 643 mg/m³	repeated dose toxicity
Acute /short term:	No hazard identified	
Local Effects		
Long-term:	No hazard identified	
Acute /short term:	No hazard identified	

DERMAL Exposure	Threshold	Most sensitive study
Systemic Effects		
Long-term:	(DNEL) 214 mg/kg bw/day	repeated dose toxicity
Acute /short term:	No hazard identified	
Local Effects		
Long-term:	No hazard identified	
Acute /short term:	No hazard identified	