



Summary report

Interlaboratory comparison of three low-sulfur marine fuel oils between laboratories in Canada, China, Sweden, USA, and Norway

WP3 – PAME/EPPR characterization methodology

Author(s):

Liv-Guri Faksness and Per S. Daling

Report No:

2023:2023:00369 - Unrestricted

Client(s):

The Norwegian Coastal Administration

Summary report

Interlaboratory comparison of three low-sulfur marine fuel oils between laboratories in Canada, China, Sweden, USA, and

KEYWORDS:

Interlaboratory comparison; Low sulfur fuel oil; Oil characterization; Toxicity

VERSION

Final

DATE

2023-03-20

AUTHOR(S)

Liv-Guri Faksness and Per S. Daling

CLIENT(S)

The Norwegian Coastal Administration

CLIENT'S REFERENCE

Jon-Arve Røyset

PROJECT NO.

302006392

NUMBER OF PAGES:

118

SUMMARY

As a part of the WP3 - PAME/EPPR project "*Low sulfur fuels, fate and behavior in cold water conditions*", an interlaboratory comparison of three low sulfur fuels has been performed.

SINTEF has prepared the present report based on results and input from the participating laboratories:

- Sweden: Ida-Maja Hassellöv, Anders Walstad, Jonas Malmberg
- Canada: Michael Goldthorp, Robert Faragher, Megan Bauer
- USA: Mace Barron, Devi Sundaravadivelu
- China: Sijie Lin, Zhibo Lu, Hongying Zhao, Weixian Zhang
- Norway: Liv-Guri Faksness, Kristin R. Sørheim Per S. Daling, Dag Altin.

PREPARED BY

Liv-Guri Faksness

SIGNATURE

Liv-Guri Faksness

Liv-Guri Faksness (20. mar. 2023 14:05 GMT+1)

CHECKED BY

Kristin R. Sørheim

SIGNATURE

Kristin R. Sørheim

Kristin R. Sørheim (20. mar. 2023 14:13 GMT+1)

APPROVED BY

Trond R. Størseth

SIGNATURE

Trond R. Størseth

Trond R. Størseth (20. mar. 2023 14:35 GMT+1)

REPORT NO

2023:00369

ISBN

978-82-14-07790-2

CLASSIFICATION

Unrestricted

CLASSIFICATION THIS PAGE

Unrestricted

Table of contents

1	Introduction	4
2	Materials	5
3	Methods	6
4	Results interlaboratory comparison of physico-chemical properties.....	9
4.1	Water content.....	10
4.2	Density	10
4.3	Pour point	10
4.4	Flash point.....	11
4.5	Viscosity	12
4.6	Temperature-sweep (viscosity).....	12
4.7	Interfacial tension	13
4.8	Wax	14
4.9	Asphaltenes.....	15
4.10	Sulfur	16
4.11	CHN and metals.....	16
4.12	True boiling point (TBP)	17
5	Results of chemical characteristics and toxicity testing of WAFs.....	18
5.1	Oil chemistry	18
5.2	Chemistry of the WAFs	28
5.3	Toxicity of the WAFs	41
5.4	Diagnostic ratios for oil fingerprinting	44
6	Summary and recommendations	48
7	References	52
Appendix A	Reported results physico-chemical properties	55
Appendix B	Reported results chemistry of the oils	62
B1	Reported results chemistry of oils – USA.....	62
B2	Reported results chemistry of oils – Canada	65
B3	Reported results chemistry of oils – China	71
B4	Reported results chemistry of oils – Sweden.....	74
B5	Reported results chemistry of oils – Norway.....	75

Appendix C	Reported result chemistry of the WAFs	79
C1	Reported results chemistry of WAFs – USA	79
C2	Reported results chemistry of WAFs – Canada.....	83
C3	Reported results chemistry of WAFs – China	86
C4	Reported results chemistry of WAFs – Sweden.....	90
C5	Reported results chemistry of WAFs – Norway	94
Appendix D	Reported results toxicity	98
D1	Toxicity results – USA	98
D2	Toxicity results – Canada.....	101
D3	Toxicity results – China	104
D4	Toxicity results – Sweden.....	107
D5	Toxicity results – Norway	110
Appendix E	Calculated diagnostic ratios for oil fingerprinting.....	114
E1	Calculated diagnostic ratios for oil fingerprinting – USA	114
E2	Calculated diagnostic ratios for oil fingerprinting – Canada.....	114
E3	Calculated diagnostic ratios for oil fingerprinting – China.....	115
E4	Calculated diagnostic ratios for oil fingerprinting – Sweden.....	115
E5	Calculated diagnostic ratios for oil fingerprinting – Norway	117
Appendix F	Overview chemical component groups.....	118

1 Introduction

As a part of the WP3 - PAME/EPPR project "*Low sulfur fuels, fate and behavior in cold water conditions*", an interlaboratory comparison to characterize three low sulfur fuel oils (LSFO) has been performed. The present report summarizes the results from the five participants at USA, Canada, China, Sweden, and Norway. These countries have accepted to participate in the interlaboratory comparison study that refers to the suggested methodology guidelines for screening testing of fuel oil samples in project memo (Daling et al. 2021) "*WP3-3- PAME-EPPR Methodology for screening properties for new low sulfur marine fuels*". The guidelines include characterization of oil properties relevant for fate, behavior, fingerprinting characterization, and relative toxicity when spilled in cold or Arctic seawater. A suggested guideline for sampling and handling of representative oil samples for testing has also been a part of this project.

Table 1-1 gives an overview of the participating countries and their accompanying laboratories. Furthermore, Norway (SINTEF) has undertaken the role to distribute three relevant test oils to the other laboratories, see Materials in chapter 2 below, and to collect the results shown in this report from each participant. As a part of this project, there were outlined suggested reporting templates that were submitted to the laboratories, and a short description (memo) of methods used from the individual laboratories was also asked for. Furthermore, the variability between the test results obtained between the laboratories such as statistical calculations or method validations were not performed for comparison of results due to limited data sets. However, the results are tabulated to show similarities or differences between the laboratories and are illustrated in figures when appropriate.

Table 1-1 Overview of the participating countries and the accompanying laboratories /institutions.

Country	Laboratory	Contact person	Comments
Sweden	Chalmers University	Ida-Maja Hassellöv	Subcontractors: Saybolt, ALS Toxicon AB, and NFC
Canada	ECCC	Michael Goldthorp	Subcontractors: Intertek and Valor labs
USA	EPA	Mace Barron	
China	Tongji University (TJU)	Sijie Lin	Subcontractors: Ningbo Customs District Technology Centers, State Key Laboratory of Pollution Control and Resource Reuse, Shanghai Key Laboratory of Chemical Assessment and Sustainability
Norway	SINTEF	Faksness/Sørheim	Subcontractors: Intertek, Biotrix

SINTEF has prepared the present report based on results and input from the participating laboratories:

- Sweden: Ida-Maja Hassellöv, Anders Walstad, Jonas Malmberg
- Canada: Michael Goldthorp, Robert Faragher, Megan Bauer
- USA: Mace Barron, Devi Sundaravadivelu
- China: Sijie Lin, Zhibo Lu, Hongying Zhao, Weixian Zhang
- Norway: Liv-Guri Faksness, Kristin R. Sørheim, Per S. Daling, Dag Altin

2 Materials

The test oils (LSFOs) used for the interlaboratory study are listed in Table 2-1. The oils arrived at the SINTEF laboratory in Trondheim June 28, 2021, and the samples were registered in the SINTEF LIMS system given unique LIMS identification of each oil. An aliquot (ca. 3 L) of each of the test oils was further shipped to USA, Canada, China, and Sweden for testing. In this project, the selected oil types for testing were a Wide range gas oil (WRG), Marine gas oil (MGO), and a Very low sulfur fuel oil (VLSFO) to give a span of oil properties among low sulfur fuel oils. GC chromatograms of the oils are shown in Figure 2-1 are analyzed by USA and Norway, but the oils are analyzed under different instrumental conditions.

Table 2-1 Overview of the three LSFOs for interlaboratory study with SINTEF LIMS ID.

LIMS ID	Oil type	Comments
2021-5427	Wide Range Gas oil (WRG)	<0.05% S (From ST1 Refinery, Gothenburg, Sweden)
2021-5428	Marine Gas Oil (MGO)	<0.1% S (From Aagotnes Refinery, Norway)
2021-5429	Very Low Sulfur Fuel Oil (VLSFO)	< 0.5% S (From ExxonMobil, Antwerpen, Belgium, "Eemslift Hendrika")

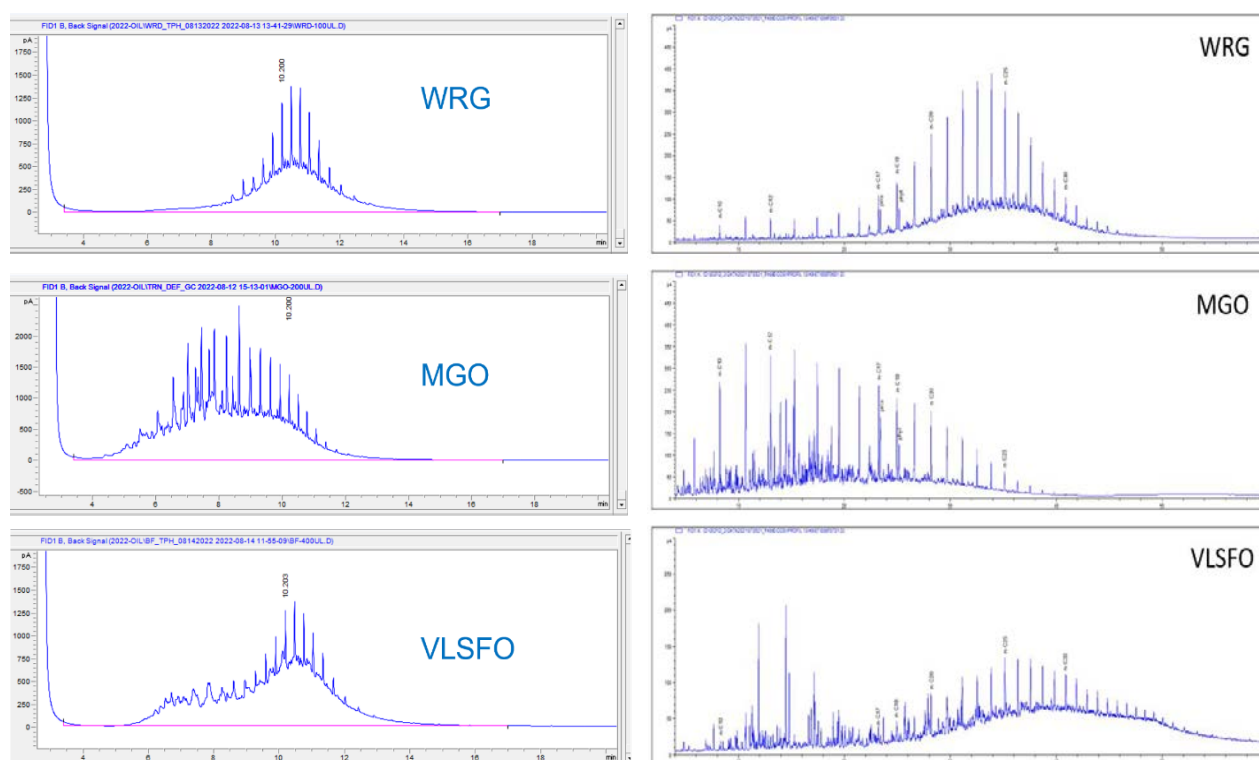


Figure 2-1 GC chromatograms of the oils from USA (left) and Norway (right).

3 Methods

The methods and test parameters are based on a best practice methodology for characterization properties that are relevant for screening the diversity of different marine low sulfur fuel oils (LSFOs) connected to fate and behavior and relative toxicity when spilled in particularly cold climate seawater. Table 3-1 and Table 3-2 give a brief overview of test parameters, methods, or instrumentation for screening of physico-chemical properties of the LSFOs from each participant. Table 3-3 attempts to give an overview indicating the methods applied, species tested, and the number of components within each component group the different laboratories have reported. Refers also to the project memo (Daling et al. 2021) "WP3-3- PAME-EPPR Methodology for screening properties for new low sulfur marine fuels" for recommendations.

Table 3-1 Overview of physical test parameters, analytical methods, or instruments.

Test parameters	USA	Canada	China	Sweden	Norway
Water content	NA	ASTM E203 (Karl Fischer Titration)	NA	ASTM D 6304	Volumetric Karl Fisher titration, Metrohm 841 Titando
Density	Gravimetric method Measured at room temp (22±1 °C)	ASTM D5002 measured at 0 and 15 °C	ASTM D4052-18a measured at 20 °C	EN ISO 12185	ASTM D4052 measured at 15.5 °C
Pour point	NA	ASTM D5949 *	ASTM D97-17b	ISO316	ASTM D97 Standard.
Flash point	NA	ASTM D7094	ASTM D93-20	EN ISO2719	ASTM D93 Pensky-Martens Closed Cup
Viscosity – temp.sweep	NA	Dynamic viscosity. 10-s, 50 to 0 °C (WRG and VLSFO a P35 and MGO a P60 plate-plate geometry.	NA	Viscosity, Kinematic, (mm ² s ⁻¹), ASTM D 7042	Dynamic viscosity measured from 50 down to 0 °C. Shear rate 10 s ⁻¹ . Temperature rate: 1°C/min
Viscosity	NA	ASTM 7042, Viscosity measurement at 15 and 0 °C	ASTM D445-19a Kinematic viscosity, (mm ² s ⁻¹) 20°C (MGO)	ASTM D 7042 Kinematic viscosity at 0°C (mm ² s ⁻¹)	Anton Paar / Physica MCR 300 /302 / PP50 Rheometer at 2 °C
Interfacial tension	Spinning drop tensiometer, measured at 25 °C	Pendant drop technique at air, water and saltwater interfaces at 0 and 15 °C. Krüss Drop Shape Analyzer DSA 100	NA	NA	Pendant drop, 5 min. equilibrium time (25 °C) Krüss Drop Shape Analyzer DSA 100
True boiling point	NA	ASTM D 7169	NA	ASTM D 2887	ASTM D 7169
Gas chromatographic analysis (GC/FID)	No info	In-house method Agilent 7890A, DB-5HT, 30 m x 0.1um	EPA Method 8015D Agilent 6890N, 30m DB1 column	No info	EPA method 8015 Agilent 6890N, 30m DB1 column

NA: Not analyzed or reported

*Canada: Pour point: A Phase Technology 70Xi Pour Point Analyzer was used for this analysis. The detection of pour point in the 70Xi Analyzer is performed by directing a pulse of compressed gas onto the sample surface. The pressure of the pulsed gas creates a disturbance at the surface of a fluid sample and the analyzer's optical sensors detect this movement. Absence of movement indicates that the liquid is below its pour point. The pour point is tested at 3°C intervals and reported as the last test temperature prior to detection of flow. This method is viable down to temperatures of -57°C. Pour point analysis was performed following ASTM

D5949, “Standard Test Method for Pour Point of Petroleum Products Automatic Pressure Pulsing Method”. Method and operator performance is monitored by periodic measurement of a lubricant check standard from Phase Technology (Vancouver, BC) in accordance with ASTM method D5949. The average of triplicate measurements is reported as the pour point in degrees Celsius.

Table 3-2 Overview of chemical test parameters and analytical methods or instruments (Yellow cells: No info).

Test parameters	USA	Canada	China	Sweden	Norway
Asphaltenes	NA	ECCC-ESTS house method is used for asphaltene precipitation and gravimetric determination *)	ASTM D6560-17	IP 143. Heptane-insoluble asphaltene	IP 143. Precipitation in n-Heptane
Wax	NA	ECCC-ESTS house method is used for wax crystallization and gravimetric determination **)	EN 12606-1:2015	NA	Bridiè et al, 1980, modified. Precipitation of the maltene fraction in a 1:1 2-MEK /DCM solvent mixture at minus 10°C for 4 hours
Sulfur	No info	ASTM D4294	ASTM D4294-16e1	EN ISO 8754	ASTM D4294***) and ASTM D2622
CHN elements	NA	NA	ASTM D5291–16 (C,H) ASTM D5762-18a (N)	ASTM D5291 (C, H) ASTM D5762 (N)	ASTM D5291
Metals	NA	ICP/MS or ICP/AES (Inductively Coupled Plasma Atomic Emission Spectrometry).	IP 501/05 ASTM D5762-18a	IP501	ICP/MS or ICP/AES (Inductively Coupled Plasma Atomic Emission Spectrometry).

NA: Not analyzed or reported

*) Asphaltenes are precipitated by using excess n-pentane as the precipitating medium (30 mL n-pentane/g of oil).

**) Waxes are separated by crystallization in a polar solvent. After quantification of resin, the remaining diluted maltene is rotary-evaporated. Then, it is filtered after mixing with 50 mL of 1:1 (v:v) dichloromethane (DCM)/methyl ethyl ketone (MEK). The flask, funnel, filtering flask, and 1:1 DCM/MEK are placed in the -30 °C freezer to chill overnight before use to be able to crystallize the wax.

***) Similar as ISO 8754. Standard Test Method for Sulfur in Petroleum and Petroleum Products by Energy Dispersive X-ray Fluorescence Spectrometry).

Table 3-3 Overview of test parameters and methods for chemical composition of the oils and their WAFs, and the species tested for acute toxicity. (x: reported in accordance with Daling et al. (2021).

Test parameters	USA	Canada	China	Sweden	Norway
Methods					
TPH	GC/FID EPA 8015C	GC/FID in-house	GC/FID EPA 8015D	GC/FID EPA 8015 /ISO 9377-2	GC/FID EPA 8015D
SVOC/PAH	GC/MS EPA 8070D	GC-MS in-house	GC/MS EPA 8270E	GC/MS DIN 38407-39	GC/MS EPA 8270E
VOC	GC/MS headspace EPA 524.3	NA	P&T GC/MS EPA 5030C & EPA 8260D	GC/FID and GC/MS EPA 624,8260,8015	P&T GC/MS EPA 8260D
WAF	23 °C / 18 h, settle for 6 h	NA	4 °C / 72 h, settle for 0.5 h	4 °C / 72 h, settle for 1 h	2 °C / 72 h
Oil chemistry					
SVOC/PAH	45 of 56 comp	45 of 56 comp	31 of 56 comp	NA	56 of 56 comp
Decalins	NA	NA	1 of 5 comp	NA	x
Naphthalenes	x	x	4 of 5 comp	NA	x
2-3 ring PAH	x	x	8 of 20 comp	NA	x
4-6 ring PAH	x	x	14 of 19 comp	NA	x
C0-C5 phenols	NA	NA	4 of 6 comp	NA	x
VOC	NA	NA	31 of 33 comp	NA	33 of 33 comp
BTEX	NA	NA	5 of 6 comp	NA	x
C3-benzenes	NA	NA	6 of 7 comp	NA	x
Other VOC	NA	NA	20 of 21 comp	NA	x
Diagnostic ratios	NA	x	NA	x	x
WAF chemistry					
TPH	x		x	x	x
SVOC/PAH	45 of 56 comp	45 of 56 comp	31 of 56 comp	26 of 56 comp	56 of 56 comp
Decalins	NA	NA	1 of 5 comp	NA	x
Naphthalenes	x	x	(4 of 5 comp	4 of 5 comp	x
2-3 ring PAH	x	x	8 of 20 comp	12 of 20 comp	x
4-6 ring PAH	x	x	14 of 19 comp	10 of 19 comp	x
C0-C5 phenols	NA	NA	4 of 6 comp	NA	x
UCM	NQ	NA	x	x	x
VOC	6 of 33 comp	NA	31 of 33 comp	14 of 33 comp	33 of 33 comp
BTEX	x	NA	5 of 6 comp	x	x
C3-benzenes	NA	NA	6 of 7 comp	4 of 7 comp	x
Other VOC	NA	NA	20 of 21 comp	4 of 21 comp	x
WAF: Acute toxicity					
<i>A. tonsa</i>	NA	x	NA	NA	x
Alternative species	<i>A. bahia</i> <i>M. beryllina</i>		Zebrafish <i>M. mongolica</i>	<i>N. spinipes</i>	<i>C. finmarcicus</i>
Toxic Unit (TU)	NQ	NQ	x	NQ	x

4 Results interlaboratory comparison of physico-chemical properties

The results from the interlaboratory comparison of physico-chemical properties of WRG, MGO, and VLSFO are summarized in this chapter.

The results from the physico-chemical properties are summarized in Table 4-1, and the results from the element analysis are summarized in Table 4-2. Density, pour point, flash point, temperature-sweep (viscosity), asphaltenes, wax, and elements of sulfur (S), carbon (C) and nitrogen (N), and the true boiling point (TBP) are also illustrated in figures (histograms / graphs) as shown in the subchapters below.

Table 4-1 Overview of physico-chemical analysis of WRG, MGO, and VLSFO from the interlaboratory comparison.

Oils	Country	Water content (vol.%)	Density, 15°C (g/mL)	Pour Point (°C)	Flash Point (°C)	Viscosity (mPa.s) 10s ⁻¹	Viscosity (mPa.s) 100s ⁻¹	Viscosity (mPa.s) 1000s ⁻¹	IFT (mN/m)	Asph. (wt.%), "Hard or Soft"	Wax (wt.%)
WRG											
	Sweden	0.004	0.874	-9	117	*	44.6 (20 °C) ^{a)}		X	<0.50	X
	Canada	0.100	0.876	27	118	NA	897 (0 °C)	227 (0 °C)		0.07	11.78
	USA		0.861						19.0		
	China		0.873	-6	108		90.4 (20 °C) ^{a)}			<0.05	
	Norway	0.233	0.873	-6**	113	218 (2°C)	186 (2°C)		28	0.01	6.54
MGO											
	Sweden	0.003	0.865	-21	70	9.2 (0 °C) ^{a)}			X	<0.50	X
	Canada	0.030	0.865	-15	69	NA	NA	8.4 (0 °C)	27	0.02	2.26
	USA		0.857						18.9		
	China		0.865	-30	70		8.2 (20 °C) ^{a)}			<0.05	
	Norway	0.200	0.865	-18**	68	6.6 (2°C)	6.3 (2°C)		11	0.01	0.62
VLSFO											
	Sweden	0.100	0.970	15	108	*	77.8 (50 °C) ^{a)}		X	2.30	X
	Canada	0.143	0.971	24	115	21977 (0°C)	11187 (0°C)	3229 (0 °C)		5.03	7.64
	USA		0.966						22.5		
	China		0.970	12	>120		1156 (20 °C) ^{a)}			2.78	0.80
	Norway	0.367	0.969	15**	109	19755 (2°C)	7766 (2°C)		58 ^{b)}	2.64	6.02

* Not possible to monitor viscosity under room temperature due to separation of waxes in the sample (Sweden)

** Pour point: Intertek subcontractor (Norway)

X: Analysis not offered by the lab. (Sweden)

^{a)} Kinematic viscosity (Sweden and China)

^{b)} Uncertain measurement of IFT at 50 °C (Norway)

Table 4-2 Overview of element analysis of WRG, MGO and VLSFO from the interlaboratory comparison.

Table 1: ICP/MS or ICP/AES (mg/kg), WGC, WGC and WGC from the Mineral Industry Company													
Oil	Country	ICP/MS or ICP/AES (mg/kg)								(mass%)	(mass%)		
		Aluminium (Al)	Calcium (Ca)	Iron (Fe)	Nickel (Ni)	Silicon (Si)	Sodium (Na)	Vanadium (V)	Copper (Cu)	Sulfur (S)	C	H	N
WRG													
	Sweden	<5	<3	x	x	<10	<1	<1	x	0.04	86.5	13.4	0.03
	Canada*			1.2	<0.01			0.1		0.05			
	USA									0.03			
	China	<1	<1	<1	<1	13	<1	<1	<1	0.04	86.5	13.1	0.016
	Norway**	<1	<5	<1	<1	<5	<2	<1	<1	0.04	87.0	14.0	<0.1
MGO													
	Sweden	<5	<3	x	x	<10	<1	<1	x	0.09	87	12.8	0.01
	Canada*			1.2	<0.01			0.01		0.08			
	USA									0.06			
	China	<1	<1	<1	<1	10	<1	<1	<1	0.08	85.1	11.7	0.01
	Norway**	<1	<5	<1	<1	<5	<2	<1	<1	0.08	86.9	13.2	<0.1
VLSFO													
	Sweden	<5	5	x	x	<10	9	10	x	0.51	87.5	10.8	0.29
	Canada*			8.3	4.7			15		0.51			
	USA									0.33			
	China	2	6	7	10	15	16	10	<1	0.48	88.2	10.5	0.31
	Norway**	1	5	3	10	<5	6	10	<1	0.54	87.7	11.2	0.3

*: Element analysis from Intertek subcontractor (Canada)

**.: Element analysis from Intertek subcontractor (Norway)

X: Analysis not offered by the lab. (Sweden)

4.1 Water content

Overall, Sweden, Canada and Norway reported all low water contents (<0.5%) in the oil phase of WRG, MGO, and VLSFO. The results are tabulated in Table 4-1. The modest deviation among the laboratories can be explained by the methods used, and handling of the test oils.

4.2 Density

The comparison of densities is illustrated in Figure 4-1, and tabulated in Table 4-1. Overall, minor variations in densities between the laboratories were reported for WRG, MGO, and VLSFO with a relatively good variability of <0.02 g/mL. As shown in Figure 4-1, the USA reported lower densities of the test oils compared with the other laboratories. The lower densities can be explained due to the gravimetric analytical method used. Note, Norway measured density of VLSFO at 40 °C due to the stiffness of the oil and recalculated the value to 15 °C that was reported, whilst China measured the densities at 20 °C.

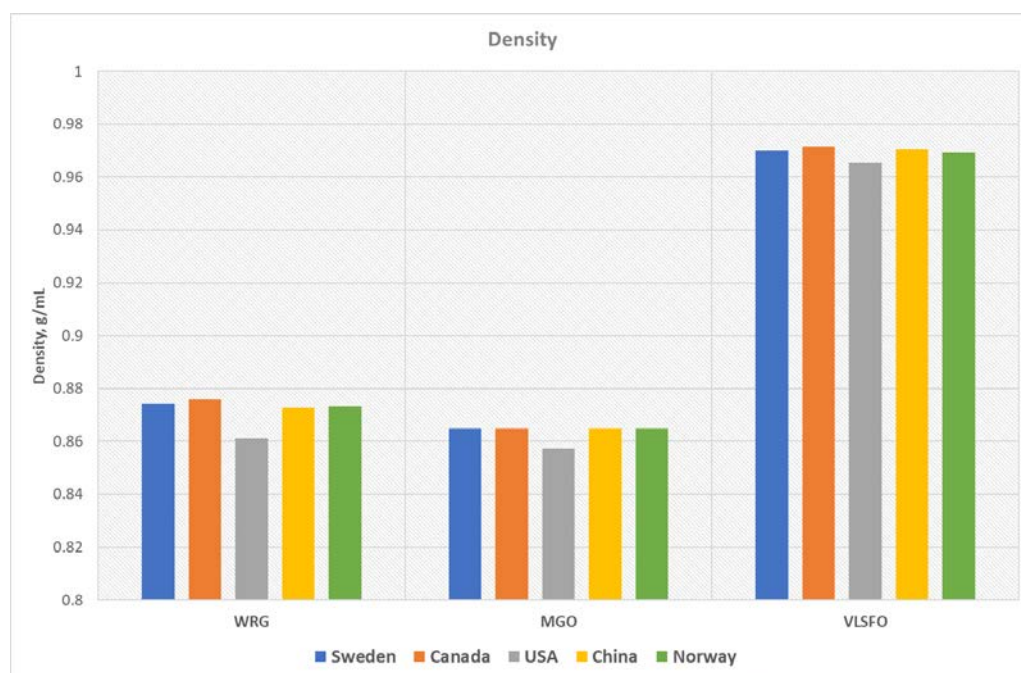


Figure 4-1 Comparison of density at 15 °C of WRG, MGO, and VLSFO.

4.3 Pour point

The comparison of pour points of WRG, MGO, and VLSFO is illustrated in Figure 4-2, and given in Table 4-1. Pour points were not reported by the USA. For WRG, the pour points varied between -9 °C to +27 °C, which is considered as a major difference. For MGO, the results were in the range of -30 °C to -15 °C, i.e., the laboratories reported low pour points for this oil. The pour point of VLSFO is high, and the pour points of this oil varied from +12°C to +24 °C between the laboratories. However, the Canadian laboratory used a method with another principle than the other laboratories, which may have caused the difference.

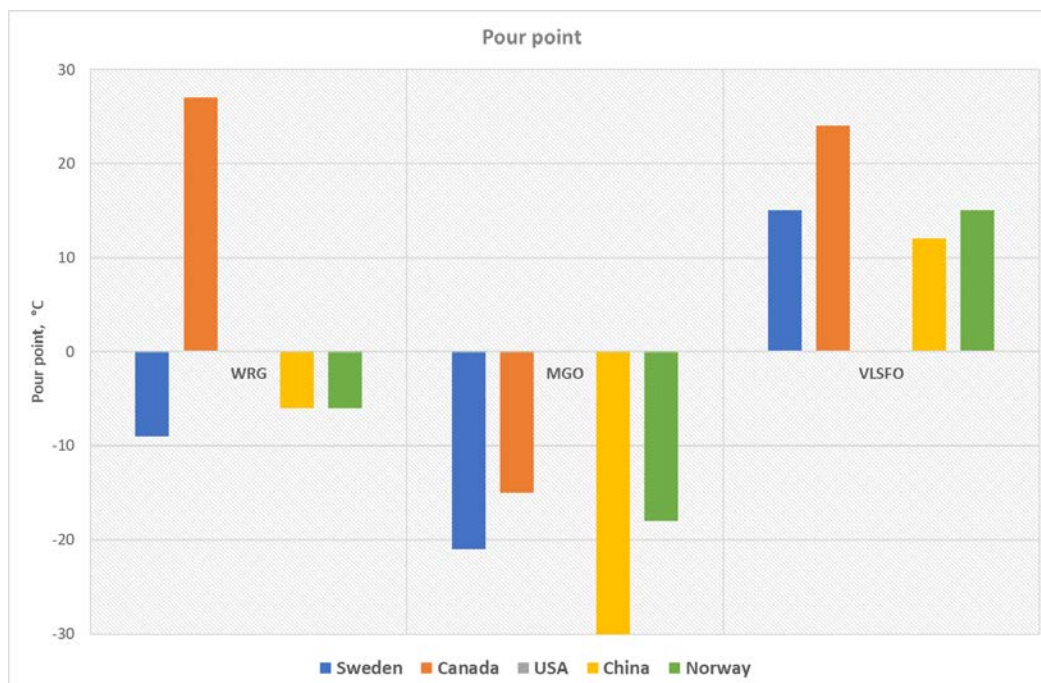


Figure 4-2 Comparison of pour point of WRG, MGO, and VLSFO. No data from USA.

4.4 Flash point

The flash points of WRG, MGO, and VLSFO reported by the different laboratories are illustrated in Figure 4-3, and tabulated in Table 4-1. No data of flash points were reported by the USA. Overall, the flash points reported did not differ highly between the laboratories, meaning they were in the same range within the different oil types.

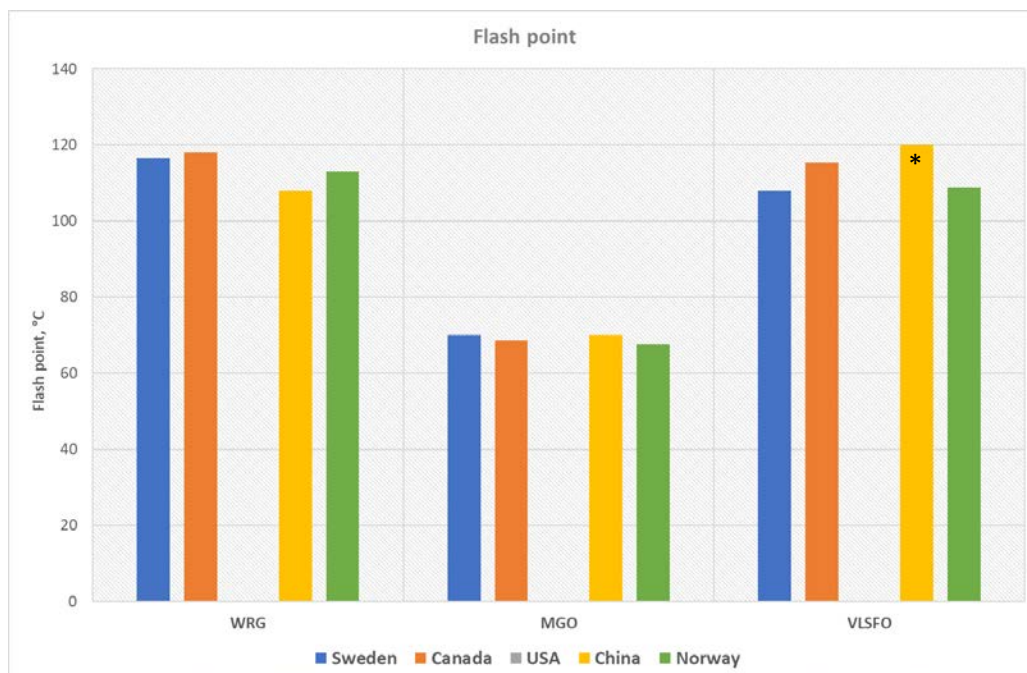


Figure 4-3 Comparison of flash point of WRG, MGO, and VLSFO. No data from USA. *The value is reported as >120 °C.

4.5 Viscosity

The results from the viscosity measurements are shown in Table 4-1. However, the viscosities were difficult to compare since they were reported at different test temperatures and different shear rates. China reported viscosities at 20 °C and Canada at 0 °C, whilst Norway reported viscosities at 2 °C according to the recommended project memo (Daling et al. 2021). In addition, there were also used different analytical methods among the laboratories, i.e., dynamic viscosity (Canada and Norway) vs. kinematic viscosity (Sweden and China) that also explain differences in viscosities between the laboratories.

4.6 Temperature-sweep (viscosity)

The temperature-sweep (viscosity) of WRG, MGO, and VLSFO were reported by Sweden, Canada, and Norway. The results (curves) are illustrated in Figure 4-4 to Figure 4-5, and tabulated in Appendix A.1. Note, Sweden reported temperature-sweeps starting from low temperatures that varied from 0 °C (MGO), 20 °C (WRG), and 50 °C (VLSFO) to a high temperature of 100 °C, whilst Canada and Norway have a method that starting from a high temperature (~50 °C) and then cooling down to a lower temperature to about 0 °C. Moreover, Sweden reported temperature-sweep based on kinematic viscosity, whilst Canada and Norway reported dynamic viscosity at shear rate 10 s⁻¹.

The results from Norway (Figure 4-5) and Canada (Figure 4-6) and were correlating very well.

Despite the differences in the methods, the temperature-sweep of MGO shows similarities between Sweden and the other two laboratories. For WRG, the viscosities in the range of 20-50 °C is lower by Sweden than and Norway, but at 50 °C the viscosities are comparable; Sweden 11 (mm²s⁻¹) vs. Norway 9 (mPa.s). Similarly, the viscosity of VLSFO at 50 °C is also comparable; Sweden 78 (mm²s⁻¹) vs. Norway 66 (mPa.s), see the green circles in Figure 4-4 and Figure 4-5. Moreover, the abrupt hump in the temperature-sweep of WRG around 23 °C reported by Norway (Figure 4-5) can be explained by the relatively high cloud point of the WRG (28 °C, ref. Certificate of Analysis).

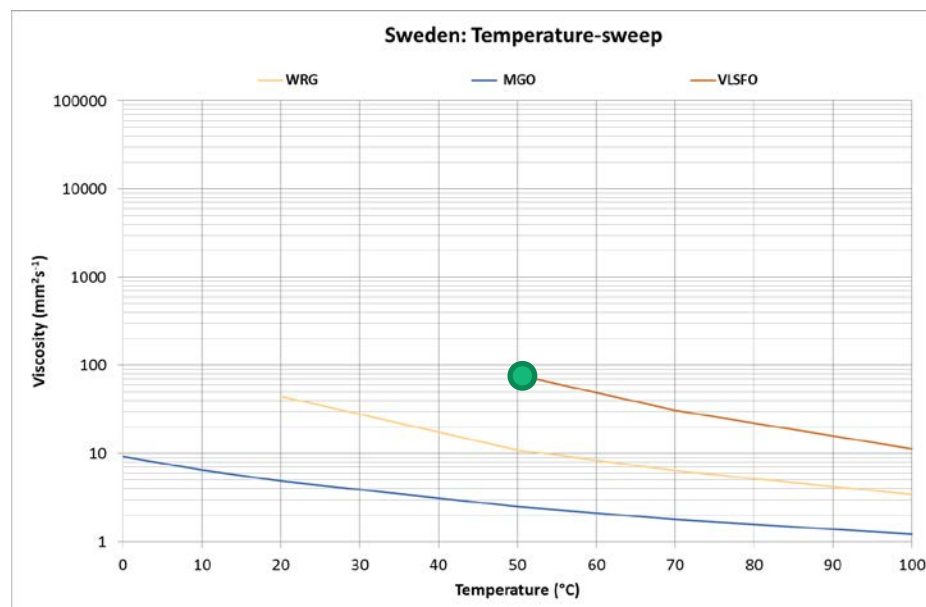


Figure 4-4 Temperature-sweep of WRG, MGO and VLSFO reported by Sweden.

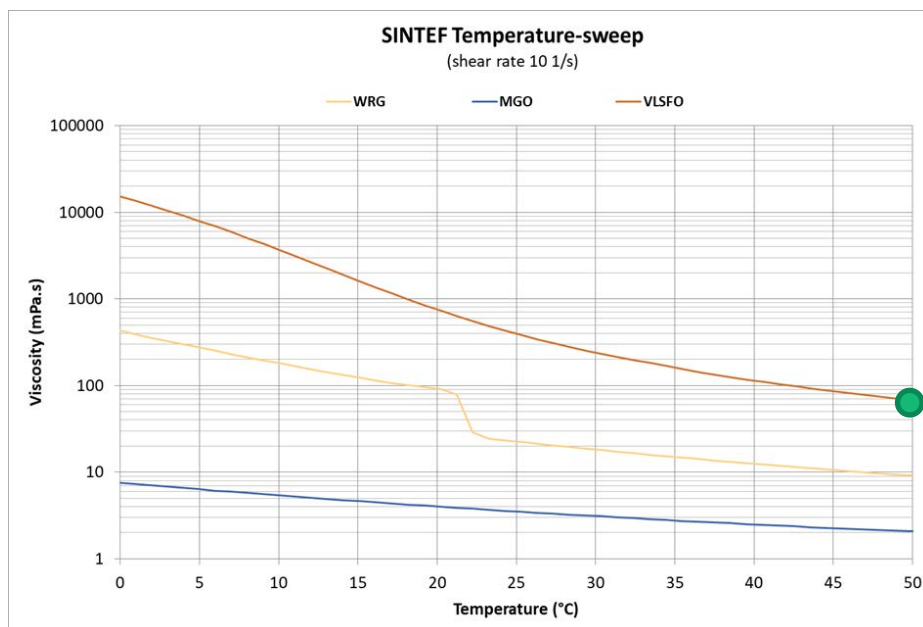


Figure 4-5 Temperature-sweep of WRG, MGO, and VLSFO reported by Norway.

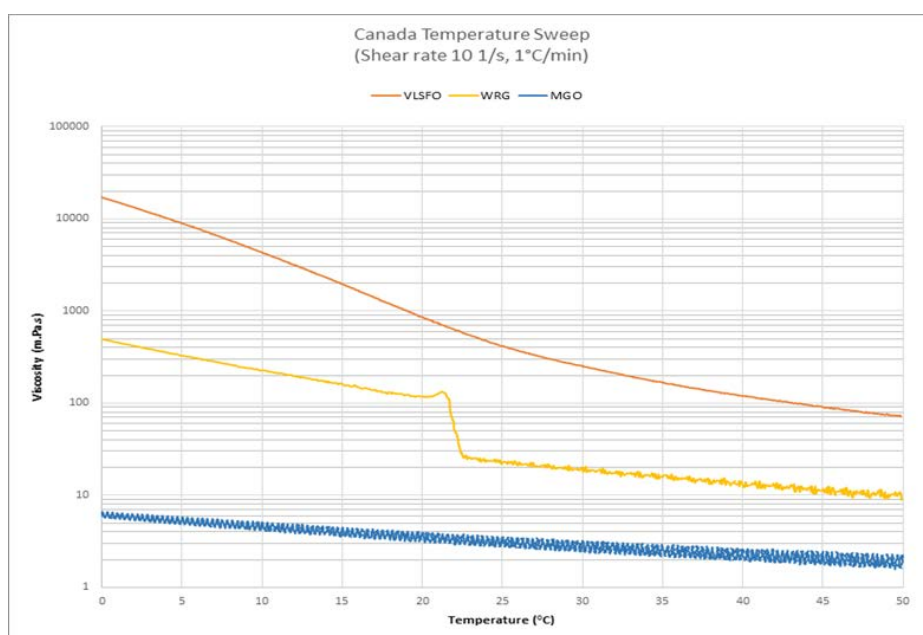


Figure 4-6 Temperature-sweep of WRG, MGO and VLSFO reported by Canada.

4.7 Interfacial tension

The interfacial tension (IFT) of WRG, MGO, and VLSFO was reported by the USA and Norway, whilst Canada reported IFT on the MGO. However, the laboratories used two different test methods (USA: Spinning drop, and Norway and Canada: Pendant drop). The results are given in Table 4-1 and Figure 4-7. For WRG, the USA reported a lower IFT than Norway, 19 mN/m vs. 28 mN/m, respectively. Whilst for MGO, Norway reported a lower IFT (11 mN/m) than USA (18.9 mN/m) and Canada (27 mN/m). For VLSFO, USA reported a IFT of 22.5 mN/m, whilst Norway measured an unexpected high IFT of 58 mN/m (50 °C) with the Pendant drop method. Such a high value of IFT may be considered uncertain.

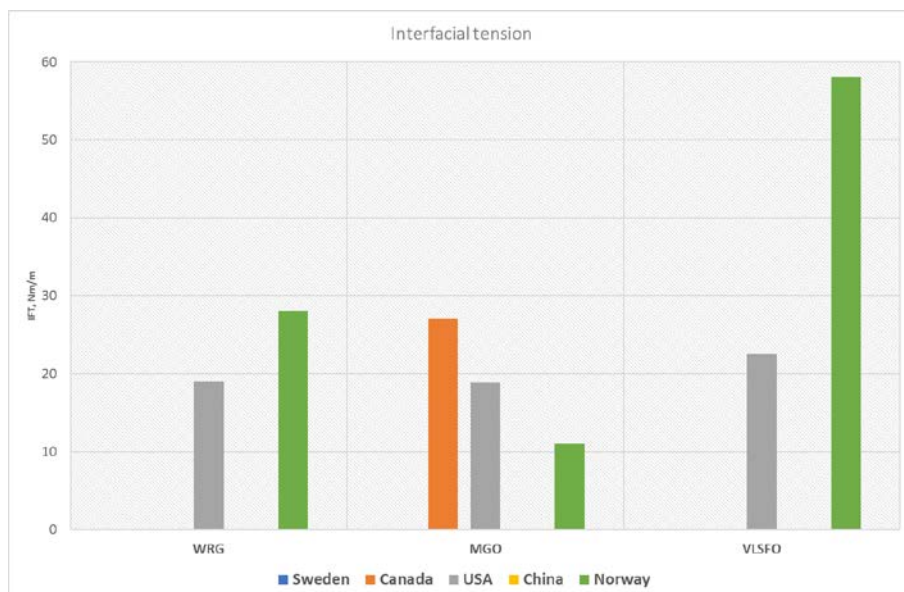


Figure 4-7 Comparison of IFT of WRG, MGO, and VLSFO. USA used the Spinning drop method, whilst Canada and Norway used the Pendant drop method). No data reported by Sweden, Canada, and China.

4.8 Wax

The wax contents of MGO, WRG, and VLSFO reported by the different laboratories are illustrated in Figure 4-8, and tabulated in Table 4-1. No data were reported by Sweden and the USA, and no data from China were reported for the WRG and MGO. For WRG, the wax content varied from 5.6 wt.% (Norway) to 11.8 wt.% (Canada). For MGO, the content of wax varied from 0.62 wt.% (Norway) to 2.3 wt.% (Canada). For VLSFO, a major deviation of wax was observed from the lowest value of 0.8 wt.% (China) to the highest value of 7.6 wt.% (Canada). Norway and Canada reported wax content of VLSFO of 6.0 wt.% vs. 7.6 wt%, respectively. The systematic higher content of wax reported by Canada vs. Norway may be explained by different precipitation temperature used (minus 30 vs. minus 10°C respectively).

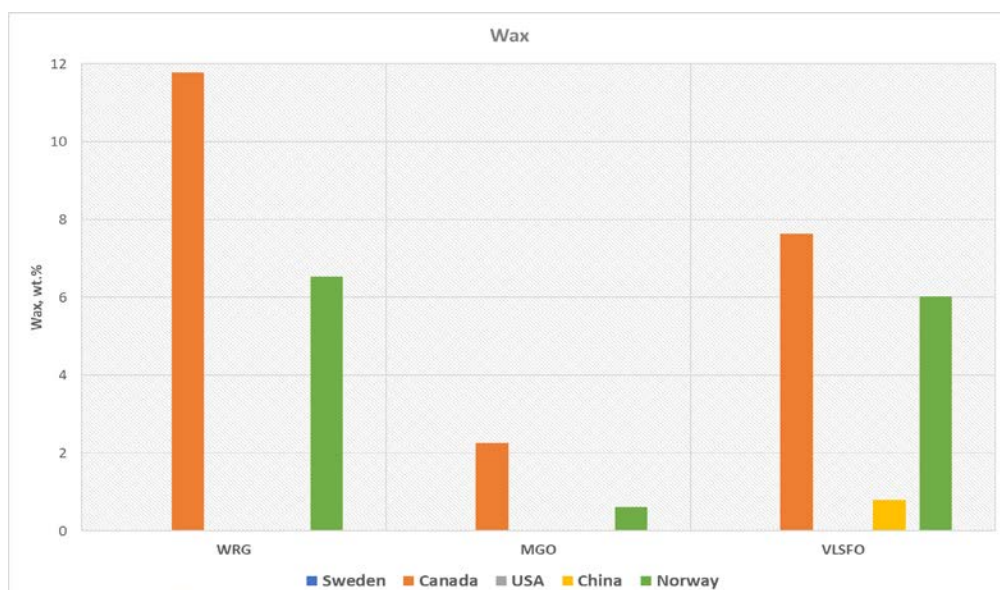


Figure 4-8 Comparison of wax content of WRG, MGO, and VLSFO. No data reported by Sweden and the USA. No data from China for WRG and MGO.

4.9 Asphaltenes

The comparison of the asphaltenes content is illustrated in Figure 4-9 for the WRG and MGO (figure above), and for the VLSFO (figure below). The bars (histograms) with asterisks indicate the detection limits given as "lower than <" and probably explain the high values of asphaltenes for the WRG and MGO reported by Sweden. The results are also tabulated in Table 4-1. The other laboratories (no data from the USA) reported very low content of asphaltenes for the WRG and MGO in the range of 0.01 to <0.50 wt.%. For VLSFO, Sweden, China and Norway reported very similar content of asphaltenes in the range of 2.3 wt.% to 2.8 wt.% ("hard" asphaltenes / n-Heptane precipitated, IP 143 method), whilst Canada reported a considerable higher value of 5.0 wt.% ("soft" /n-pentane precipitated asphaltenes)

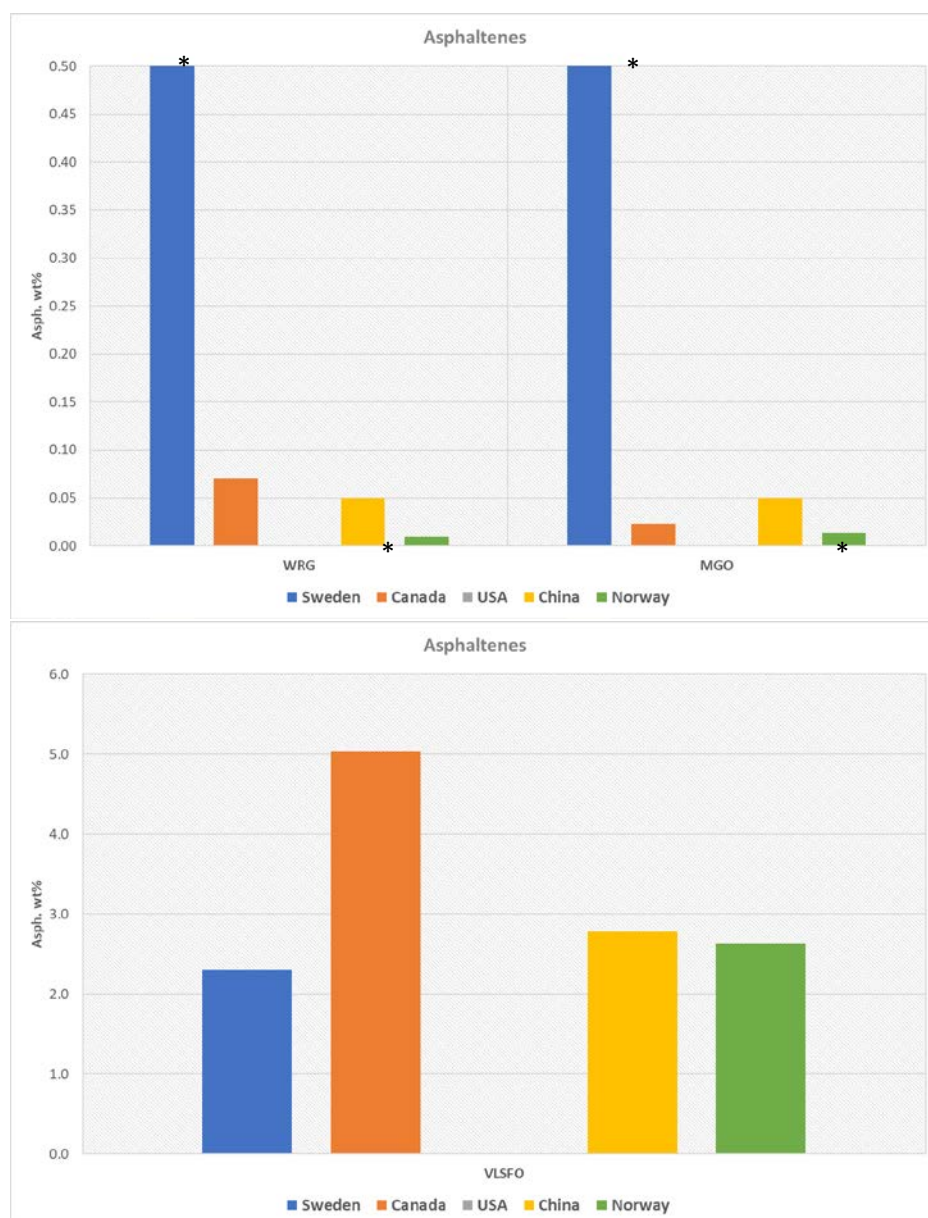


Figure 4-9 Comparison of asphaltenes of WRG and MGO (above) and VLSFO (below). No data reported by USA. *The value is given as <0.5 wt.% (Sweden) and <0.05 wt.% (China) for WRG and MGO.

4.10 Sulfur

The sulfur content of WRG, MGO, and VLSFO are illustrated in Figure 4-10, and tabulated in Table 4-2. For WRG, the laboratories reported low sulfur content in the range of 0.03-0.05 wt.%. All the laboratories reported low sulfur content of MGO in the range of 0.06-0.09 wt.%, i.e., the values are below the IMO sulfur limit of ultra-low sulfur oils, $S < 0.10$ wt.%. However, for the VLSFO, three of the laboratories reported a sulfur content slightly higher than the sulfur limit of $S < 0.50$ wt.%. Norway reported two values of sulfur of VLSFO with use of the ASTM methods D4294 and D2622, where D4294 gave 0.54 wt.% (S) just above the "IMO-limit" of VLSFO < 0.50 % m/m, whilst D2622 gave 0.479 wt.% (S) that is below the IMO sulfur cap (both are shown in Figure 4-10).

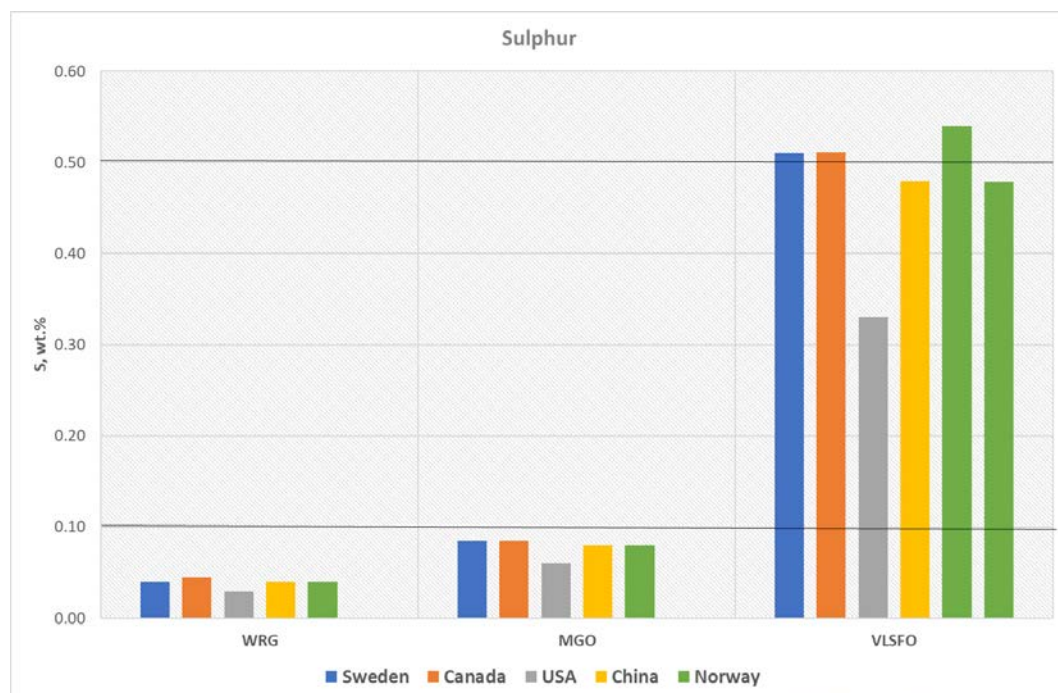


Figure 4-10 Comparison of sulfur (S) content of WRG, MGO, and VLSFO. The black lines show the sulfur IMO limits for VLSFO ($S < 0.5$ wt.%) and ULSFO ($S < 0.1$ wt.%). Norway reported two values of sulfur for VLSFO based on two different ASTM methods (ECCC used subcontractor for analysis)

4.11 CHN and metals

The mass percentage of carbon (C), hydrogen (H), and nitrogen (N) in WRG, MGO, and VLSFO were reported by Sweden, China, and Norway. The results are tabulated in Table 4-2 and illustrated in Figure 4-11 for carbon and hydrogen. The content of nitrogen was very low in the range of 0.01-0.31%, and therefore not shown in the same figure as for carbon and hydrogen. Overall, the laboratories reported comparable results of CHN for the three test oils.

The content of metals in WRG, MGO, and VLSFO also showed comparable values between the same laboratories as mentioned above for the CHN analysis, as shown in Table 4-2. The metals analyzed were aluminum (Al), calcium (Ca), iron (Fe), nickel (Ni), silicon (Si), sodium (Na), vanadium (V), and copper (Cu).

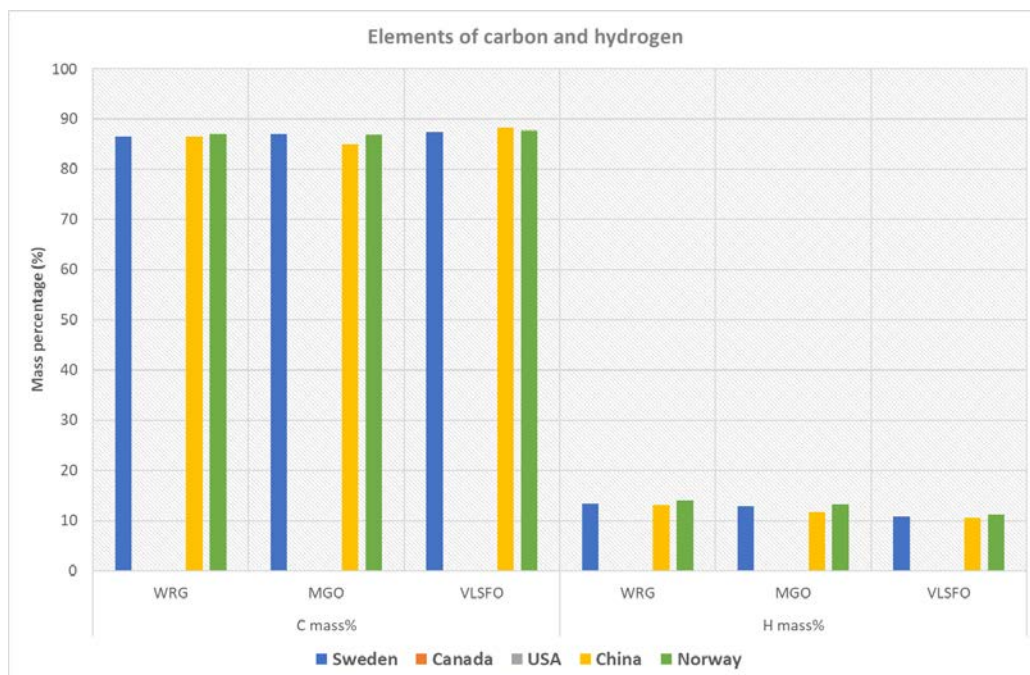


Figure 4-11 Comparison of carbon (C) and hydrogen (H) of WRG, MGO, and VLSFO.

4.12 True boiling point (TBP)

The comparison of the true boiling point (TBP) or distillation curve of the WRG, MGO, and VLSFO reported by Sweden, Canada, and Norway, is illustrated in Figure 4-12. Overall, the TBPs reported were relatively comparable within each oil type. The TBPs from Sweden seemed to be approx. 5-10 % higher for all the three oils than reported by the other laboratories. Norway on the other hand reported slightly higher TBPs than Canada, except for the WRG where Canada and Norway show overlapping curves.

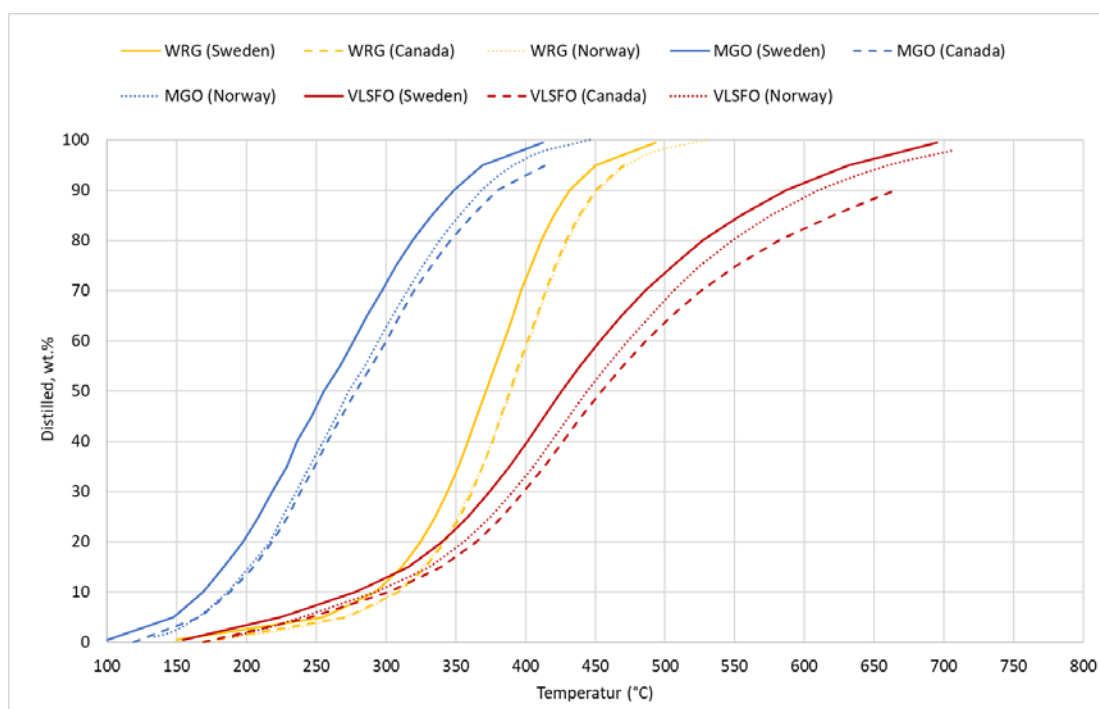


Figure 4-12 Comparison of true boiling point curves (TBP) of WRG, MGO, and VLSFO.

5 Results of chemical characteristics and toxicity testing of WAFs

The recommended SVOC and VOC components are given in Table F 1 (Appendix F).

It seems that the analytical parameters agreed on for performing chemical characterization of the oils and their WAFs, including the toxicity testing, were more challenging than expected. As indicated in Table 3-3, all laboratories, but one, have not delivered a complete data set. Therefore, using statistical methods to compare the results was not feasible, as the number of analyzed analytes vary from the participating laboratories. The results are presented in tables for each oil, both in summary tables and in tables giving the detailed results.

The results from each laboratory are given in the appendices:

Appendix B: Reported results chemistry of the oils

- B1 Reported results chemistry of the oils - USA
- B2 Reported results chemistry of the oils - Canada
- B3 Reported results chemistry of the oils - China
- B4 Reported results chemistry of the oils - Sweden
- B5 Reported results chemistry of the oils - Norway

Appendix C: Reported results chemistry of the WAFs

Appendix D: Reported results toxicity

Appendix E: Calculated diagnostic ratios for oil fingerprinting

In addition to the Excel template file, USA, Sweden, and Norway have submitted a memo/report describing the methodology they have used and reported the results. Canada has submitted a description of sample preparation and analytical methods. These files are not included in the report.

5.1 Oil chemistry

No data of the oil chemistry was reported from Sweden. The remaining laboratories have reported SVOC data, but only China and Norway have done analysis of volatiles (Table 5-7). A summary of the reported SVOC and VOC results are given in Table 5-1 for WRG, Table 5-2 for MGO, and Table 5-3 for VLSFO. Detailed SVOC results are shown in Table 5-4 for WRG, Table 5-5 for MGO, and Table 5-6 for VLSFO. Reported results from each laboratory are shown in Appendix B.

Figure 5-1 presents the concentrations of the naphthalenes, 2-3 ring PAHs and 4-6 ring PAHs. USA, Canada, and Norway have reported the same components, while China has reported 28 of 45 components. The figure shows that there is relatively good correlation between the results from Canada and Norway. The results from the volatile analysis (Table 5-7) give very different results from China and Norway, might be due to different settings of parameters used.

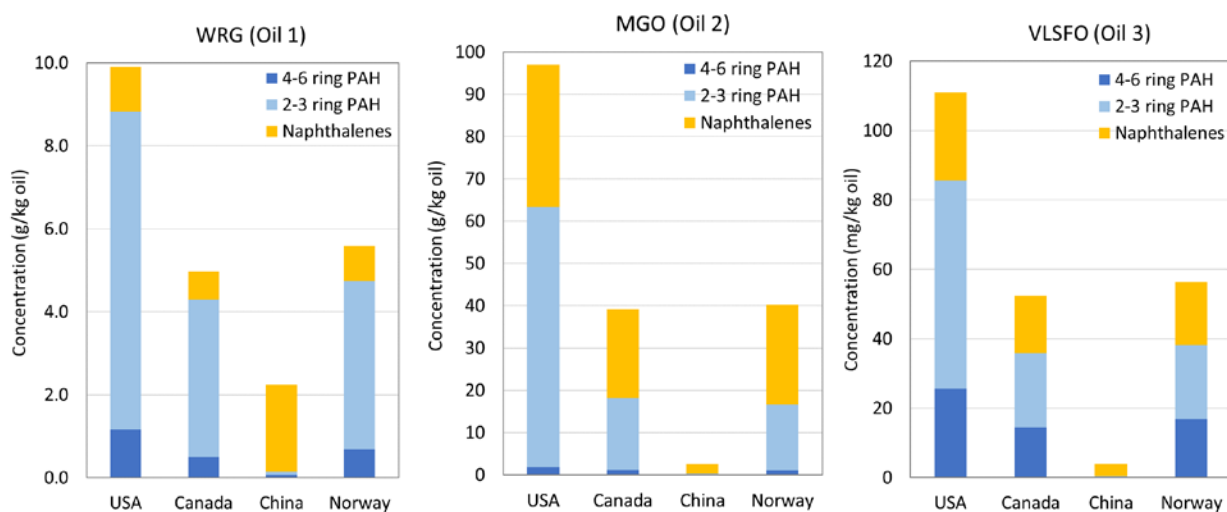


Figure 5-1 Naphthalenes and PAHs in the oils (mg/kg oil). No results from Sweden. USA, Canada and Norway have reported the same 45 components, while China has reported 28 of 45 components.

Table 5-1 Summary of reported results of the chemical composition of the WRG oil. Description of the component groups are given in Table F 1 (Appendix F). NA: Not analyzed.

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	WRG	2021-5427	2021-5427		
Internal Lab ID	LSFO 1	2021-09-17-6081			2021-5427
Oil type	WRG	WRG	WRG	No data reported	WRG
	mg/kg oil	mg/kg oil	mg/kg oil		mg/kg oil
Sum SVOC	8832	4973	2399		7122
Sum VOC	NA	NA	2962		1137
Decalins	NA	NA	26.8		1527
Naphthalenes	1063	677	2102		857
2-3 ring PAH	7669	3791	87.7		4051
4-6 ring PAH	1162	505	60.1		683
C0-C5 phenols	NA	NA	122		3.81
BTEX	NA	NA	1632		183
C3-benzenes	NA	NA	882		223
Other VOC	NA	NA	447		731

Table 5-2 *Summary of reported results of the chemical composition of MGO. Description of the component groups are given in Table F 1 (Appendix F). NA: Not analyzed.*

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	MGO	2021-5428	2021-5428		
Internal Lab ID	LSFO 2	2021-09-17-6082			2021-5428
Oil type	MGO	MGO	MGO	No data reported	MGO
	mg/kg oil	mg/kg oil	mg/kg oil		mg/kg oil
Sum SVOC	63301	39199	2838		52094
Sum VOC	NA	NA	7129		49267
Decalins	NA	NA	29.9		11829
Naphthalenes	33668	21108	2350		23616
2-3 ring PAH	61444	16969	254		15591
4-6 ring PAH	1857	1122	55.4		1049
C0-C5 phenols	NA	NA	149		9.69
BTEX	NA	NA	3632		5283
C3-benzenes	NA	NA	2726		16554
Other VOC	NA	NA	771		27430

Table 5-3 *Summary of reported results of the chemical composition of VLSFO. Description of the component groups are given in Table F 1 (Appendix F). NA: Not analyzed.*

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	VLSFO	2021-5429	2021-5429		
Internal Lab ID	LSFO 3	2021-09-17-6083			2021-5429
Oil type	VLSFO	VLSFO	VLSFO	No data reported	VLSFO
	mg/kg oil	mg/kg oil	mg/kg oil		mg/kg oil
Sum SVOC	85530	52460	4119		56545
Sum VOC		NA	1571		1459
Decalins		0	19.2		278
Naphthalenes	25555	16486	3462		18063
2-3 ring PAH	59895	21581	325		21431
4-6 ring PAH	25635	14393	168		16765
C0-C5 phenols		0	146		9.22
BTEX		NA	981		271
C3-benzenes		NA	498		695
Other VOC		NA	91.5		489

Table 5-4 *Semi-volatile components reported for the WRG oil. No results reported from Sweden. (NA: Not analyzed; ND: Not detected). Comments given by the laboratories to their results are given in Appendix B.*

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	WRG	2021-5427	2021-5427		2021-5427
Internal Lab ID	LSFO 1	2021-09-17-6081	2021-5427		2021-5427
Oil type	WRG	WRG	WRG	No data reported	WRG
	mg/kg oil	mg/kg oil	mg/kg oil		mg/kg oil
Decalin	NA	NA	26.8		232
C1-decalins	NA	NA	NA		369
C2-decalins	NA	NA	NA		371
C3-decalins	NA	NA	NA		337
C4-decalins	NA	NA	NA		219
Benzo(b)thiophene	NA	NA	2.64		1.98
Naphthalene	31.3	22.7	12.2		61.0
C1-naphthalenes	109	75.0	254		120
C2-naphthalenes	223	165	1836		191
C3-naphthalenes	326	223	NA		237
C4-naphthalenes	373	190	NA		247
Biphenyl	67.9	57.6	NA		78.0
Acenaphthylene	4.44	1.66	NA		2.40
Acenaphthene	4.00	4.01	NA		ND
Dibenzofuran	14.7	NA	NA		10.3
Fluorene	40.2	27.3	21.5		29.5
C1-fluorenes	297	208	NA		158
C2-fluorenes	1045	468	NA		459
C3-fluorenes	1466	663	NA		601
Phenanthrene	76.8	50.6	8.43		70.9
Anthracene	24.3	12.2			10.8
C1-phenanthrenes/anthracenes	432	321	2.21		317
C2-phenanthrenes/anthracenes	766	542	43.5		578
C3-phenanthrenes/anthracenes	909	634			645
C4-phenanthrenes/anthracenes	800	560			688
Dibenzothiophene	13.7	0.00	6.37		1.01
C1-dibenzothiophenes	66.4	27.9			41.3
C2-dibenzothiophenes	171	97.2	2.98		108
C3-dibenzothiophenes	225	117			117
C4-dibenzothiophenes	182				133
Fluoranthene	12.0	4.26	26.6		5.24
Pyrene	17.7	22.6			20.7
C1-fluoranthrenes/pyrenes	183	63.3	8.31		106
C2-fluoranthrenes/pyrenes	256	109			87.5
C3-fluoranthrenes/pyrenes	251	133			211
Benz(a)anthracene	7.22	2.20	2.44		1.94
Chrysene	28.7	17.2			30.7
C1-chrysenes	82.5	29.1	13.8		49.4

Project no. 302006392	Report No 2023:00369	Version Final	21 of 118
---------------------------------	--------------------------------	-------------------------	------------------

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	WRG	2021-5427	2021-5427		2021-5427
Internal Lab ID	LSFO 1	2021-09-17-6081	2021-5427		2021-5427
Oil type	WRG	WRG	WRG	No data reported	WRG
	mg/kg oil	mg/kg oil	mg/kg oil		mg/kg oil
C2-chrysenes	107	47.3	0.61		60.4
C3-chrysenes	97.3	63.8			44.9
C4-chrysenes	74.6				32.1
Benzo(b)fluoranthene	8.23	2.84	1.399		11.0
Benzo(k)fluoranthene	4.02	0.00			ND
Benzo(e)pyrene	10.6	6.72	4.586		9.20
Benzo(a)pyrene	6.64	0.67	1.546		8.63
Perylene	3.86	1.09			1.26
Indeno(1,2,3-c,d)pyrene	2.78	0.29	0.777		0.48
Dibenz(a,h)anthracene	3.03	0.25			0.10
Benzo(g,h,i)perylene	4.76	1.69			2.23
Phenol	NA	NA	24.4		3.81
C1-Phenols	NA	NA	57.9		ND
C2-Phenols	NA	NA			ND
C3-Phenols	NA	NA			ND
C4-Phenols	NA	NA			ND
C5-Phenols	NA	NA			ND
30 ab hopane	132	159	NA		251
Sum all compounds (not hopane)	8832	4973	2359		7122
Decalins		0	26.8		1527
Naphthalenes	1063	677	2102		857
2-3 ring PAHs	7669	3791	87.7		4051
4-6 ring PAHs	1162	505	60.1		683
C0-C5 Phenols		0	122		3.81

Table 5-5 *Semi-volatile components reported for the MGO. No results reported from Sweden. (NA: Not analyzed; ND: Not detected). Comments given by the laboratories to their results are given in Appendix B.*

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	MGO	2021-5428	2021-5428		2021-5428
Internal Lab ID	LSFO 2	2021-09-17-6082			2021-5428
Oil type	MGO	MGO	MGO	No data reported	MGO
	mg/kg oil	mg/kg oil	mg/kg oil		mg/kg oil
Decalin	NA	NA	29.9		1554
C1-decalins	NA	NA	NA		2847
C2-decalins	NA	NA	NA		3002
C3-decalins	NA	NA	NA		2783
C4-decalins	NA	NA	NA		1642
Benzo(b)thiophene	NA	NA	23.0		28.1
Naphthalene	1749	1107	167		2193
C1-naphthalenes	7042	3719	182		5246
C2-naphthalenes	11015	6676	2001		7515
C3-naphthalenes	9047	6241			5590
C4-naphthalenes	4815	3364			3072
Biphenyl	867	569			886
Acenaphthylene	47.8	38.0			31.1
Acenaphthene	100	90.2			108
Dibenzofuran	266				249
Fluorene	602	479	111		583
C1-fluorenes	2601	1856			1427
C2-fluorenes	5988	2835			2309
C3-fluorenes	5330	2357			1816
Phenanthrene	822	581	19.4		789
Anthracene	114	95.2			91.7
C1-phenanthrenes/anthracenes	2879	2194	17.7		2071
C2-phenanthrenes/anthracenes	3274	2465	62.7		2288
C3-phenanthrenes/anthracenes	2290	1688			1403
C4-phenanthrenes/anthracenes	1021	770			688
Dibenzothiophene	71.5	55.8	16.9		52.4
C1-dibenzothiophenes	326	254			178
C2-dibenzothiophenes	501	397	2.79		254
C3-dibenzothiophenes	456	246			211
C4-dibenzothiophenes	220				128
Fluoranthene	46.8	36.7	20.7		32.9
Pyrene	254	255			267
C1-fluoranthrenes/pyrenes	710	380	24.6		403
C2-fluoranthrenes/pyrenes	443	236			54.6
C3-fluoranthrenes/pyrenes	218	115			157
Benz(a)anthracene	10.3	7.04	0.687		7.60
Chrysene	24.5	24.7			40.6
C1-chrysenes	46.7	28.5	3.38		39.4

Project no. 302006392	Report No 2023:00369	Version Final	23 of 118
---------------------------------	--------------------------------	-------------------------	------------------

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	MGO	2021-5428	2021-5428		2021-5428
Internal Lab ID	LSFO 2	2021-09-17-6082			2021-5428
Oil type	MGO	MGO	MGO	No data reported	MGO
	mg/kg oil	mg/kg oil	mg/kg oil		mg/kg oil
C2-chrysenes	37.5	24.9	0.66		25.3
C3-chrysenes	27.2	8.97			11.7
C4-chrysenes	16.2				3.12
Benzo(b)fluoranthene	4.96	1.57	0.166		2.24
Benzo(k)fluoranthene	1.08	0.00			ND
Benzo(e)pyrene	2.46	1.79	5.253		1.82
Benzo(a)pyrene	2.90	0.52	0.000		0.67
Perylene	2.60	0.43			0.68
Indeno(1,2,3-c,d)pyrene	2.95	0.06	0.000		0.06
Dibenz(a,h)anthracene	3.13	0.09			0.07
Benzo(g,h,i)perylene	2.48	0.10			0.14
Phenol	NA	NA	27.2		9.69
C1-Phenols	NA	NA	67.2		ND
C2-Phenols	NA	NA			ND
C3-Phenols	NA	NA			ND
C4-Phenols	NA	NA	54.9		ND
C5-Phenols	NA	NA			ND
30 ab hopane	6.64	6.04	NA		7.22
Sum all compounds (not hopane)	63301	39199	2838		52094
Decalins	NA	NA	29.9		11829
Naphthalenes	33668	21108	2350		23616
2-3 ring PAHs	61444	16969	254		15591
4-6 ring PAHs	1857	1122	55.4		1049
C0-C5 Phenols	NA	NA	149		9.69

Table 5-6 *Semi-volatile components reported for VLSFO. No results reported from Sweden. (NA: Not analyzed; ND: Not detected). Comments given by the laboratories to their results are given in Appendix B.*

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	VLSFO	2021-5429	2021-5429		2021-5429
Internal Lab ID	LSFO 3	2021-09-17-6083			2021-5429
Oil type	VLSFO	VLSFO	VLSFO	Not reported	VLSFO
	mg/kg oil	mg/kg oil	mg/kg oil		mg/kg oil
Decalin	NA	NA	19.2		22.4
C1-decalins	NA	NA			46.3
C2-decalins	NA	NA			74.3
C3-decalins	NA	NA			77.7
C4-decalins	NA	NA			56.9
Benzo(b)thiophene	NA	NA	38.5		47.6
Naphthalene	2973	1730	166		2503
C1-naphthalenes	5694	3128	2720		3820
C2-naphthalenes	7482	4924	576		5604
C3-naphthalenes	6456	4433			4037
C4-naphthalenes	2950	2271			2099
Biphenyl	147	108			151
Acenaphthylene	54.0	36.8			33.3
Acenaphthene	152	112			154
Dibenzofuran	69.1				56.3
Fluorene	197	151	57.6		203
C1-fluorenes	1053	758			637
C2-fluorenes	3586	1458			1373
C3-fluorenes	3958	1640			1481
Phenanthrene	903	612	14.3		925
Anthracene	161	130			24.6
C1-phenanthrenes/anthracenes	4016	3091	15.8		2929
C2-phenanthrenes/anthracenes	6534	4686	160		4611
C3-phenanthrenes/anthracenes	6225	4213			4359
C4-phenanthrenes/anthracenes	3940	2525			2541
Dibenzothiophene	102	78.8	18.5		85.0
C1-dibenzothiophenes	542	388			319
C2-dibenzothiophenes	978	785	20.2		570
C3-dibenzothiophenes	1059	809			517
C4-dibenzothiophenes	664				414
Fluoranthene	116	80.1	69.1		86.4
Pyrene	504	489			589
C1-fluoranthrenes/pyrenes	3313	1653	33.3		1825
C2-fluoranthrenes/pyrenes	5132	2507			697
C3-fluoranthrenes/pyrenes	4827	2635			4030
Benz(a)anthracene	259	228	5.95		283
Chrysene	422	337			578
C1-chrysenes	2109	1464	15.1		1962
C2-chrysenes	3189	2304	6.76		2754

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	VLSFO	2021-5429	2021-5429		2021-5429
Internal Lab ID	LSFO 3	2021-09-17-6083			2021-5429
Oil type	VLSFO	VLSFO	VLSFO	Not reported	VLSFO
	mg/kg oil	mg/kg oil	mg/kg oil		mg/kg oil
C3-chrysenes	3050	1955			2124
C4-chrysenes	1885				923
Benzo(b)fluoranthene	125	91.1	7.31		114
Benzo(k)fluoranthene	28.7	9.24			ND
Benzo(e)pyrene	239	219	12.2		224
Benzo(a)pyrene	153	161	4.53		171
Perylene	72.3	66.3			177
Indeno(1,2,3-c,d)pyrene	37.4	35.8	13.8		27.9
Dibenz(a,h)anthracene	59.3	46.4			54.8
Benzo(g,h,i)perylene	114	113			143
Phenol	NA	NA	38.6		9.22
C1-Phenols	NA	NA	69.8		ND
C2-Phenols	NA	NA			ND
C3-Phenols	NA	NA			ND
C4-Phenols	NA	NA	37.2		ND
C5-Phenols	NA	NA			ND
30 ab hopane	158	119			193
Sum all compounds (not hopane)	85530	52460	4119		56545
Decalins	NA	NA	19.2		278
Naphthalenes	25555	16486	3461		18063
2-3 ring PAHs	59895	21581	324		21431
4-6 ring PAHs	25635	14393	168		16765
C0-C5 Phenols	NA	NA	146		9.22

Table 5-7 Volatile components reported for WRG, MGO and VLSFO. No results reported from Sweden, USA, and Canada. (NA: Not analyzed; ND: Not detected). Comments given by the laboratories to their results are given in Appendix B.

Laboratory Sample ID Oil type	China	Norway	China	Norway	China	Norway
	2021-5427	2021-5427	2021-5428	2021-5428	2021-5429	2021-5429
	WRG mg/kg	WRG mg/kg	MGO mg/kg	MGO mg/kg	VLSFO mg/kg	VLSFO mg/kg
Isopentane	0.00	ND	0.00	ND	0.00	ND
n-C5 (Pentane)	0.00	ND	0.00	ND	0.00	ND
Cyclopentane	0.00	ND	0.00	ND	0.00	ND
2-methylpentane	1.16	ND	5.42	ND	0.00	ND
3-Methylpentane	2.11	ND	7.11	ND	1.97	ND
n-C6 (Hexane)	1.27	ND	4.02	ND	0.00	ND
Methylcyclopentane	10.3	ND	30.1	ND	0.00	ND
Benzene	280	ND	405	ND	68.6	ND
Cyclohexane	36.8	ND	27.0	90.2	0.00	ND
2,3-Dimethylpentane	3.48	ND	10.1	ND	0.00	ND
3-methylhexane	3.80	ND	0.00	ND	0.00	ND
n-C7 (Heptane)	1.52	ND	11.9	ND	0.00	ND
Methylcyclohexane	23.5	75.7	25.7	604	0.00	ND
Toluene	548	48.4	1749	435	278	42.0
2,4 dimethylhexane	0.00	ND	55.3	ND	0.00	ND
2-Methylheptane	0.00	ND	0.00	ND	0.00	ND
n-C8 (Octane)	322	ND	366	1794	0.00	4.51
Ethylbenzene	290	20.2	399	568	99.2	31.0
m-Xylene	381	64.6	896	2377	0.00	106
p-Xylene		21.4		654	536	39.6
o-Xylene	133	28.2	183	1250	0.00	52.2
n-C9 (Nonane)	27.3	71.5	37.4	7044	51.0	32.1
Propylbenzene	45.5	10.6	128	1016	38.5	22.8
1-Methyl-3-ethylbenzene	184	40.9	1074	3394	272	131
1-Methyl-4-ethylbenzene	66.2	18.7		1235		58.0
1,3,5-trimethylbenzene	73.8	21.9		1776	0.00	59.8
1-Methyl-2-ethylbenzene		22.2		1598		44.6
1,2,4-Trimethylbenzene	274	68.7	1524	5087	0.00	289
n-C10 (Decane)		511		14368		101
1,2,3-Trimethylbenzene	240	40.4		2448	188	89.4
n-Butylbenzene	12.4	19.0	12.1	1169	30.7	34.2
1,2,4,5-Tetramethylbenzene	0.629	13.4	113	1755	0.0000	260
n-Pentylbenzene	1.21	39.9	65.5	606	7.77	61.4
Sum VOC	2962	1137	7129	49267	1571	1459
BTEX	1632	183	3632	5283	981	271
C3-benzenes	882	223	2726	16554	498	695
Other VOC	447	731	770	27430	91.5	489

5.2 Chemistry of the WAFs

The experimental conditions for generating WAFs are given in Table 5-8. China has prepared WAFs in both seawater and freshwater. Data from the seawater WAFs are used in comparison with the other laboratories and the results of the freshwater WAFs are given in Appendix C3.

Table 5-8 Experimental conditions for WAF preparation, including the recommended conditions given in the protocol (Daling et al., (2021)).

Laboratory	Recommended in protocol	USA	Canada	China	Sweden	Norway
Oil to water ratio	1:40	1:40	1:40	1:40	1:40	1:40
Temperature	2 °C	23 °C	4°C	4°C	4 °C	2 °C
Time	72 h	18 h	72 h	72h	72 h	72 h
Settling time	Not given	6 h	Not recorded	0.5h	1 h	< 5 min

The laboratories were asked to submit the GC chromatograms for the WAFs. GC chromatograms from USA and Norway are shown in Figure 5-2, and from Canada and Sweden in Figure 5-3. No chromatograms are reported from China. The chromatogram of WRG from Sweden indicates that there were oil droplets in the WAF, as n-alkane peaks from C9 to C24 seems to be detected in their LE-WAF. There also an UCM-hump (unresolved complex materials) present in their WAF that is not observed in the chromatograms from USA and Norway.

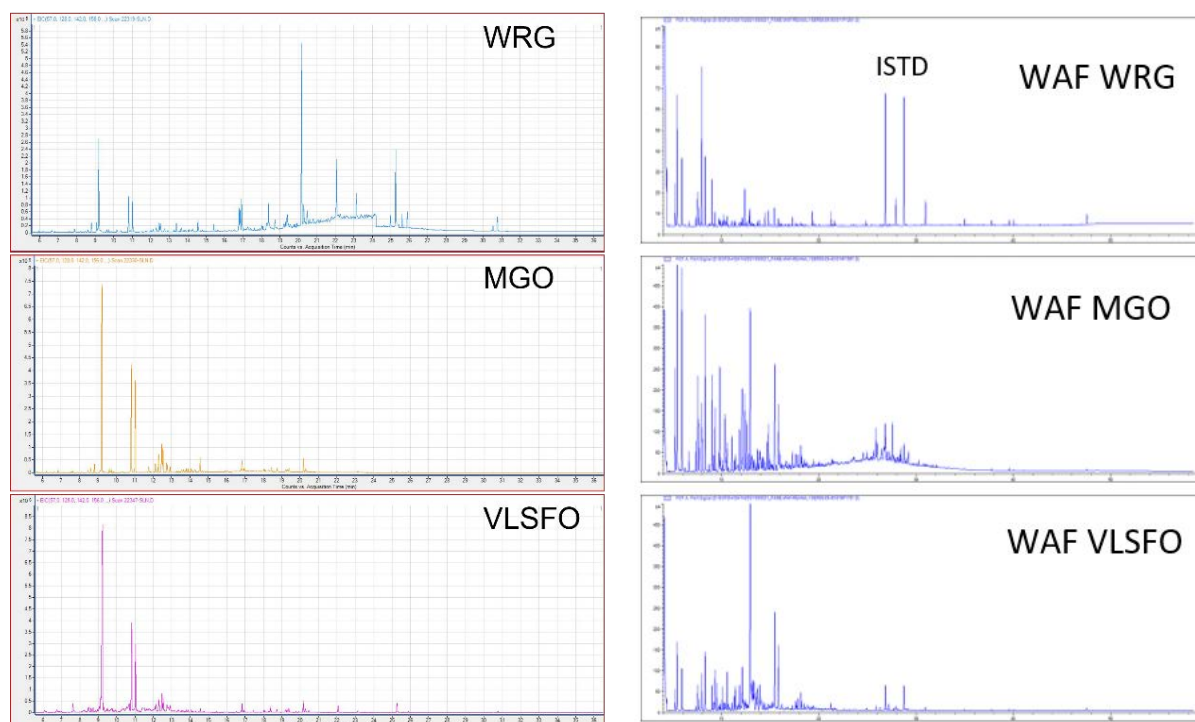


Figure 5-2 GC chromatograms of the WAFs from USA (left) and Norway (right).

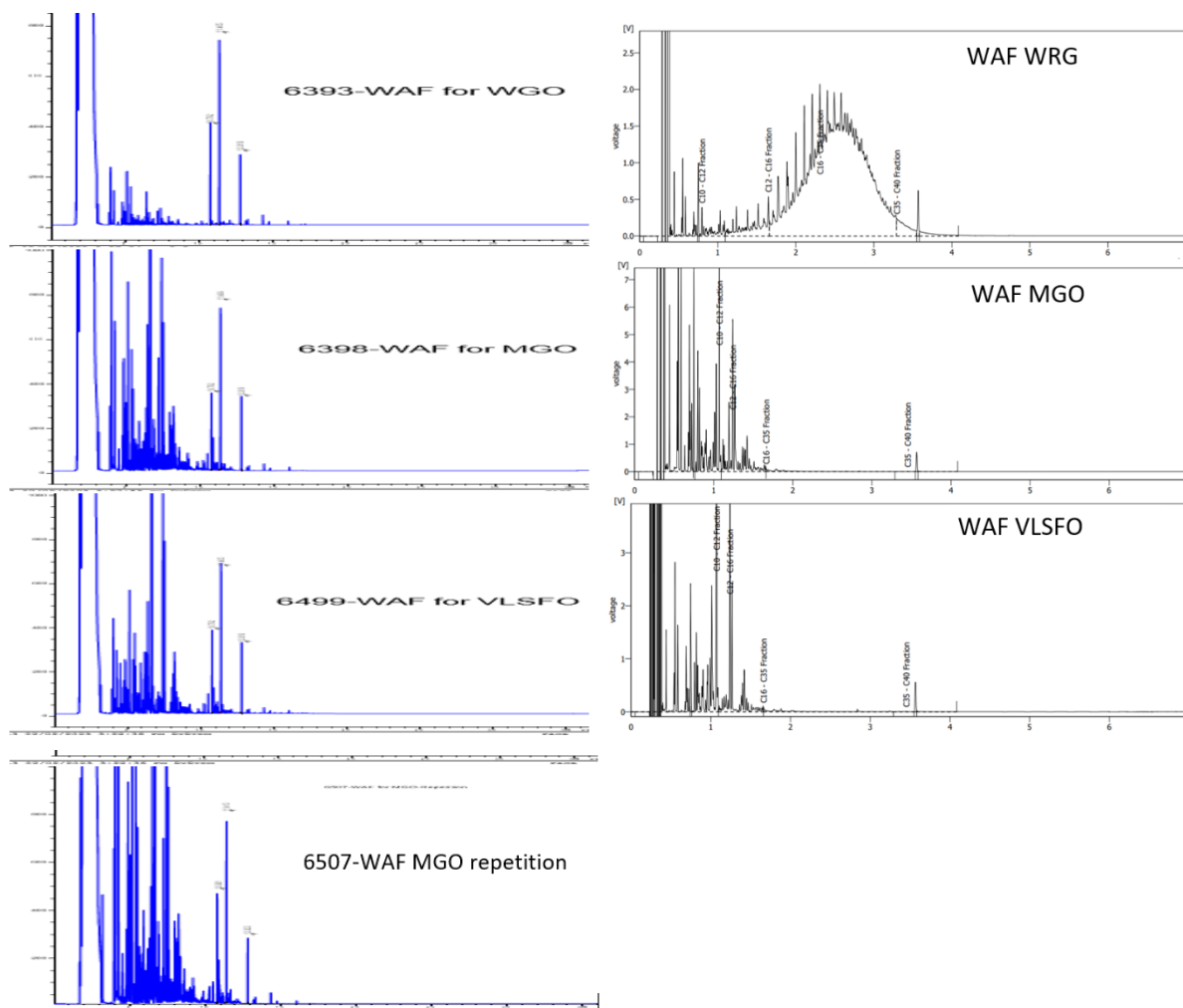


Figure 5-3 GC chromatograms of the WAFs from Canada and Sweden (No chromatograms reported from China)

A summary of the reported WAF results is shown in Figure 5-4 and is given in Table 5-9 for WRG, Table 5-10 for MGO, and Table 5-11 for VLSFO. Detailed results from the SVOC analyses in the WAFs are given in Table 5-12 for WRG, Table 5-13 for MGO, and Table 5-14 for VLSFO. Results from the VOC analyses in the WAFs are given in Table 5-15 for WRG, Table 5-16 for MGO, and Table 5-17 for VLSFO. Canada has not reported any volatiles. The reported results from the SVOC and VOC analyses of the WAFs from each laboratory are given in Appendix C.

Preparing WAFs in different laboratories, even with the same oils, may give different results although the same protocols have been followed. The results will be impacted of details such as the temperatures on water and oil when the WAFs are prepared, oil droplets in the water phase, different methods for sample preparation, instrument conditions, and quantification methods.

A summary of the quantified components and UCM in the WAFs is summarized in Figure 5-4 and illustrates that the composition of the WAFs prepared by the participating laboratories varied. Although the total WAF concentration for MGO are in the same range for WAFs prepared by USA and Norway (6.3 mg/L and 7.2 mg/L), and by China and Sweden (2.6 mg/L and 2.3 mg/L), the chemical composition of the WAFs were different. In WAF of VLSFO, Sweden reported higher concentration of total SVOC (mainly naphthalenes (1629 of 1670 µg/L)) than TPH, resulting in a negative UCM concentration ($UCM = TPH - SVOC = -811 \mu\text{g/L}$).

WAF composition

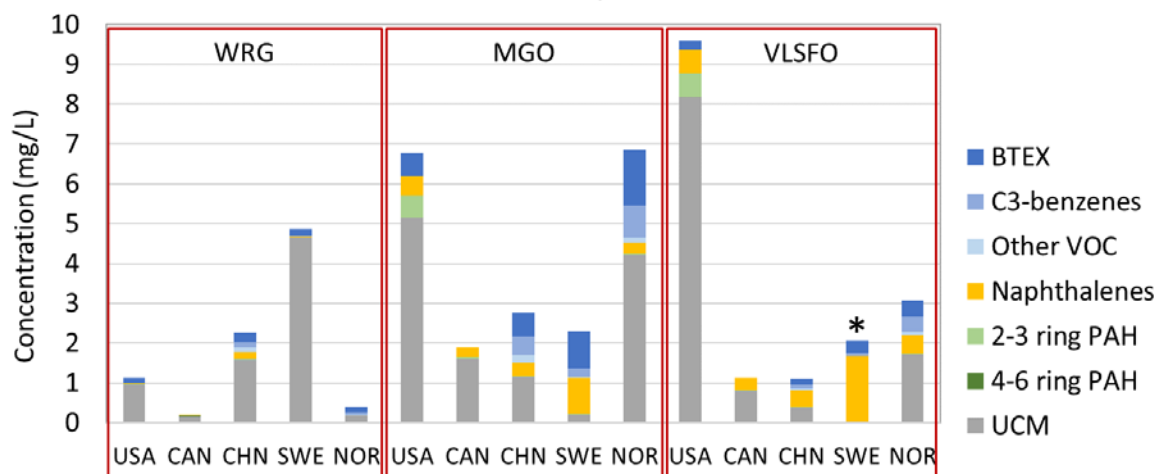


Figure 5-4 Summary of the quantified components and UCM in the WAFs. The groups compositions are given in Table F 1. Canada has not reported volatiles. *UCM not included for WAF of VLSFO for SWE, as the concentration of naphthalenes was reported higher than TPH (gives negative UCM).

Table 5-9 Summary of reported results of the chemical composition of WAF of WRG oil in seawater. Description of the component groups are given in Table F 1 (Appendix F). NA: Not analyzed; * Total WAF for USA is sum of TPH and BTEX. No volatiles reported from Canada.

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	WRG	WGO	2021-5427		2021-5427
Internal Lab ID	LSFO 1	WAF1	TO1	E21-055-1	2021-5427
Oil type	WRG	WRG	WRG	WRG	WRG
	µg/L	µg/L	µg/L	µg/L	µg/L
Tot WAF	1118*		1967	4865	392
TPH	981	185	1820	4670	187
Sum SVOC	25.0	19.3	464	16.0	18.2
Sum VOC		NA	147	195	205
UCM (TPH-SVOC)	956	166	1356	4654	169
Decalins	NA	NA	0.00	NA	0.177
Naphthalenes	9.35	10.1	293	11.1	8.00
2-3 ring PAH	22.1	8.32	29.6	4.30	5.08
4-6 ring PAH	2.92	0.89	13.5	0.55	0.295
C0-C5 phenols	NA	NA	128	NA	4.64
BTEX	137	NA	102	164	140
C3-benzenes	NA	NA	42.8	30.3	49.4
Other VOC	NA	NA	2.00	ND	15.6

Table 5-10 Summary of reported results of the chemical composition of WAF of MGO in seawater. Description of the component groups are given in Table F 1 (Appendix F). NA: Not analyzed. * Total WAF for USA is sum of TPH and BTEX. No volatiles reported from Canada.

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	MGO	MGO-repetition	2021-5428		2021-5428
Internal Lab ID	LSFO 2	WAF1	TO2	E21-055-3	2021-5428
Oil type	MGO	MGO	MGO	MGO	MGO
	µg/L	µg/L	µg/L	µg/L	µg/L
Tot WAF	6299*		2582	2295	7237
TPH	5702	1894	1440	1120	4911
Sum SVOC	554	302	523	925	702
Sum VOC		NA	1142	1175	2326
UCM (TPH-SVOC)	5148	1592	917	195	4209
Decalins	NA	NA	0.00	NA	1.12
Naphthalenes	479	247	296	907	276
2-3 ring PAH	553	53.1	27.9	18.0	36.3
4-6 ring PAH	0.937	1.29	19.9	0.500	1.54
C0-C5 phenols	NA	NA	180	NA	387
BTEX	597	NA	656	922	1406
C3-benzenes	NA	NA	471	226	796
Other VOC	NA	NA	14.9	26.0	125

Table 5-11 Summary of reported results of the chemical composition of WAF of VLSFO in seawater. Description of the component groups are given in Table F 1 (Appendix F). NA: Not analyzed. * Total WAF for USA is sum of TPH and BTEX.

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	VLSFO	VLSFO	2021-5429		2021-5429
Internal Lab ID	LSFO 3	WAF2	TO3	E21-055-2	2021-5429
Oil type	VLSFO	VLSFO	VLSFO	VLSFO	VLSFO
	µg/L	µg/L	µg/L	µg/L	µg/L
Tot WAF	9017*		1008	1243	3127
TPH	8787	1122	693	859	2250
Sum SVOC	615	329	420	1670	540
Sum VOC		NA	315	384	877
UCM (TPH-SVOC)	NQ	793	273	-811	1710
Decalins	NA	NA	0.00	NA	0.26
Naphthalenes	574	303	350	1653	471
2-3 ring PAH	612	23.5	15.5	16.8	25.9
4-6 ring PAH	2.68	2.50	12.7	0.519	1.28
C0-C5 phenols	NA	NA	42.3	NA	41.9
BTEX	230	NA	155	296	418
C3-benzenes	NA	NA	139	86.5	392
Other VOC	NA	NA	20.8	1.60	66.9

Table 5-12 *Semi-volatile components reported in the WAFs of WRG oil in seawater. (NA, / or *: Not analyzed; ND: Not detected). Comments given by the laboratories to their results are given in Appendix C.*

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	WRG	WGO	2021-5427		WRG
Internal Lab ID	LSFO 1	WAF 1	TO1	E21-055-1	2021-5427
Oil type	WRG	WRG	WRG	WRG	WRG
	µg/L	µg/L	µg/L	µg/L	µg/L
Decalin	NA	/	0.000	*	0.051
C1-decalins	NA	/		*	0.020
C2-decalins	NA	/		*	0.023
C3-decalins	NA	/		*	0.028
C4-decalins	NA	/		*	0.055
Benzo(b)thiophene	NA	/	8.45	*	ND
Naphthalene	2.49	2.88	198	4.00	3.43
C1-naphthalenes	2.95	3.57	43.1	7.14	2.18
C2-naphthalenes	2.18	2.20	51.9	<1.00	1.38
C3-naphthalenes	1.16	0.98		<1.00	0.844
C4-naphthalenes	0.573	0.44		*	0.167
Biphenyl	1.68	1.97		*	2.23
Acenaphthylene	0.043	0.01		<0.040	0.034
Acenaphthene	0.034	0.03		<0.20	0.022
Dibenzofuran	0.283	/		*	0.223
Fluorene	0.566	0.45		0.56	0.444
C1-fluorenes	1.45	1.07		*	0.513
C2-fluorenes	1.18	0.64		*	0.354
C3-fluorenes	0.684	0.30		*	0.136
Phenanthrene	0.641	0.43	2.79	0.880	0.381
Anthracene	0.090	0.06		0.180	0.015
C1-phenanthrenes/anthracenes	1.47	0.96		2.68	0.307
C2-phenanthrenes/anthracenes	1.35	1.13	12.30	<1.50	0.209
C3-phenanthrenes/anthracenes	1.01	0.74		<1.00	0.055
C4-phenanthrenes/anthracenes	1.02	0.31		*	0.021
Dibenzothiophene	0.093	0.14	6.01	<1.00	0.005
C1-dibenzothiophenes	0.307	0.04		<1.00	0.031
C2-dibenzothiophenes	0.302	0.03		<1.00	0.036
C3-dibenzothiophenes	0.301	0.01		<1.00	0.029
C4-dibenzothiophenes	0.233	/		*	0.030
Fluoranthene	0.088	0.10	2.45	0.330	0.007
Pyrene	0.041	0.05		0.170	0.025
C1-fluoranthrenes/pyrenes	1.11	0.33	5.04	*	0.038
C2-fluoranthrenes/pyrenes	0.623	0.23		*	0.050
C3-fluoranthrenes/pyrenes	0.267	0.10		*	0.050
Benz(a)anthracene	0.016	0.02	3.86	<0.040	0.021
Chrysene	0.026	0.01		0.038	0.004
C1-chrysenes	0.199	0.01		*	0.008
C2-chrysenes	0.165	0.01		*	0.007

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	WRG	WGO	2021-5427		WRG
Internal Lab ID	LSFO 1	WAF 1	TO1	E21-055-1	2021-5427
Oil type	WRG	WRG	WRG	WRG	WRG
	µg/L	µg/L	µg/L	µg/L	µg/L
C3-chrysenes	ND	0.01		*	0.028
C4-chrysenes	ND	/		*	ND
Benzo(b)fluoranthene	0.090	0.01		<0.030	0.008
Benzo(k)fluoranthene	0.029	0.00		<0.020	0.005
Benzo(e)pyrene	0.112	0.00		*	0.006
Benzo(a)pyrene	0.121	0.00	2.12	<0.020	0.005
Perylene	0.027	0.00		*	0.003
Indeno(1,2,3-c,d)pyrene	ND	0.00		<0.010	0.012
Dibenz(a,h)anthracene	ND	0.00		<0.010	0.008
Benzo(g,h,i)perylene	ND	0.00		0.013	0.012
Phenol		/	23.9	*	0.925
C1-Phenols		/	82.8	*	0.935
C2-Phenols		/		*	0.443
C3-Phenols		/		*	1.20
C4-Phenols		/	20.9	*	0.445
C5-Phenols		/		*	0.685
30 ab hopane	0.004	nd		*	ND
Sum all SVOC (not hopane)	25.0	19.3	464	16.0	18.2
Decalins	NA	/		NA	0.177
Naphthalenes	9.35	10.1	293	11.1	8.00
2-3 ring PAHs	22.1	8.32	29.6	4.30	5.08
4-6 ring PAHs	2.92	0.89	13.5	0.551	0.295
C0-C5 Phenols	NA	/	128	NA	4.64

Table 5-13 *Semi-volatile components reported in the WAFs of MGO in seawater. (NA or *: Not analyzed; ND: Not detected). Comments given by the laboratories to their results are given in Appendix C.*

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	MGO	MGO repetition	2021-5428		MGO
Internal Lab ID	LSFO 2	WAF1	TO2	E21-055-3	2021-5428
Oil type	MGO	MGO	MGO	MGO	MGO
	µg/L	µg/L	µg/L	µg/L	µg/L
Decalin	NA	/	ND	*	0.40
C1-decalins	NA	/		*	0.16
C2-decalins	NA	/		*	0.13
C3-decalins	NA	/		*	0.18
C4-decalins	NA	/		*	0.26
Benzo(b)thiophene	NA	/	8.89	*	0.06
Naphthalene	183	65.1	221	380	130
C1-naphthalenes	188	95.2	28.5	501	102
C2-naphthalenes	85.1	60.1	46.1	25.5	32.7
C3-naphthalenes	19.6	20.8		<1.00	8.69
C4-naphthalenes	3.88	6.19		*	3.21
Biphenyl	19.9	11.3		*	10.6
Acenaphthylene	0.427	0.31		0.480	0.643
Acenaphthene	1.77	1.17		<2.5	1.11
Dibenzofuran	5.50	/		*	2.49
Fluorene	9.96	5.13		9.50	5.05
C1-fluorenes	10.8	5.97		*	3.45
C2-fluorenes	3.93	3.01		*	1.97
C3-fluorenes	1.67	0.89		*	0.56
Phenanthrene	5.54	2.80	2.79	3.90	2.66
Anthracene	0.515	4.15		0.320	0.580
C1-phenanthrenes/anthracenes	6.23	10.6		3.76	2.45
C2-phenanthrenes/anthracenes	2.12	5.59	13.10	<1.00	0.894
C3-phenanthrenes/anthracenes	0.445	1.24		<1.00	0.344
C4-phenanthrenes/anthracenes	ND	0.24		*	0.229
Dibenzothiophene	0.530	0.25	3.10	<1.00	0.282
C1-dibenzothiophenes	1.85	0.25		<1.00	0.758
C2-dibenzothiophenes	1.05	0.12		<1.00	1.10
C3-dibenzothiophenes	0.854	0.03		<1.00	0.792
C4-dibenzothiophenes	0.327	/		*	0.299
Fluoranthene	0.115	0.34	4.94	0.23	0.251
Pyrene	0.335	0.27		0.27	0.272
C1-fluoranthrenes/pyrenes	0.438	0.51	7.26	*	0.281
C2-fluoranthrenes/pyrenes	ND	0.12		*	0.492
C3-fluoranthrenes/pyrenes	ND	0.02		*	0.172
Benz(a)anthracene	0.016	0.01	2.05	<0.010	0.012
Chrysene	0.032	0.01		<0.010	0.004
C1-chrysenes	ND	0.01	0.07	*	0.020
C2-chrysenes	ND	0.01	0.23	*	0.008

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	MGO	MGO repetition	2021-5428		MGO
Internal Lab ID	LSFO 2	WAF1	TO2	E21-055-3	2021-5428
Oil type	MGO	MGO	MGO	MGO	MGO
	µg/L	µg/L	µg/L	µg/L	µg/L
C3-chrysenes	ND	0.00		*	0.011
C4-chrysenes	ND	/		*	ND
Benzo(b)fluoranthene	ND	0.00	0.00	<0.010	0.003
Benzo(k)fluoranthene	ND	0.00		<0.010	0.002
Benzo(e)pyrene	ND	0.00	0.88	*	0.002
Benzo(a)pyrene	ND	0.00	5.61	<0.010	0.002
Perylene	ND	0.00		*	0.002
Indeno(1,2,3-c,d)pyrene	ND	0.00		<0.010	0.003
Dibenz(a,h)anthracene	ND	0.00		<0.010	0.002
Benzo(g,h,i)perylene	ND	0.00		<0.010	0.00
Phenol	NA	/	70.8	*	63.1
C1-Phenols	NA	/	92.3	*	111
C2-Phenols	NA	/		*	112
C3-Phenols	NA	/		*	62.3
C4-Phenols	NA	/	16.8	*	30.9
C5-Phenols	NA	/		*	7.47
30 ab hopane	0.004	nd		*	ND
Sum all SVOC (not hopane)	554	302	523	925	702
Decalins	NA	/		NA	1.12
Naphthalenes	479	247	296	907	276
2-3 ring PAHs	553	53.1	27.9	18.0	36.3
4-6 ring PAHs	0.937	1.29	19.9	0.50	1.54
C0-C5 Phenols	NA	/	180	NA	387

Table 5-14 *Semi-volatile components reported in the WAFs of VLSFO in seawater. (NA or *: Not analyzed; ND: Not detected). Comments given by the laboratories to their results are given in Appendix C.*

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	VLSFO	VLSFO	2021-5429		2021-5429
Internal Lab ID	LSFO 3	WAF 1	TO3	E21-055-2	2021-5429
Oil type	VLSFO	VLSFO	VLSFO	VLSFO	VLSFO
	µg/L	µg/L	µg/L	µg/L	µg/L
Decalin	NA	/	ND	*	0.007
C1-decalins	NA	/		*	0.015
C2-decalins	NA	/		*	0.055
C3-decalins	NA	/		*	0.088
C4-decalins	NA	/		*	0.092
Benzo(b)thiophene	NA	/	4.30	*	3.87
Naphthalene	345	94.7	210	1100	296
C1-naphthalenes	148	101	88.4	529	120
C2-naphthalenes	62.4	48.6	51.2	24	43.4
C3-naphthalenes	16.0	16.0		<1.00	9.34
C4-naphthalenes	3.17	2.71		*	1.63
Biphenyl	3.72	3.08		*	3.59
Acenaphthylene	0.287	0.50		0.89	1.22
Acenaphthene	2.63	2.15		3.5	2.84
Dibenzofuran	1.26	/		*	0.886
Fluorene	2.83	1.95		3.30	2.50
C1-fluorenes	3.82	2.79		*	1.35
C2-fluorenes	2.14	1.92		*	0.797
C3-fluorenes	0.851	1.02		*	0.671
Phenanthrene	5.10	3.12	2.79	3.90	3.19
Anthracene	0.690	0.49		0.540	0.402
C1-phenanthrenes/anthracenes	6.69	5.19		4.71	2.29
C2-phenanthrenes/anthracenes	3.31	3.74	5.99	<1.00	1.05
C3-phenanthrenes/anthracenes	0.958	2.12		<1.00	0.235
C4-phenanthrenes/anthracenes	ND	1.22		*	0.047
Dibenzothiophene	0.727	0.43	2.43	<1.00	0.376
C1-dibenzothiophenes	2.04	0.58		<1.00	0.344
C2-dibenzothiophenes	0.696	0.49		<1.00	0.164
C3-dibenzothiophenes	ND	0.32		<1.00	0.041
C4-dibenzothiophenes	ND	/		*	0.018
Fluoranthene	0.129	0.11	4.02	0.11	0.098
Pyrene	0.536	0.50		0.35	0.433
C1-fluoranthrenes/pyrenes	0.866	0.84	2.69	*	0.298
C2-fluoranthrenes/pyrenes	0.488	1.19		*	0.073
C3-fluoranthrenes/pyrenes	0.326	1.16		*	0.224
Benz(a)anthracene	0.063	0.69	2.36	0.024	0.031
Chrysene	0.057	0.18		0.035	0.024
C1-chrysenes	0.120	0.64	0.161	*	0.033
C2-chrysenes	0.037	0.92	0.292	*	0.011

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	VLSFO	VLSFO	2021-5429		2021-5429
Internal Lab ID	LSFO 3	WAF 1	TO3	E21-055-2	2021-5429
Oil type	VLSFO	VLSFO	VLSFO	VLSFO	VLSFO
	µg/L	µg/L	µg/L	µg/L	µg/L
C3-chrysenes	ND	0.80		*	0.027
C4-chrysenes	ND	/		*	ND
Benzo(b)fluoranthene	ND	0.03	ND	<0.010	0.004
Benzo(k)fluoranthene	0.024	0.01		<0.010	0.001
Benzo(e)pyrene	ND	0.08		*	0.005
Benzo(a)pyrene	ND	0.06	3.58	<0.010	0.003
Perylene	ND	0.02		*	0.002
Indeno(1,2,3-c,d)pyrene	0.039	0.01		<0.010	0.004
Dibenz(a,h)anthracene	ND	0.01		<0.010	0.003
Benzo(g,h,i)perylene	ND	0.04		<0.010	0.004
Phenol	NA	/	17.4	*	6.05
C1-Phenols	NA	/	13.2	*	5.30
C2-Phenols	NA	/		*	10.3
C3-Phenols	NA	/		*	12.1
C4-Phenols	NA	/	11.7	*	6.10
C5-Phenols	NA	/		*	2.06
30 ab hopane	0.005	0.07		*	ND
Sum all SVOC (not hopane)	615	329	420	1670	540
Decalins	NA	/		NA	0.257
Naphthalenes	574	303	350	1653	471
2-3 ring PAHs	612	23.5	15.5	16.8	25.9
4-6 ring PAHs	2.68	2.50	12.7	0.52	1.28
C0-C5 Phenols	NA	/	42.3	NA	41.9

Table 5-15 Volatile components reported in the WAFs of WRG in seawater. (NA or *: Not analyzed; ND: Not detected). Comments given by the laboratories to their results are given in Appendix C.

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	WRG		2021-5427		2021-5427
Internal Lab ID	LSFO 1			E21-055-1	2021-5427
Oil type	WRG	Not reported	WRG	WRG	WRG
	µg/L		µg/L	µg/L	µg/L
Isopentane			0.03	*	ND
n-C5 (Pentane)				*	ND
Cyclopentane			0.23	*	ND
2-methylpentane			0.04	*	ND
3-Methylpentane			0.01	*	ND
n-C6 (Hexane)			0.15	*	ND
Methylcyclopentane			0.07	*	1.19
Benzene	15.6		13.5	19.8	9.72
Cyclohexane			0.01	*	6.51
2,3-Dimethylpentane				*	ND
3-methylhexane			0.01	*	ND
n-C7 (Heptane)			0.44		ND
Methylcyclohexane			0.04	*	3.43
Toluene	50.7		40.74	66.9	49.8
2,4 dimethylhexane				*	ND
2-Methylheptane			0.14	*	ND
n-C8 (Octane)			0.30	*	ND
Ethylbenzene	6.75		7.11	10.4	9.10
m-Xylene	44.2		25.7	45.9	39.6
p-Xylene			15.0	*	11.1
o-Xylene	19.6		0.09	21.3	20.9
n-C9 (Nonane)			0.00	*	ND
Propylbenzene			1.68	3.10	1.71
1-Methyl-3-ethylbenzene			13.0	*	9.22
1-Methyl-4-ethylbenzene			2.72	*	3.49
1,3,5-trimethylbenzene			5.98	5.30	4.11
1-Methyl-2-ethylbenzene			9.62	1.60	4.66
1,2,4-Trimethylbenzene			5.98	20.3	16.4
n-C10 (Decane)				*	ND
1,2,3-Trimethylbenzene			3.92	*	9.81
n-Butylbenzene			0.00	<1.0	0.407
1,2,4,5-Tetramethylbenzene			0.04	<1	0.417
n-Pentylbenzene			0.00	*	3.63
Sum VOC			147	195	205
BTEX	137		102	164	140
C3-benzenes	NA		42.8	30.3	49.4
Other VOC	NA		1.51	NA	15.6

Table 5-16 Volatile components reported in the WAFs of MGO in seawater. (NA or *: Not analyzed; ND: Not detected). Comments given by the laboratories to their results are given in Appendix C.

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	MGO		2021-5428		2021-5428
Internal Lab ID	LSFO 2			E21-055-3	2021-5428
Oil type	MGO	Not reported	MGO	MGO	MGO
	µg/L		µg/L	µg/L	µg/L
Isopentane			0.02	*	ND
n-C5 (Pentane)				*	ND
Cyclopentane			0.21	*	ND
2-methylpentane			0.00	*	ND
3-Methylpentane			0.01	*	ND
n-C6 (Hexane)			0.07	*	ND
Methylcyclopentane			0.14	*	1.58
Benzene	44.6		31.0	60.4	62.7
Cyclohexane			0.00	*	8.41
2,3-Dimethylpentane				*	ND
3-methylhexane			0.06	*	ND
n-C7 (Heptane)			7.40		ND
Methylcyclohexane			3.43	*	10.1
Toluene	177		171	243	358
2,4 dimethylhexane				*	ND
2-Methylheptane			0.16	*	ND
n-C8 (Octane)			0.10	*	ND
Ethylbenzene	60.8		84.4	146	128
m-Xylene	204		218	308	463
p-Xylene			150	*	126
o-Xylene	111		1.35	165	268
n-C9 (Nonane)			2.75	*	ND
Propylbenzene			27.0	44.5	58.1
1-Methyl-3-ethylbenzene			121	*	235
1-Methyl-4-ethylbenzene			31.7	*	79.4
1,3,5-trimethylbenzene			78.8	61.5	98.6
1-Methyl-2-ethylbenzene			81.6	29.7	130
1,2,4-Trimethylbenzene			78.8	90.5	ND
n-C10 (Decane)				*	ND
1,2,3-Trimethylbenzene			52.4	*	195
n-Butylbenzene			0.00	7.00	11.8
1,2,4,5-Tetramethylbenzene			0.58	*	27.0
n-Pentylbenzene			0.01	*	65.9
Sum VOC			1142	1156	2326
BTEX	597		656	922	1406
C3-benzenes			471	226	796
Other VOC			14.9	7.0	125

Table 5-17 Volatile components reported in the WAFs of VLSFO in seawater. (NA or *: Not analyzed; ND: Not detected). Comments given by the laboratories to their results are given in Appendix C.

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	VLSFO		2021-5429		2021-5429
Internal Lab ID	LSFO 3			E21-055-2	2021-5429
Oil type	VLSFO	Not reported	VLSFO	VLSFO	VLSFO
	µg/L		µg/L	µg/L	µg/L
Isopentane			1.78	*	ND
n-C5 (Pentane)				*	ND
Cyclopentane			0.05	*	ND
2-methylpentane			0.00	*	ND
3-Methylpentane			0.00	*	ND
n-C6 (Hexane)			0.00	*	ND
Methylcyclopentane			0.00	*	2.38
Benzene	34.4		13.6	24.7	24.9
Cyclohexane			0.00	*	1.06
2,3-Dimethylpentane				*	ND
3-methylhexane			0.00	*	ND
n-C7 (Heptane)			12.7		ND
Methylcyclohexane			4.74	*	0.920
Toluene	83.6		44.0	94.1	112
2,4 dimethylhexane				*	ND
2-Methylheptane			0.35	*	ND
n-C8 (Octane)			0.87	*	ND
Ethylbenzene	29.1		16.3	25.6	34.6
m-Xylene	53.9		48.0	99.6	124
p-Xylene			33.4	*	38.1
o-Xylene	29.3		0.00	51.9	83.7
n-C9 (Nonane)			0.01	*	ND
Propylbenzene			4.22	5.70	10.7
1-Methyl-3-ethylbenzene			43.9	*	76.7
1-Methyl-4-ethylbenzene			8.07	*	26.5
1,3,5-trimethylbenzene			22.8	13.3	30.2
1-Methyl-2-ethylbenzene			25.5	1.00	32.7
1,2,4-Trimethylbenzene			22.8	66.5	147
n-C10 (Decane)				*	ND
1,2,3-Trimethylbenzene			11.7	*	68.1
n-Butylbenzene			0.00	1.60	4.18
1,2,4,5-Tetramethylbenzene			0.03	*	57.0
n-Pentylbenzene			0.00	*	1.38
Sum VOC			315	384	877
BTEX	230		155	296	418
C3-benzenes			139	86.5	392
Other VOC			20.5	1.60	66.9

5.3 Toxicity of the WAFs

Initially, it was decided that the laboratories should test the copepod *Acartia tonsa*, but only Norway and Canada (not reported yet) tested *A. tonsa*. Norway tested *Calanus finmarchicus* as the second specie. The US laboratory tried to set up testing with *A. tonsa*, but it was not successful. They tested the WAFs with mysids (*A. bahia*) and menidia (*M. beryllina*). It was too challenging to ship *A. tonsa*, so China tested zebra fish and *Moina monolica Daday*. Sweden decided to test *N. spinipes*.

An overview of the test organisms and test conditions are given in Table 5-18. In addition, toxic units were calculated. The reported results from the different laboratories are given in Appendix D. The observed toxicity results and the calculated toxic units are reported in Table 5-19 for WAF of WRG, Table 5-20 for WAF of MGO, and Table 5-21 for WAF of VLSFO.

Table 5-18 Test organisms and test conditions for the toxicity testing of the WAFs. Conditions for WAF preparation (test solution) are given in Table 5-8.

Laboratory	USA	Canada	China	Sweden	Norway
Test specie 1	<i>Americamysis bahia</i> Mysid	<i>Acartia tonsa</i> Marine copepod	Zebra fish Freshwater vertebrate	<i>Nitocra spinipes</i> Marine copepod	<i>Acartia tonsa</i> Marine copepod
Test temperature	25 °C	20°C	28 °C	20 °C	20 °C
Test endpoint	48 h	48 hr	120 h	48 h	48 h
Test specie 2	<i>Menidia beryllina</i> Estuarine fish		<i>Moina mongolica Daday</i> Marine cladoceran		<i>Calanus finmarchicus</i> Marine copepod
Test temperature	25 °C		28 °C		10 °C
Test endpoint	96 h		48 h		96 h

The acute toxicity, expressed as LC_{50} , can be given in percent dilution of the undiluted (or 100%) WAF (relative toxicity, LC_{50} reported in percent (%)), or as normalized to the total WAF concentration (specific toxicity, LC_{50} given in mg/L or ppm). A low value of LC_{50} indicates high toxicity, while a high value of LC_{50} corresponds to lower toxicity.

Relative and specific toxicity of the tested species are shown in Figure 5-5. However, as mentioned earlier, and shown in Table 3-3, the number of the recommended components analyzed and quantified varied among the laboratories. Therefore, with the different species tested and varying components quantified, it was not possible to do a direct comparison of the toxicity results, but only evaluate the trends.

In WAFs of WRG, the lethal immobilization was too low to calculate LC_{50} s for all species, except *N. spinipes* (Sweden) and *A. tonsa* (Canada). The GC chromatogram of the WAF used to expose *N. spinipes* contained oil droplets (Table 5-3), so they have been exposed higher WAF concentration of WRG than the other species. *A. tonsa* was tested of Canada and Norway, and the relative toxicity in WAFs of VLSFO were comparable (LC_{50} of 42 and 43%). Relative toxicity indicates that the LC_{50} s are in the same range in WAFs of MGO and VLSFO, but when expressed as specific toxicity, the results indicate that WAFs of VLSFO were more toxic than WAFs of MGO to all tested organisms, except *M. bahia* and *M. beryllina* (both species tested by USA). In WAFs of MGO the LC_{50} s are relatively comparable for *M. bahia*, *M. beryllina*, zebrafish, *A. tonsa* (NOR), and *C. finmarchicus*.

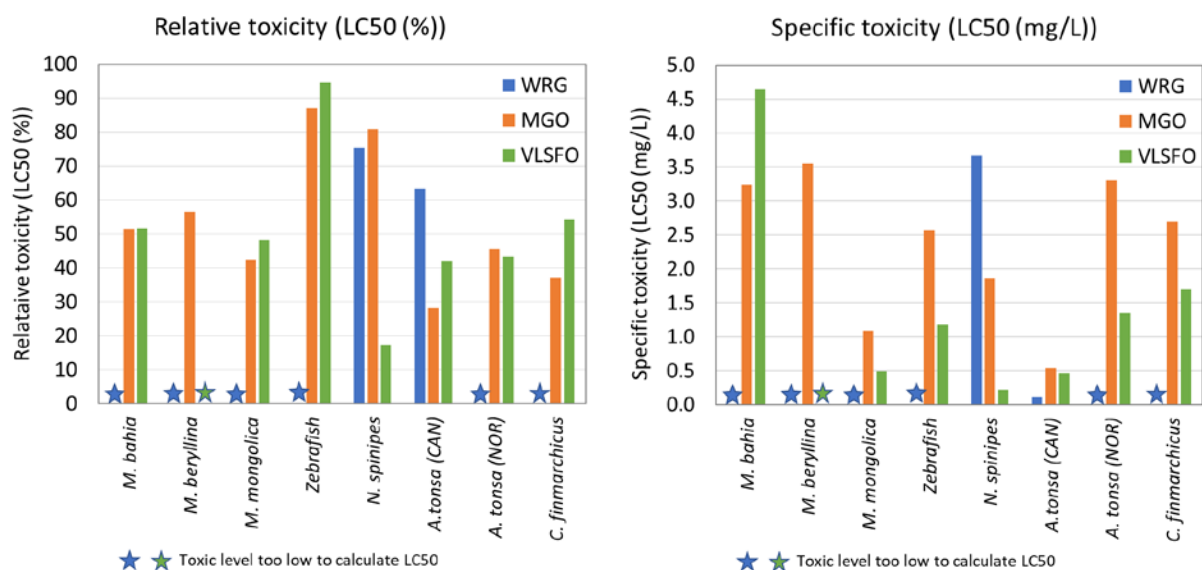


Figure 5-5 Acute toxicity (LC50) expressed as relative toxicity (left figure) and specific toxicity (right figure). The blue and green stars indicate that the toxic level is too low for calculation of LC₅₀ for in WAF of WRG (blue) and VLSFO (green). Canada has not reported VOCs, so the TPH concentration to quantify specific toxicity.

Acute toxicity, expressed as toxic unit (TU), was predicted based on the chemical composition of the WAFs and the logK_{ow} for the individual components. The UCM (unresolved complex materials), which could include thousands of unidentified components in the WAFs, is not included in the TU calculations. A TU>1 for the total WAF implies that it is expected to cause more than 50% mortality in the test organisms. All laboratories used the same input data and equations to calculate TU, but as their WAF concentrations varies, the TU will also vary among the laboratories (Figure 5-6). China predicts highest TUs in all systems, but the large contribution of 4-6 rings indicates that there are oil droplets present in their WAFs.

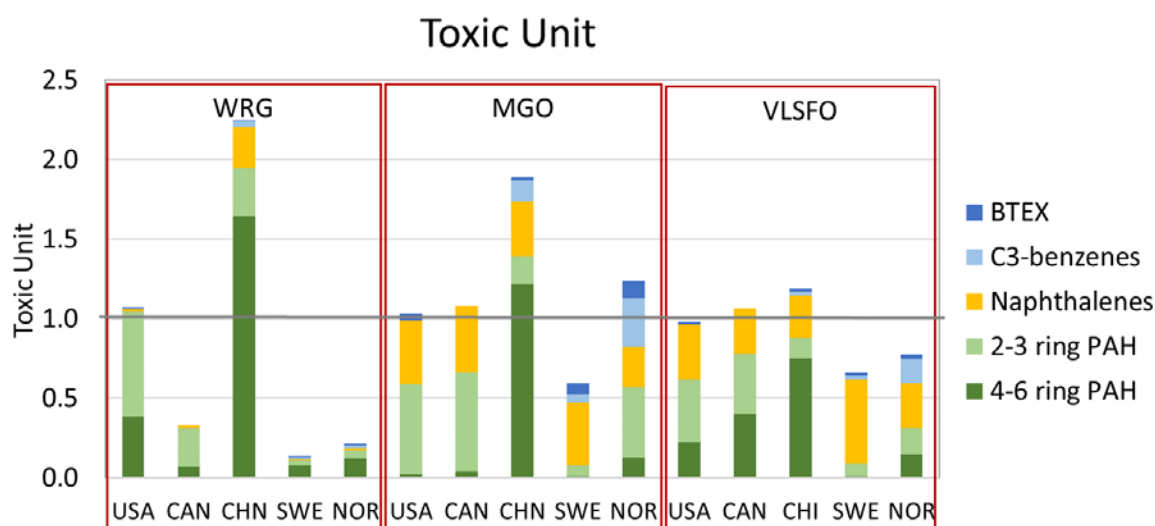


Figure 5-6 Predicted toxicity expressed as toxic unit. A TU > 1 implies that it is expected to cause more than 50% mortality in the test organisms. Canada did not report BTEX and C3-benzenes.

Table 5-19 *Reported results from toxicity testing of WAF of WRG (* USA: Total WAF concentration is the sum of BTEX and TPH; **: Toxic unit not reported, but calculated by SINTEF; ***: Tot WAF Canada is only TPH (no volatiles reported); ****: Before "/" stands for seawater WAF data, after "/" stands for freshwater WAF data).*

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	WRG	WRG	2021-5427	Sweden	WRG
Internal Lab ID	LSFO 1	21-11-2022		E21-055-1	2021-5427
Oil type	WRG	WRG	WRG	WRG	WRG
Oil to water ratio	1:40	1:40	1:40	1:40	1:40
Tot WAF conc (mg/L)	1.118*	0.185***	1.97/2.43****	4.865	0.392
Tot SVOC (mg/L)	0.025	0.019	0.46/0.37****	0.016	0.018
	A. bahia	A. tonsa	M. mongolica	N. spinipes	A. tonsa
LC50 (%)	>100%	63.3	>100%	75.3	>100
LC50 (mg/L)	>1.118*	0.117***	>1.97	3.67	>0.392
Observed toxicity at end point in 100% WAF	0%	85%	32%	90%	2.5%
	M. beryllina		Zebrafish		C. finmarcicus
LC50 (%)	>100%		>100%		>100
LC50 (mg/L)	>1.118		>2.43		>0.392
Observed toxicity at end point in 100% WAF	13%		6%		None
TU	1.07**	0.33**	1.77/2.28****	0.14**	0.23

Table 5-20 *Reported results from toxicity testing of WAF of MGO (* USA: Total WAF concentration is the sum of BTEX and TPH; **: Toxic unit not reported, but calculated by SINTEF; ***: Tot WAF Canada is only TPH (no volatiles reported); ****: Before "/" stands for seawater WAF data, after "/" stands for freshwater WAF data).*

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	MGO	MGO repetition	2021-5428		2021-5428
Internal Lab ID	LSFO 2	WAF1		E21-055-3	2021-5428
Oil type	MGO	MGO	MGO	MGO	MGO
Oil to water ratio	1:40	1:40	1:40	1:40	1:40
Tot WAF conc (mg/L)	6.299*	1.894***	2.58/2.96****	2.276	7.237
Tot SVOC (mg/L)	0.554	0.302	0.52/0.54****	0.925	0.702
	A. bahia	A. tonsa	M. mongolica	N. spinipes	A. tonsa
LC50 (%)	51.5	28.3	42.35	80.9	45.5
LC50 (mg/L)	3.24*	0.536***	1.09	1.86	3.30
Observed toxicity at end point in 100% WAF	100%	100%	87%	60%	100%
	M. beryllina		Zebrafish		C. finmarcicus
LC50 (%)	56.34		87.09		37.2
LC50 (mg/L)	3.55*		2.57		2.70
Observed toxicity at end point in 100% WAF	100%		70%		100%
TU	1.03**	1.08**	3.15/1.92****	0.60**	1.36

Table 5-21 *Reported results from toxicity testing of WAF of VLSFO (* USA: Total WAF concentration is the sum BTEX and TPH; **: Toxic unit not reported, but calculated by SINTEF; ***: Tot WAF Canada is only TPH (no volatiles reported); ****: Before "/" stands for seawater WAF data, after "/" stands for freshwater WAF data).*

Laboratory	USA	Canada	China	Sweden	Norway
Sample ID	VLSFO	VLSFO	2021-5429		2021-5429
Internal Lab ID	LSFO 3	WAF2		E21-055-2	2021-5429
Oil type	VLSFO	VLSFO	VLSFO	VLSFO	VLSFO
Oil to water ratio	1:40	1:40	1:40	1:40	1:40
Tot WAF conc (mg/L)	9.017*	1.122***	1.01/1.25****	1.243	3.127
Tot SVOC (mg/L)	0.615	0.329	0.42/0.58	1.670	0.540
	<i>A. bahia</i>	<i>A. tonsa</i>	<i>M. mongolica</i>	<i>N. spinipes</i>	<i>A. tonsa</i>
LC50 (%)	51.6	41.9	48.23	17.4	43.3
LC50 (mg/L)	4.65*	0.470***	0.49	0.22	1.35
Observed toxicity at end point in 100% WAF	93%	95%	87%	100%	100%
	<i>M. beryllina</i>		<i>Zebrafish</i>		<i>C. finmarcicus</i>
LC50 (%)	>100%		94.63		54.2
LC50 (mg/L)	>9.02		1.18		1.70
Observed toxicity at end point in 100% WAF	None		58%		81%
TU	0.98**	1.06**	2.00/1.21****	0.66**	0.81

5.4 Diagnostic ratios for oil fingerprinting

The recommended diagnostic ratios in the oils were calculated by Sweden, Canada, and Norway. Sweden used manual integration for all ratios (Table E 2), Canada a combination of concentrations ratios and area ratios (see Table E 1), and Norway a combination of COSI and manual integration (Table E 3).

The calculated ratios are given in Table 5-22 for WRG, in Table 5-23 or MGO, and in Table 5-24 for VLSFO. The correlation between the different laboratories is in general relatively good, except for a few outliers.

The objective with the additional DRs with PAHs that contain sulfur, was to test if some of the ratios could be used to get an indication of the sulfur content in the oils, e.g. if it is a ULSFO (<0.1% S) or a VLSFO (<0.5% S). The data set is limited with only three oils, but the oils have different sulfur content. The average sulfur contents based on results from four laboratories (not USA) were 0.04% S in WRG, 0.08% S in MGO, and 0.5% in VLSFO (Table 4-2).

The trends in the calculated ratios show that no ratios could indicate the difference in sulfur content in MGO and VLSFO. The results indicate that some of the ratios could indicate sulfur content <0.05% (WRG) when compared with the oils with >0.1% S (MGO and VLSO). These ratios were 4MD/1MD, 1-MDT/30ab, and 4M-DBT. However, these findings are based on the analysis of only three low sulfur oils and did not include a non-LSFO. A larger data set might give different or other conclusions. However, no high sulfur oils were included (> 1% S), but it is likely that their sulfur containing ratios will be much higher than in LSFOs and that the ratios could indicate if it is a LSFO.

Table 5-22 Calculated diagnostic ratios for screening fingerprinting analysis of WRG (no data China and USA)

Laboratory			Sweden	Canada	Norway
Sample ID			Product WRG		no-1-41.1 (COSI)
Internal Lab ID			12669825	2021-09-17-6081	2021-5427
Oil type	m/z	Ratios	WRG	WRG	WRG
GC/FID		C17/pristane	1.47	1.76	1.60
		C18/phytane	1.86	1.26	2.03
		Pristane/phytane	1.07	0.63	0.98
GC/MS	191	Ts/30ab	0.30	0.32	0.31
	191	Tm/30ab	0.22	0.21	0.20
	191	28ab/30ab	0.26	/	0.28
	191	29ab/30ab	0.50	0.66	0.50
	191	30O/30ab	0.06	/	0.000
	191	31abS/30ab	0.34	0.31	0.34
	191	30G/30ab	0.05	/	0.05
	217	27dbR/27dbS	0.62	/	0.62
	218	27bb/29bb	1.56	1.26	1.43
	231	TASC26/RC26+SC27	0.31	0.30	0.18
	231	TASC28/RC26+SC27	0.54	0.64	0.51
	231	TARC27/RC26+SC27	0.55	0.51	0.50
	231	TARC28/RC26+SC27	0.39	0.49	0.43
	192	2MP/1MP	0.66	0.81	0.68
	192	MA/1MP	<LOD (MA)	0.05	0.000
	198	4MD/1MD	<LOD (1-MD)	/	3.65
	216	2MF/4MPy	<LOD (2MF)	0.06	0.09
	216	B(a)F/4MPy	0.20	0.18	0.21
	216	B(b+c)F/4MPy	<LOD (B(b+c)F)	0.09	0.09
	216	2MPy/4MPy	0.32	0.41	0.41
	216	1MPy/4MPy	0.50	0.58	0.60
	234	Retene/TMPhe	2.12	/	1.91
	234	BNT/TMPhe	<LOD (BNT)	0.00	0.000
Sulfur content					
GC/MS	198/191	1M-DBT/30ab	<LOD (1M-DBT)	0.00	0.05
	198/191	4M-DBT/30ab	0.07	0.14	0.17
	234/191	BNT/30ab	<LOD (BNT)	0.00	0.04
	If 30ab is small or not present				
	198/192	1M-DBT/1MP	<LOD (1M-DBT)	0.00	0.07
	198/192	4M-DBT/1MP	0.20	0.28	0.26
	234/192	BNT/TMPhe	<LOD (BNT)	0.00	0.15
	Optional ratios sulfur content				
	212/206	C2-DBT/C2-Phe	0.19	0.18	0.19
	212/206	C3-DBT/C2-Phe	0.24	0.22	0.22
	234/206	BNT/C2-Phe	<LOD (BNT)	0.00	0.003
	No pattern				
	162/206	C2-BT/C2-Phe	recognition C2-BT	/	0.023

Table 5-23 Calculated diagnostic ratios for screening fingerprinting analysis of MGO (no data China and USA).

Laboratory			Sweden	Canada	Norway
Sample ID			Product MGO		no-1-41.2
Internal Lab ID			12670165	2021-09-17-6082	2021-5428
Oil type	m/z	Ratios	MGO	MGO	MGO
GC/FID		C17/pristane	1.41	2.21	1.48
		C18/phytane	1.90	1.44	
		Pristane/phytane	1.69	0.82	1.73
GC/MS	191	Ts/30ab	0.75	0.65	0.57
	191	Tm/30ab	0.45	0.41	0.35
	191	28ab/30ab	0.00	/	0.30
	191	29ab/30ab	0.68	0.78	0.59
	191	30O/30ab	<LOD (30O)	/	ND
	191	31abS/30ab	<LOD (31abS)	0.25	0.31
	191	30G/30ab	<LOD (30G)	/	0.06
	217	27dbR/27dbS	0.57	/	0.57
	218	27bb/29bb	2.16	1.78	1.91
	231	TASC26/RC26+SC27	0.40	0.35	0.36
	231	TASC28/RC26+SC27	0.51	0.58	0.44
	231	TARC27/RC26+SC27	0.42	0.44	0.42
	231	TARC28/RC26+SC27	0.27	0.37	0.31
	192	2MP/1MP	1.93	1.95	1.74
	192	MA/1MP	0.03	0.10	0.06
	198	4MD/1MD	4.62	5.26	5.63
	216	2MF/4MPy	0.22	0.31	0.19
	216	B(a)F/4MPy	0.37	0.57	0.45
	216	B(b+c)F/4MPy	0.12	0.26	0.17
	216	2MPy/4MPy	1.43	1.55	1.59
	216	1MPy/4MPy	0.63	0.66	0.67
	234	Retene/TMPhe	1.93	/	1.66
	234	BNT/TMPhe	0.15	0.01	0.39
Sulfur content					
GC/MS	198/191	1M-DBT/30ab	5.56	4.58	6.09
	198/191	4M-DBT/30ab	25.7	24.5	35.9
	234/191	BNT/30ab	0.98	1.67	3.64
		If 30ab is small or not present			
	198/192	1M-DBT/1MP	0.07	0.08	0.06
	198/192	4M-DBT/1MP	0.32	0.42	0.38
	234/192	BNT/TMPhe	0.15	0.01	0.41
		Optional ratios sulfur content			
	212/206	C2-DBT/C2-Phe	0.14	0.16	0.12
	212/206	C3-DBT/C2-Phe	0.11	0.10	0.11
	234/206	BNT/C2-Phe	0.0005	0.00	0.002
		No pattern			
	162/206	C2-BT/C2-Phe	recognition C2-BT	/	0.11

Table 5-24 *Calculated diagnostic ratios for screening fingerprinting analysis of VLSFO (no data China and USA).
(*: Ratios integrated from GC/MS)*

Laboratory			Sweden	Canada	Norway
Sample ID			Product VLSFO		no-1-41.3
Internal Lab ID			12670191	2021-09-17-6083	2021-5429
Oil type	m/z	Ratios	VLSFO	VLSFO	VLSFO
GC/FID		C17/pristane	4.09*	4.01	1.92
		C18/phytane	4.15*	3.06	2.43
		Pristane/phytane	0.79*	0.68	1.04
GC/MS	191	Ts/30ab	0.17	0.21	0.18
	191	Tm/30ab	0.44	0.44	0.43
	191	28ab/30ab	0.04	/	ND
	191	29ab/30ab	0.69	0.92	0.71
	191	30O/30ab	0.09	/	0.20
	191	31abS/30ab	0.32	0.32	0.33
	191	30G/30ab	0.06	/	0.09
	217	27dbR/27dbS	0.85	/	0.06
	218	27bb/29bb	1.04	0.95	1.03
	231	TASC26/RC26+SC27	0.51	0.38	0.67
	231	TASC28/RC26+SC27	0.59	0.73	0.58
	231	TARC27/RC26+SC27	0.59	0.54	0.55
	231	TARC28/RC26+SC27	0.55	0.62	0.58
	192	2MP/1MP	2.17	1.82	1.99
	192	MA/1MP	0.39	0.44	0.48
	198	4MD/1MD	4.18	5.56	4.87
	216	2MF/4MPy	0.14	0.20	0.14
	216	B(a)F/4MPy	0.21	0.29	0.26
	216	B(b+c)F/4MPy	0.11	0.20	0.15
	216	2MPy/4MPy	0.83	0.85	0.94
	216	1MPy/4MPy	0.81	0.77	0.89
	234	Retene/TMPhe	0.00	/	ND
	234	BNT/TMPhe	0.19	0.02	0.30
Sulfur content					
GC/MS	198/191	1M-DBT/30ab	0.26	0.28	0.34
	198/191	4M-DBT/30ab	1.09	1.54	1.70
	234/191	BNT/30ab	0.68	0.40	0.70
		If 30ab is small or not present			
	198/192	1M-DBT/1MP	0.07	0.06	0.07
	198/192	4M-DBT/1MP	0.30	0.35	0.33
	234/192	BNT/TMPhe	0.14	0.02	0.31
		Optional ratios sulfur content			
	212/206	C2-DBT/C2-Phe	0.15	0.17	0.14
	212/206	C3-DBT/C2-Phe	0.14	0.17	0.15
	234/206	BNT/C2-Phe	0.0024	0.01	0.004
	162/206	C2-BT/C2-Phe	0.022	/	0.15

6 Summary and recommendations

Three low sulfur fuel oils have been characterized through this interlaboratory comparison study by laboratories from USA, Canada, China, Sweden, and Norway. The oils analyzed were a WRG (<0.05% S), a MGO (<0.1% S) and a VLSFO (<0.5% S). A common guideline for the methodology was accepted by all laboratories that included characterization of oil properties relevant for fate, behavior, fingerprinting, and relative toxicity when spilled in cold or Arctic seawater.

However, it turned out to be more challenging than expected to accomplish a complete set of analyses for all laboratories. Due to the limited data set, statistical variability and validation of the methods used have not been performed. An overview of the methods used and the parameters analyzed by each laboratory was given in Table 3-1 (physical test parameters), Table 3-2 (chemical test parameters), and Table 3-3 (chemical composition of oils and WAFs, including acute toxicity).

A summary of the results from the analyses of the oils is given in Table 6-1, describing the number of laboratories that have reported the parameters and the robustness of the results based on the reported results:

- Pour point: Variation in the measurements is of concern. This is likely due to that Canada uses another method than the other laboratories. It is recommended that one of the methods (ASTM D-97) is selected and that a systematic comparison of the two methods is performed.
- Temperature sweep for viscosity: Especially for LSFOs with high pour point. According to the memo (Daling et al., 2021) it is recommended to measure from 50 °C down to 0 °C.
- Dynamic viscosity should be measured at low temperature according to the memo (Daling et al., 2021), and at different shear rates (e.g. 10, 100, and 1000 s⁻¹).
- Interfacial tension: Measurements a challenge for oils with high pour points for all labs. Discuss if this parameter should be recommended in the characterization of new LSFOs.
- Only USA and Norway provided GC chromatograms of the oils. Must be mandatory for all labs.
- Asphaltenes: Content below detection limit for 2 of 3 oils for China and Sweden. Canada reports soft asphaltenes, Norway hard asphaltenes. Agree on a common method.
- Wax: Canada and Norway use different method. Recommends that Norway could revise the method and crystallize the wax at -20 °C instead of -10 °C (Canada uses -30 °C). Suggests using -20 °C in the next phase.
- Sulfur: Good correlation between all laboratories (ASTM D4294).
- CHN: The German representative requested this analysis. In the literature the amount of these elements is usually 82-87% for C, 11-15% for H, and 0-1% for N (Butt et al., 1986), and the reported values are within these limits. It is recommended that these elements are excluded in further analysis as it gives limited information.
- Metals: Below detection limit in WRG and MGO. Skip metals or select the most analyzed metals, such as Fe, Ni and V.
- SVOC/PAH: USA, Canada and Norway analyze same components (only Norway reports decalins and phenols). China analyzed fewer components and reports lower values on most single components. Relatively good correlation between component groups for NOR and CAN, but USA higher. This could be due to different quantification methods (relative response factors (RRF)). Recommends that a common practice for use of RRF is implemented.
- VOC: Only reported by China and Norway. Very large variation in the results, even BTEX. Could be caused by different sample preparation and/or instrument conditions.
- Diagnostic ratios: Relatively good correlations on most ratios. The sulfur containing ratios not suited to indicate if it is a ULSFO or VLSFO, but it is likely that they could indicate if it is a LSFO or a fuel with

high sulfur content. As the information is limited, it is recommended that calculation of DRs is excluded in further studies. Will be removed from the revised memo (Daling et al., 2021).

Table 6-1 **A summary of the reported parameters for the oil analyses and an evaluation of the results, including a recommendation of further analysis of the specific test parameters, and laboratories that seem to have the capability to perform the analyses.**

Test parameters	Laboratory					Evaluation of results		
	USA	CAN	CHN	SWE	NOR	Indication of variability	Comments	Recommendation
In oil								
Water content	NA	x	NA	x	x	Low, but varies	Diff. methods used	
Density	x	x	x	x	x	Minor variation	Robust parameter	CAN, CHN, SWE, NOR
Pour point	NA	x	x	x	x	Too large variation	CAN diff. method	A systematic comparison of the methods, or select one of the methods
Flash point	NA	x	x	x	x	Low	Robust	CAN, CHN, SWE, NOR
Viscosity – temp.sweep	NA	x	NA	x	x	Low between CAN and NOR	SWE reported different temp range	CAN and NOR
Viscosity	NA	x	x	x	x	OK between CAN and NOR (dynamic visc)	SWE and CHN rep kinematic visc.	Dynamic visc recommended, compared with temp sweep. CAN and NOR
Interfacial tension	x	x	NA	NA	x	Large variation	Oils with high PP challenging for all labs	Exclude parameter?
True boiling point	NA	x	NA	x	x	Relative comparable, but minor diff	Larger variation bp>350 °C	SWE, CAN and NOR
GC/FID	x				x	Yes	Diff GC conditions?	Only reported by USA and NOR, but must be included by all
Asphaltenes	NA	x	x	x	x	Some, but diff methods (hard or soft).	Detect limit for SWE (0.5wt%) and CHN (0.05 wt%)	Select soft or hard asphaltenes.
Wax	NA	x	x	NA	x	NOR reports lower wax content on all oils	CHN rep only VLSFO. CAN use -30°C, NOR use -10°C	If NOR decrease temp from -10 to -20°C: CAN and NOR
Sulfur	x	x	x	x	x	Low	USA lower than other labs	CAN, CHN, SWE, NOR (ASTM D4294)
CHN	NA	NA	x	x	x	Low	Specific request from Germany	Exclude parameter, gives limited info
Metals	NA	x	x	x	x	Rel. low conc, but OK	Most metals below detection limits	Exclude, or analyze only Ni and V (+ Fe?)
SVOC/PAH	x	x	x	NA	x	Rel low variation CAN and NOR, USA higher conc	CHN quant fewer comp. RRF applied different USA	Exclude decalins and phenols. Agree on use of RRF
VOC			x		x	Large variation, also for BTEX	Only reported by two laboratories	Difference between labs too large to give any recommendation
Diagnostic ratios (DR)		x		x	x	Rel good	Only NOR used COSI (automatic integr)	CAN, SWE, NOR, but recommend that DRs are excluded.

The results from the chemical and toxicological characterization of the WAFs are evaluated in Table 6-2. However, one of the laboratories (China) has not reported the GC-FID chromatograms of their WAFs. To evaluate the results, the chromatograms are necessary as they will give information on the success of the preparation of the low-energy WAFs. The presence of oil droplets in the WAFs result in increased concentrations of PAHs and other less water-soluble oil components.

Initially, it was decided that all laboratories should test the copepod *Acartia tonsa*, but only Norway and Canada have tested *A. tonsa*. The US laboratory tried to set up testing with *A. tonsa*, but it was not successful, and it was too challenging to ship *A. tonsa* to China. An overview of the test organisms and test conditions was given in Table 5-18.

Preparing WAFs in different laboratories, even with the same oils, may give different results although the same protocols have been followed. The results will be impacted of details such as the temperatures on water and oil when the WAFs are prepared, oil droplets in the water phase, different methods for sample preparation, and analytical and quantification methods.

Eight different species have been tested in the laboratories. Although some trends can be observed, the variation in the WAF chemistry make it to challenging to give any recommendations regarding other future test organisms than *A. tonsa*. *A. tonsa* was tested of Canada and Norway, and the relative toxicity in WAFs of VLSFO were comparable (LC₅₀ of 42 and 43%) and was in the same range in WAFs of MGO.

Table 6-2 A summary of the reported parameters for characterization of chemistry and toxicity of the WAFs, and an evaluation of the results, including a recommendation of further analysis of the specific test parameters.

Test parameters	Laboratory					Evaluation of results	Comments	Recommendation
	USA	CAN	CHN	SWE	NOR	Indication of variability		
WAF chemistry								
GC chrom of WAF	x	x		x	x		One WAF from SWE (WRG) contained oil droplets.	Labs must report GC-chrom to show that a LE-WAF is prepared
TPH	x	x	x	x	x	Large variation on all WAFs for all labs	High conc SWE on WRG can be explained by oil droplets	
SVOC/PAH	x	x	x	x	x	Large variation on all WAFs for all labs	SWE higher SVOC than TPH in VLSFO. CHN higher 4-6 ring PAH than other labs, indicates oil droplets in all WAFs	
VOC	x	ND	x	x	x	BTEX analysed of 4 labs: better correlation for some WAFs than for SVOC	BTEX: CHN lower than other labs in WAFs of WRG and VLSFO, NOR higher in MGO and VLSO	Reduce component list to only BTEX?
Toxicity								
Toxic Unit	x	x	x	x	x	As chemistry varies, TU varies (NOR calc TU for USA, CAN and SWE)	CHN: Mainly contrib from 4-6 ring PAH (60-80%) to TU	
<i>Acartia tonsa</i>		x			x	Rel good correlations WAFs of VLSFO and MGO, but diff for WRG.		Test <i>A. tonsa</i> in next phase (CAN and NOR)

Test parameters	Laboratory					Evaluation of results	Comments	Recommendation
	USA	CAN	CHN	SWE	NOR	Indication of variability		
All species	x		x	x	x	USA, CHN and NOR observed low tox in WAFs of WRG (<LC ₅₀). Rel comparable LC ₅₀ s of WAF of MGO <i>M. bahia</i> , <i>M. beryllina</i> , zebrafish, <i>A. tonsa</i> (NOR), and <i>C. finmarchicus</i> .		8 different species tested, some trends can be observed, but as the tests have been performed in different labs the value of the trends are uncertain.

7 References

ASTM D93 (Standard Test Methods for Flash Point by Pensky-Martens Closed Cup Tester)

ASTM D97 (Standard Test Method for Pour Point of Petroleum Products)

ASTM D445-19a (Standard Test Method for Kinematic Viscosity of Transparent and Opaque Liquids (and Calculation of Dynamic Viscosity))

ASTM D1250-80 (Standard Guide for Use of the Petroleum Measurement Tables).

ASTM D2622 (Standard Test Method for Sulfur in Petroleum Products by Wavelength Dispersive X-ray Fluorescence Spectrometry)

ASTM D4052 (Standard Test Method for Density, Relative Density, and API Gravity of Liquids by Digital Density Meter)

ASTM D4294 (Standard Test Method for Sulfur in Petroleum and Petroleum Products by Energy Dispersive X-ray Fluorescence Spectrometry)

ASTM D5002 (Standard Test Method for Density, Relative Density, and API Gravity of Crude Oils by Digital Density Analyzer)

ASTM D5291:2012 (Standard test method for instrumental determination of carbon, hydrogen, and nitrogen in petroleum products and lubricants).

ASTM D5762 (Standard Test Method for Nitrogen in Liquid Hydrocarbons, Petroleum and Petroleum Products by Boat-Inlet Chemiluminescence)

ASTM D5949 (Standard Test Method for Pour Point of Petroleum Products (Automatic Pressure Pulsing Method))

ASTM D6377 (Standard Test Method for Determination of Vapor Pressure of Crude Oil: VPCRx (Expansion Method))

ASTM D6378 (Standard Test Method for Determination of Vapor Pressure (VPX) of Petroleum Products, Hydrocarbons, and Hydrocarbon-Oxygenate Mixtures (Triple Expansion Method)).

ASTM D6560-17 (Standard Test Method for Determination of Asphaltenes (Heptane Insolubles) in Crude Petroleum and Petroleum Products)

ASTM D7042 (Standard Test Method for Dynamic Viscosity and Density of Liquids by Stabinger Viscometer (and the Calculation of Kinematic Viscosity))

ASTM D7094 (Standard Test Method for Flash Point by Modified Continuously Closed Cup (MCCCFP) Tester)

ASTM D7169 (Standard Test Method for Boiling Point Distribution of Samples with Residues Such as Crude Oils and Atmospheric and Vacuum Residues by High Temperature Gas Chromatography)

ASTM E203 (Standard Test Method for Water Using Volumetric Karl Fischer Titration)

Aurand, D., Coelho G. (2005). Cooperative Aquatic Toxicity Testing of Dispersed Oil and the "Chemical Response to Oil Spills: Ecological Research Forum (CROSERF)". Ecosystem Management & Associates, Inc., Lusby, MD. Technical report 07-03, 105 pages + Appendices.

Bridié, A.L., Wanders, T. H., Zegveld, W. V. and den Heijde, H. B., 1980. Formation, Prevention and Breaking of Seawater in Crude Oil Emulsions, Chocolate Mousse. Marine Poll. Bull., vol. 11, pp. 343-348.

Butt, J.A., Duckworth, D.F., Perry, S.G. (1986). Characterization of spilled oil samples. Purpose, sampling, analysis and interpretation. Institute of Petroleum, Great Britain, ISBN 0 471 90890 8.

CEN (2012). Oil spill identification – Waterborne petroleum and petroleum products – Part 2: Analytical methodology and interpretation of results based on GC-FID and GC-MS low resolution analyses. CEN/TR 15522-2:2012.

Dahlmann, G., Kienhuis, P. (2016). Development and application of online computerized oil spill identification – COSIWeb. In Stout and Wang (eds): Standard Handbook Oil Spill Environmental Forensics. Fingerprinting and Source Identification. Second Edition. Elsevier Academic Press, ISBN 978-0-12-809659-8, pp. 729-745.

Daling, P.S., L.G. Faksness, T.A. Pettersen (2021). WP-3 PAME – EPPR Methodology for screening properties of new Low Sulfur Marine Fuels. Selection of test parameters. SINTEF Project memo dated March 22, 2021.

DiToro, D.M., McGrath, J.A, Stubblefield, W.A. (2007). Predicting the toxicity of neat and weathered crude oil: Toxic potential and the toxicity of saturated mixtures. Environmental Toxicity and Chemistry. 26: 24-36.

EN 12606-1:2015 (Bitumen and bituminous binders - Determination of the paraffin wax content - Part 1: Method by distillation)

IP 143 (Determination of asphaltenes (heptane insolubles) in crude petroleum and petroleum products)

IP 501/05 (Determination of aluminium, silicon, vanadium, nickel, iron, sodium, calcium, zinc and phosphorous in residual fuel oil by ashing, fusion and inductively coupled plasma emission spectrometry)

ISO [International Organization for Standardization] (1999). Water quality - Determination of acute lethal toxicity to marine copepods (Copepoda, Crustacea). ISO 14669:1999.

ISO (2017). Petroleum products — Fuels (class F) — Specifications of marine fuels. ISO 8217:2017.

Kienhuis, P.G.M., Hansen, A.B., Faksness, L.G., Stout, S.A. Dahlmann, G. (2016). CEN methodology for oil spill identification. In Stout and Wang (eds): Standard Handbook Oil Spill Environmental Forensics. Fingerprinting and Source Identification. Second Edition. Elsevier Academic Press, ISBN 978-0-12-809659-8, pp. 685-728.

McCarty, L.S., Mackay, D., Smith, A.D., Ozburn, G.W., Dixon, D.G. (1992). Residue-based interpretation of toxicity and bioconcentration QSARs from aquatic bioassays: Neutral narcotic organics. *Environmental Toxicology and Chemistry* 11, 917-930.

McCarty, L.S., Mackay, D., Smith, A.D., Ozburn, G.W., Dixon, D.G. (1993). Residue-based interpretation of toxicity and bioconcentration QSARs from aquatic bioassays: Polar narcotic organics. *Ecotoxicology and Environmental Safety*. 25, 253-270.

McDonagh, M., Hokstad, J. N., Nordvik, A. B. (1995). "Standard procedure for viscosity measurement of water-in-oil emulsions". Marine Spill Response Corporation, Washington, D.C. MRSC Technical Report Series 95-030, 36 p.

McGrath, J.A., DiToro, D.M. (2009). Validation of the target lipid model for toxicity assessment of residual petroleum constituents: Monocyclic and polycyclic aromatic hydrocarbons. *Environ. Toxicol. Chem.* 28: 1130-1148.

Neff, J.M., Stout, S.A., Gunster D.G. (2005). Ecological risk assessment of polycyclic aromatic hydrocarbons in sediments: Identifying sources and ecological hazard. *Integr. Environ. Assess. Manag.* 1 (1): 22-33.

Philibert, D. A., Philibert, C. P., Lewis, C., Tierney, K. B. (2016). Comparison of diluted bitumen (dilbit) and conventional crude oil toxicity to developing zebrafish. *Environmental science & technology*. 50 (11): 6091-6098.

Sørheim, K., Daling, P.S., Cooper, D., Buist, I., Faksness, L.G., Altin, D., Pettersen, T.A., Bakken, O.M. (2020). Characterization of Low Sulfur Fuel Oils (LSFO) – A new generation of marine fuel oils. SINTEF report OC2020 A-050, ISBN 978-82-7174-385-7.

US EPA, Method 3510C (2015). Separatory Funnel Liquid-Liquid Extraction.
<https://www.epa.gov/sites/production/files/2015-12/documents/3510c.pdf>

US EPA, Method 8260D (2018). Volatile organic compounds by gas chromatography/mass spectrometry (GC/MS). https://www.epa.gov/sites/production/files/2018-06/documents/method_8260d_update_vi_final_06-11-2018.pdf

US EPA, Method 8270E (2018). Semivolatile Organic Compounds by Gas Chromatography/Mass Spectrometry (GC-MS). https://www.epa.gov/sites/production/files/2020-10/documents/method_8270e_update_vi_06-2018_0.pdf

US EPA, Method 8015D (2015). Non-halogenated organics using GC/FID.
https://www.epa.gov/sites/production/files/2015-12/documents/8015d_r4.pdf

Wang, Z., Dong, H., Wang, Y., Ren, R., Qin, X., Wang, S. (2020). Effects of microplastics and their adsorption of cadmium as vectors on the cladoceran *Moina monogolica* Daday: implications for plastic-ingesting organisms. *Journal of Hazardous Materials*. 400: 123239.

Appendix A Reported results physico-chemical properties

Table A 1 Template physico-chemical properties (fresh non-weathered samples) reported by Sweden.

Laboratory	SAYBOLT											
					ASTM D 6304 (mg/kg)	EN ISO 12185	ISO316	EN ISO2719	20 °C (WRG), 50 °C(VLSFO)			
									Viscosity, Kinematic at 0°C (mm ² s ⁻¹), ASTM D		IP 143 (Heptane Insolubles asphaltene)	
Oil name	Oil type	Sample ID	Internal Lab ID	Water content (vol.)	Density, 15°C (g/ml)	Pour Point (upper, °C)	Flash Point (°C)	Viscosity, 2°C- (mPa.s), 10s ⁺	Viscosity, 2°C- (mPa.s), 100s ⁺	IFT (mN/m)	Asph. (wt.%), "Hard or Soft"	Wax (wt.%)
Received Sample Test Oil : 1 WRG	1 WRG			43.0	0.874	-9	116.5	*	44.6	X	<0.50	X
Mean from 2 replicats												
Received Sample Test Oil : 2 MGO				30.0	0.865	-21	70	9.229		X	<0.50	X
Mean from 2 replicats												
Received Sample Test Oil : 3 VLSFO				1042.0	0.970	15	108	*	77.8	X	2.30	X
Mean from 2 replicats												

Table A 2 Template physico-chemical properties (fresh non-weathered samples) reported by Canada.

Oil name	Oil type	Sample ID	Internal Lab ID	Water content (vol.)	Density, 15°C (g/mL)	Pour Point (°C)	Flash Point (°C)	Measured at 15°C and 100s ⁻¹	Measured at 15°C and 1000s ⁻¹	Measured at 0°C and 10s ⁻¹	Measured at 0°C and 100s ⁻¹	Measured at 0°C and 1000s ⁻¹	IFT (mN/m)	Asph. (wt.%), "Hard or Soft"	Wax (wt.%)
Sample 1	WRG	2021-6081	6081	0.1	0.876	27	118	152	69		897	227	0	0.07	11.78
Parallels		#1		0.1	0.876	27	118	151	69		906	235	0	0.06	11.48
		#2		0.1	0.876	27	119	154	68		867	226	0	0.08	12.86
		#3		0.1	0.876	27	117	150	70		917	219	0	0.07	11.00
Sample 2	MGO	2021-6082	6082	0.0	0.865	-15	69		5			8	0	0.02	2.26
Parallels		#1		0.0	0.865	-15	69		5			8	0	0.02	2.01
		#2		0.0	0.865	-15	68		5			9	0	0.03	2.46
		#3		0.0	0.865	-15	69		5			8	0	0.02	2.32
Sample 3	VLSFO	2021-6083	6083	0.143	0.971	24	115	1614	1102	21977	11187	3229	0	5.03	7.64
Parallels		#1		0.1	0.971	24	116	1678	1085	22240	11150	3296	0	5.17	8.02
		#2		0.1	0.972	24	114	1574	1116	21930	11220	3191	0	4.86	7.23
		#3		0.2	0.971	24	116	1591	1104	21760	11190	3199	0	5.06	7.67

Table A 3 Template physico-chemical properties (fresh non-weathered samples) reported by China.

Oil name	Oil type	Sample ID	Internal Lab ID	Water content (vol.)	Density, 15°C (g/mL)	Density, 20°C (g/cm ³)	Pour Point (°C)	Flash Point (°C)	Viscosity, 2°C (mPa.s), 10s ⁻¹	Viscosity, 2°C (mPa.s), 100s ⁻¹	Viscosity, 6°C (mm ² /s)	Viscosity, 1°C (mPa.s)	IFT (mN/m)	Asph. (wt.%), "Hard or Soft"	Wax (wt.%)
Sample 1	WRG	2021-5427				0.873	-6	108			90.42 (20)	0.08 (20)		<0.05	0.00
Parallels		#1													
		#2									°C	°C			
		#3													
Sample 2	MGO	2021-5428				0.865	-30	70			8.21 (3)	0.01 (3)		<0.05	0.00
Parallels		#1													
		#2									°C	°C			
		#3													
Sample 3	VLSFO	2021-5429				0.970	12	>120			1156 (20)	1.12 (20)		2.78	0.80
Parallels		#1													
		#2													
		#3													

Table A 4 *Template physico-chemical properties (fresh non-weathered samples) reported by Norway.*

Sample name	Internal sample ID	Oil category	Water content (vol.)	Density, 15°C (g/mL)	Pour Point (°C)	Flash Point (°C)	Viscosity, 2°C (mPa.s), 10s ⁻¹	Viscosity, 2°C (mPa.s), 100s ⁻¹	IFT (mN/m)	Asph. (wt.%), "Hard"	Wax (wt.%)
Sample 1	2021-5427	WRG	0.2	0.8733	-6	113	218	186	27.6	0.01	6.54
Parallels	#1		0.2	0.8733	-6	113.5	215	189	26.65	0.01	6.46
	#2		0.2	0.8733	-6	112.5	232	189	27.47	0.01	5.42
	#3		0.3	0.8733	-6	113	206	180	28.7	0.01	7.30
	#4										6.98
Sample 2	2021-5428	MGO	0.2	0.8648	-18	67.5	6.6	6.3	10.8	0.01	0.62
Parallels	#1		0.2	0.86479	-18	67.5	6.4	6.3	11.1	0.02	0.70
	#2		0.2	0.86483	-18	67.5	6.6	6.2	10.88	0.01	0.61
	#3		0.2	0.86487	-18	67.5	6.7	6.5	10.421	0.01	0.62
	#4										0.56
Sample 3	2021-5429	VLSFO	0.4	0.9694	15	108.8	19755	7766	58.3	2.64	6.02
Parallels	#1		0.3	0.96950	15	108.5	20499	7856	58.44	2.55	5.72
	#2		0.4	0.96940	15	108.5	19616	7780	59.36	2.62	5.85
	#3		0.4	0.96920	15	109.5	19149	7661	57.38	2.79	6.11
	#4								57.9	2.58	6.38

Table A 5 *Template Element analysis (fresh non-weathered samples) reported by Sweden.*

Sample name	Received Sample Test Oil : 1 WRG		Received Sample Test Oil : 2 MGO	Received Sample Test Oil : 3 VLSFO
Oil type	WRG			
Sample ID	Received Sample Test Oil : 1 WRG			
Internal Lab ID	11601/00064210.4/L/21			
ICP/MS or ICP/AES	mg/kg		mg/kg	mg/kg
Aluminium (Al)	<5		<5	<5
Calsium (Ca)	<3		<3	5
Iron (Fe)				
Nickel (Ni)				
Silicon (Si)	<10		<10	<10
Sodium (Na)	<1		<1	9
Vanadium (V)	<1		<1	10
Sulfur (S)	0.044 wt%		0.085 wt%	0.51 wt%
Copper (Cu)				
ASTM D5291	mass %		mass %	mass %
C	86.5		87	87.5
H	13.4		12.8	10.8
N	280*		110*	2900*
* ASTM D 5762 (µg/g)				

Table A 6 *Template Element analysis (fresh non-weathered samples) reported by Canada.*

Sample name	Sample 1	Sample 2	Sample 3
Oil type	WRG	MGO	VLSFO
Sample ID	2021-6081	2021-6082	2021-6083
Internal Lab ID	6081	6082	6083
ICP/MS or ICP/AES	mg/kg	mg/kg	mg/kg
Aluminium (Al)			
Calcium (Ca)			
Iron (Fe)	1.2	1.2	8.3
Nickel (Ni)	<0.01	<0.01	4.7
Silicon (Si)			
Sodium (Na)			
Vanadium (V)	0.1	0.01	15
Sulfur (S)	0.05 %	0.08 %	0.51 %
Copper (Cu)			
ASTM D5291	mass %	mass %	mass %
C			
H			
N			

Table A 7 *Template Element analysis (fresh non-weathered samples) reported by China.*

Sample name	Sample 1	Sample 2	Sample 3
Oil type	WRG	MGO	VLSFO
Sample ID	2021-5427	2021-5428	2021-5429
Internal Lab ID			
ICP/MS or ICP/AES	mg/kg	mg/kg	mg/kg
Aluminium (Al)	<1	<1	2
Calcium (Ca)	<1	<1	6
Iron (Fe)	<1	<1	7
Nickel (Ni)	<1	<1	10
Silicon (Si)	13	10	15
Sodium (Na)	<1	<1	16
Vanadium (V)	<1	<1	10
Sulfur (S)	0.04 %	0.08 %	0.48 %
Copper (Cu)	<1	<1	<1
ASTM D5291	mass %	mass %	mass %
C	86.5	85.07	88.19
H	13.11	11.73	10.48
N	0.016	0.011	0.31

Table A 8 *Template Element analysis (fresh non-weathered samples) reported by Norway.*

Laboratory	SINTEF	SINTEF	SINTEF
Sample name	WRG	MGO	VLSFO
Internal sample ID	2021-5427-S1-S4-S2	2021-5428-S2-S4-S2	2021-5429-S1-S4-S2
Oil category	WRG	MGO	VLSFO
ICP/MS or ICP/AES	mg/kg	mg/kg	mg/kg
Aluminium (Al)	<1	<1	1
Calcium (Ca)	<5	<5	5
Iron (Fe)	<1	<1	3
Nickel (Ni)	<1	<1	10
Silicon (Si)	<5	<5	<5
Sodium (Na)	<2	<2	6
Vanadium (V)	<1	<1	10
Sulfur (S)	-	-	-
Copper (Cu)	<1	<1	<1
ASTM D5291	mass %	mass %	mass %
Carbon (C)			
Hydrogen (H)			
Nitrogen (N)			
ASTM D4294	mass %	mass %	mass %
Sulfur (S)	0.04 (wt. %)	0.08 (wt. %)	0.54 (wt. %)
MT/ELE/21	% (m/m)	% (m/m)	% (m/m)
Oxygen (O)	<0.04	0.05	0.26
ASTM D2622	mass %	mass %	mass %
Sulfur (S)	<0.1	<0.1	0.479
MT/ELE/13	% (m/m)	% (m/m)	% (m/m)
Carbon (C)	87.0	86.9	87.7
Hydrogen (H)	14.0	13.2	11.2
Nitrogen (N)	<0.1	<0.1	0.3

Table A 9 *Temperature-sweep of WRG, MGO and VLSFO reported by Sweden. Viscosity, Kinematic, (mm²s⁻¹), ASTM D 7042*

Laboratory			Laboratory			Laboratory		
Sample name			Sample name			Sample name		
Sample ID			Sample ID			Sample ID		
Internal Lab ID			Internal Lab ID			Internal Lab ID		
Oil type			Oil type			Oil type		
Sample description			Sample description			Sample description		
Temperature	Viscosity (10 ⁻³)		Temperature	Viscosity (10 ⁻³)		Temperature	Viscosity (10 ⁻³)	
[°C]	[mPa·s]		[°C]	[mPa·s]		[°C]	[mPa·s]	
0	N/A		0		9.23	0	N/A	
10	N/A		10		6.508	10	N/A	
20		44.56	20		4.881	20	N/A	
50		11.05	50		2.505	50		77.78
70		6.378	70		1.803	70		30.81
100		3.452	100		1.22	100		11.3

Table A 10 *Temperature-sweep of WRG, MGO and VLSFO reported by Norway.*

Laboratory			Laboratory			Laboratory		
Sample name			Sample name			Sample name		
Internal sample ID			Internal sample ID			Internal sample ID		
Oil category			Oil category			Oil category		
Temperature	Viscosity (10 ⁻¹)		Temperature	Viscosity (10 ⁻¹)		Temperature	Viscosity (10 ⁻¹)	
[°C]	[mPa·s]		[°C]	[mPa·s]		[°C]	[mPa·s]	
52.09	9.1714		52.13	2.1087		52.01	64.268	
51.17	9.1001		51.19	2.0761		50.94	65.405	
49.89	9.25		49.91	2.0963		49.89	67.712	
48.76	9.4639		48.76	2.1261		48.85	70.697	
47.7	9.7215		47.7	2.1498		47.82	74.211	
46.67	10.015		46.66	2.1862		46.8	78.061	
45.65	10.326		45.64	2.2339		45.78	82.442	
44.63	10.665		44.61	2.2729		44.76	87.141	
43.61	11.012		43.59	2.3115		43.74	92.076	
42.59	11.397		42.56	2.3604		42.72	97.629	
41.57	11.791		41.54	2.4154		41.7	103.54	
40.55	12.208		40.52	2.4609		40.68	109.75	
39.53	12.66		39.51	2.5088		39.66	116.57	
38.51	13.135		38.49	2.5688		38.64	124.23	
37.5	13.625		37.47	2.6286		37.63	132.48	
36.48	14.148		36.46	2.6782		36.61	142.1	
35.46	14.705		35.44	2.7388		35.59	153.57	
34.44	15.287		34.43	2.809		34.57	167.19	
33.42	15.896		33.41	2.8722		33.55	181.12	
32.41	16.548		32.39	2.9331		32.53	195.75	
31.39	17.239		31.37	3.0064		31.51	212.27	
30.37	17.961		30.36	3.0857		30.49	230.96	
29.36	18.723		29.34	3.1599		29.47	251.74	
28.34	19.54		28.32	3.2345		28.45	276.18	
27.32	20.404		27.3	3.3204		27.43	304.34	
26.3	21.31		26.29	3.4081		26.41	336.88	
25.28	22.276		25.27	3.491		25.39	376.65	
24.26	23.309		24.27	3.5804		24.37	423.64	
23.25	24.401		23.25	3.6817		23.35	479.52	
22.23	25.566		22.23	3.7787		22.33	546.67	
21.22	26.743		21.22	3.8772		21.31	627.22	
20.2	27.988		20.2	3.987		20.29	723.81	
19.18	29.386		19.18	4.1059		19.27	838.47	
18.17	30.958		18.17	4.2201		18.26	975.24	
17.15	32.696		17.15	4.3379		17.24	1139.6	
16.14	34.614		16.13	4.472		16.22	1337.2	
15.12	36.726		15.12	4.6086		15.2	1571.7	
14.1	39.057		14.1	4.7437		14.18	1853.7	
13.09	41.713		13.08	4.888		13.16	2196.6	
12.07	44.688		12.07	5.0467		12.14	2596.8	
11.06	48.054		11.05	5.2075		11.12	3077.4	
10.05	51.827		10.04	5.367		10.1	3639.3	
9.04	56.073		9.03	5.5436		9.08	4284.1	
8.01	60.863		8	5.7342		8.06	5031	
6.99	66.233		6.99	5.9234		7.05	5879.3	
5.98	72.199		5.97	6.1218		6.03	6835.2	
4.97	78.822		4.96	6.3395		5.01	7902.2	
3.96	86.112		3.94	6.5662		3.99	9096.3	
2.94	94.182		2.93	6.7971		2.97	10433	
1.92	103.072		1.92	7.0403		1.95	11915	
0.91	112.821		0.91	7.3065		0.93	13567	
-0.1	123.462		-0.1	7.5811		-0.09	15414	
-1.11	135.086		-1.12	7.8649		-1.11	17513	
-2.12	147.725		-2.13	8.1718		-2.13	19904	

Table A 11 True boiling point (TBP) of WRG, MGO and VLSFO reported by Sweden. Simdist GC (fresh non-weathered samples).

Laboratory Saybolt Sweden Sample name WRG			Laboratory Saybolt Sweden Sample name MGO			Laboratory Saybolt Sweden Sample name VLSFO		
Sample ID Received Sample Test Oil : 1 WRG			Sample ID Received Sample Test Oil : 2 MGO			Sample ID Received Sample Test Oil : 3 VLSFO		
Internal Lab ID 12669825			Internal Lab ID 12670165			Internal Lab ID 12670191		
Oil type WRG			Oil type MGO			Oil type Fuel Oil VLSFO		
Sample description			Sample description			Sample description		
Temp. °C	Wt%		Temp. °C	Wt%		Temp. °C	Wt%	
150		0.5	100.5		0.5	154.5		0.5
255		5	148		5	224.5		5
292.5		10	169		10	278.5		10
311.5		15	184		15	316		15
325		20	198		20	340.5		20
335.5		25	209		25	359		25
344.5		30	218.5		30	374.5		30
352		35	229		35	388.5		35
359		40	236.5		40	401.5		40
365		45	247		45	413.5		45
372		50	255.5		50	426		50
378		55	267		55	439		55
385		60	277		60	453.5		60
391		65	286.5		65	469		65
397		70	297.5		70	486		70
404		75	307.5		75	505.5		75
411.5		80	319		80	527		80
420.5		85	333		85	554		85
432		90	349		90	587		90
450.5		95	369		95	632		95
493		99.5	412.5		99.5	695		99.5

Table A 12 True boiling point (TBP) of WRG, MGO and VLSFO reported by Canada. Simdist GC (fresh non-weathered samples).

Laboratory 6081 Sample name Sample 1			Laboratory 6081 Sample name Sample 2			Laboratory 6081 Sample name Sample 3		
Sample ID 2021-6081			Sample ID 2021-6082			Sample ID 2021-6083		
Internal Lab ID 6081			Internal Lab ID 6082			Internal Lab ID 6083		
Oil type WRG			Oil type MGO			Oil type VLSFO		
Sample description Test oil			Sample description Test oil			Sample description Test oil		
Temp. °C	Wt%		Temp. °C	Wt%		Temp. °C	Wt%	
169	Initial Boiling Point		119.4	Initial Boiling Point		169.3	Initial Boiling Point	
272	5		166.6	5		245.8	5	
309	10		188.7	10		302.4	10	
329	15		205.3	15		339.7	15	
342	20		218.7	20		365	20	
353	25		229.6	25		383.5	25	
362	30		239.1	30		399.2	30	
369	35		248.9	35		413.6	35	
376	40		258.1	40		427.1	40	
382	45		268.2	45		440.2	45	
389	50		278.4	50		454.5	50	
395	55		289.5	55		469.9	55	
402	60		300.5	60		486.4	60	
408	65		309.8	65		504.7	65	
415	70		320.3	70		526.2	70	
422	75		332.6	75		550.9	75	
429	80		346.2	80		581.9	80	
439	85		361.7	85		620.2	85	
451	90		380.3	90		665.1	90	
470	95		414.7	95				
519								
547	100							

Table A 13 *True boiling point (TBP) of WRG, MGO and VLSFO reported by Norway. Simdist GC (fresh non-weathered samples).*

Laboratory	SINTEF		Laboratory	SINTEF		Laboratory	SINTEF	
Sample name	WRG		Sample name	MGO		Sample name	VLSFO	
Internal sample ID	2021-5427		Internal sample ID	2021-5428		Internal sample ID	2021-5429	
Oil category	WRG		Oil category	MGO		Oil category	VLSFO	
Temp. °C	Wt%		Temp. °C	Wt%		Temp. °C	Wt%	
	188	1		135	1		191	1
	216	2		146	2		201	2
	237	3		154	3		217	3
	270	5		166	5		240	5
	289	7		175	7		261	7
	307	10		187	10		293	10
	327	15		202	15		331	15
	341	20		217	20		356	20
	352	25		226	25		375	25
	361	30		236	30		391	30
	370	35		246	35		406	35
	376	40		255	40		419	40
	383	45		265	45		432	45
	390	50		274	50		445	50
	396	55		285	55		459	55
	403	60		295	60		474	60
	409	65		305	65		490	65
	416	70		316	70		506	70
	423	75		327	75		525	75
	431	80		339	80		549	80
	440	85		353	85		576	85
	452	90		369	90		610	90
	463	93		381	93		638	93
	473	95		391	95		660	95
	486	97		405	97		674	96
	496	98		415	98		691	97
	513	99		431	99		708	98
	531	100		447	100			

Appendix B Reported results chemistry of the oils

B1 Reported results chemistry of oils – USA

USA has not reported volatiles in the oils.

Table B 1 Summary of the chemical composition of the oils (USA)

Laboratory	USA	USA	USA
Sample ID	WRG	MGO	VLSFO
Internal Lab ID	LSFO 1	LSFO 2	LSFO 3
Sample description	WRG	MGO	VLSFO
	mg/kg oil	mg/kg oil	mg/kg oil
Sum SVOC	8832	63301	85530
Sum VOC	NA	NA	NA
Decalins	NA	NA	NA
Naphthalenes	1063	33668	25555
2-3 ring PAH	7669	61444	59895
4-6 ring PAH	1162	1857	25635
C0-C5 phenols	NA	NA	NA
BTEX	NA	NA	NA
C3-benzenes	NA	NA	NA
Other VOC	NA	NA	NA

Table B 2 Semi-volatile components in the oils (in g analyte/kg oil) (USA)

Laboratory	USA	USA	USA	
Sample ID	WRG	MGO	VLSFO	
Internal Lab ID	LSFO 1	LSFO 2	LSFO 3	
Oil type	WRG	MGO	VLSFO	
PAH compound class	mg/kg oil	mg/kg oil	mg/kg oil	
Decalin				
C1-decalins				
C2-decalins				
C3-decalins				
C4-decalins				
Benzo(b)thiophene				
Naphthalene	31.3	1 749	2 973	2 ring
C1-naphthalenes	109	7 042	5 694	
C2-naphthalenes	223	11 015	7 482	
C3-naphthalenes	326	9 047	6 456	
C4-naphthalenes	373	4 815	2 950	
Biphenyl	67.9	867	147	
Acenaphthylene	4.44	47.8	54.0	3 ring
Acenaphthene	4.00	100	152	

Laboratory	USA	USA	USA	
Sample ID	WRG	MGO	VLSFO	
Internal Lab ID	LSFO 1	LSFO 2	LSFO 3	
Oil type	WRG	MGO	VLSFO	
PAH compound class	mg/kg oil	mg/kg oil	mg/kg oil	
Dibenzofuran	14.7	266	69.1	
Fluorene	40.2	602	197	
C1-fluorenes	297	2 601	1 053	
C2-fluorenes	1 045	5 988	3 586	
C3-fluorenes	1 466	5 330	3 958	
Phenanthrene	76.8	822	903	
Anthracene	24.3	114	161	
C1-phenanthrenes/anthracenes	432	2 879	4 016	
C2-phenanthrenes/anthracenes	766	3 274	6 534	
C3-phenanthrenes/anthracenes	909	2 290	6 225	
C4-phenanthrenes/anthracenes	800	1 021	3 940	
Dibenzothiophene	13.7	71.5	102	
C1-dibenzothiophenes	66.4	326	542	
C2-dibenzothiophenes	171	501	978	
C3-dibenzothiophenes	225	456	1 059	
C4-dibenzothiophenes	182	220	664	
Fluoranthene	12.0	46.8	116	4 ring+
Pyrene	17.7	254	504	
C1-fluoranthrenes/pyrenes	183	710	3 313	
C2-fluoranthrenes/pyrenes	256	443	5 132	
C3-fluoranthrenes/pyrenes	251	218	4 827	
Benz(a)anthracene	7.22	10.3	259	
Chrysene+Triphenylene	28.7	24.5	422	
C1-chrysenes	82.5	46.7	2 109	
C2-chrysenes	107	37.5	3 189	
C3-chrysenes	97.3	27.2	3 050	
C4-chrysenes	74.6	16.2	1 885	
Benzo(b)fluoranthene	8.23	4.96	125	
Benzo(k)fluoranthene	4.02	1.08	28.7	
Benzo(e)pyrene	10.6	2.46	239	
Benzo(a)pyrene	6.64	2.90	153	
Perylene	3.86	2.60	72.3	
Indeno(1,2,3-c,d)pyrene	2.78	2.95	37.4	
Dibenz(a,h)anthracene	3.03	3.13	59.3	
Benzo(g,h,i)perylene	4.76	2.48	114	
Phenol				
C1-Phenols				
C2-Phenols				
C3-Phenols				
C4-Phenols				
C5-Phenols				

Laboratory	USA	USA	USA
Sample ID	WRG	MGO	VLSFO
Internal Lab ID	LSFO 1	LSFO 2	LSFO 3
Oil type	WRG	MGO	VLSFO
PAH compound class	mg/kg oil	mg/kg oil	mg/kg oil
30 ab hopane	132	6.64	158
Sum all compounds (not hopane)	8 832	63 301	85 530
Decalins			
Naphthalenes	1 063	33 668	25 555
2-3 ring PAHs	7 669	61 444	59 895
4-6 ring PAHs	1 162	1 857	25 635
C0-C5 Phenols			

B2 Reported results chemistry of oils – Canada

As Canada did not use the template spread sheets for reporting av oil chemistry, the reporting differs from the other laboratories. They did not report any volatile components in the oil, but they reported several other components which are given in the tables below.

Table B 3 Summary of the chemical composition of the oils (Canada). Table prepared by SINTEF, as Canada did not use the template spread sheet for reporting of the oil chemistry.

Laboratory	Canada	Canada	Canada
Sample ID	2021-5427	2021-5428	2021-5429
Internal Lab ID	2021-09-17-6081	2021-09-17-6082	2021-09-17-6083
Oil type	WRG	MGO	VLSFO
	mg/kg oil	mg/kg oil	mg/kg oil
Sum SVOC	4973	39199	52460
Sum VOC	NA	NA	NA
Decalins	NA	NA	NA
Naphthalenes	677	21108	16486
2-3 ring PAH	3791	16969	21581
4-6 ring PAH	505	1122	14393
C0-C5 phenols	NA	NA	NA
BTEX	NA	NA	NA
C3-benzenes	NA	NA	NA
Other VOC	NA	NA	NA

Table B 4 TPH analysis results from Canada

ESTS code	2021-09-17-6081	2021-09-17-6082	2021-09-17-6083
Sample Location	SINTEF, 2021-5427, S1-S3 fresh	SINTEF, 2021-5428, S1-S3 fresh	SINTEF, 2021-5429, S1-S3 fresh
Sample Description	Test oil 1, WRG, 5L	Test oil 2, MGO, 5L	Test oil 3, VLSFO, 5L
	mg/g oil	mg/g oil	mg/g oil
TPH	1058	901	693
TSH	801	569	308
TAH	258	331	385
Resolved peaks (F3)	247	442	101
TSH/TPH (%)	75.7	63.2	44.5
TAH/TPH (%)	24.3	36.8	55.5
Resolved Peaks/TPH (%)	21.2	37.5	17.2
TPH fractions (%)			
TPH F1 (<n-C10)	0.45	4.71	0.33
TPH F2 (<n-C10-n-C16)	6.76	45.8	8.85
TPH F3 (n-C16-n-C34)	88.5	49.3	63.9
TPH F4 (>n-C34)	4.30	0.16	27.0

Table B 5 *n-Alkane analysis results (Canada)*

ESTS code	2021-09-17-6081	2021-09-17-6082	2021-09-17-6083
Sample Location	2021-5427, S1-S3 fresh	2021-5428, S1-S3 fresh	2021-5429, S1-S3 fresh
Sample Description	Test oil 1, WRG, 5L	Test oil 2, MGO, 5L	Test oil 3, VLSFO, 5L
Compounds	µg/g oil	µg/g oil	µg/g oil
n-Alkanes			
n-C9	330	3509	77.1
n-C10	1019	5123	162
n-C11	1311	4886	243
n-C12	1336	5105	333
n-C13	1397	5286	419
TMD	408	1869	63.0
n-C14	1628	5513	438
n-C15	1819	4743	447
n-C16	2159	4440	443
TMP	1397	3029	217
n-C17	2757	4748	514
Pristane	1570	2144	128
n-C18	3131	3747	573
Phytane	2482	2603	187
n-C19	3672	3518	755
n-C20	4271	3294	962
n-C21	4787	2819	1112
n-C22	5555	2783	1275
n-C23	5767	2419	1428
n-C24	6329	2201	1589
n-C25	5844	1665	1712
n-C26	4443	1154	1852
n-C27	3449	735	1674
n-C28	3193	406	1501
n-C29	2548	262	1424
n-C30	2235	180	1206
n-C31	1572	90	1074
n-C32	1003	46.7	875
n-C33	652	21.7	769
n-C34	542	13.3	664
n-C35	361	7.5	600
n-C36	193	4.12	505
n-C37	110	3.48	370
n-C38	73.1	3.60	306
n-C39	38.7	5.5	224
n-C40	25.0	4.63	137
Total n-alkanes	79405	78380	26259

ESTS code	2021-09-17-6081	2021-09-17-6082	2021-09-17-6083
Sample Location	2021-5427, S1-S3 fresh	2021-5428, S1-S3 fresh	2021-5429, S1-S3 fresh
Sample Description	Test oil 1, WRG, 5L	Test oil 2, MGO, 5L	Test oil 3, VLSFO, 5L
Compounds	µg/g oil	µg/g oil	µg/g oil
Diagnostic indexes			
n-C17/Pristane	1.76	2.2	4.01
n-C18/Phytane	1.26	1.44	3.06
Pr/Ph	0.63	0.82	0.68
Odd alkanes	36414	34716	12842
Even alkanes	35914	30375	12446
CPI	1.01	1.14	1.03

Table B 6 *Biomarker analysis results (Canada)*

ESTS code	2021-09-17-6081	2021-09-17-6082	2021-09-17-6083
Sample Location	SINTEF, 2021-5427, S1-S3 fresh	SINTEF, 2021-5428, S1-S3 fresh	SINTEF, 2021-5429, S1-S3 fresh
Sample Description	Test oil 1, WRG, 5L	Test oil 2, MGO, 5L	Test oil 3, VLSFO, 5L
Biomarker compounds	µg/g oil	µg/g oil	µg/g oil
C21 terpane	18.4	6.24	5.46
C22 terpane	6.64	1.47	2.86
C23 terpane	22.7	7.69	21.8
C24 terpane	27.8	6.05	11.6
C27 Ts	51.0	3.95	24.8
C27 Tm	33.6	2.47	52.2
C29aß hopane	105	4.73	109
C30aß hopane	159	6.04	119
C31(S) hopane	49.3	1.53	38.5
C31(R) hopane	37.1	1.13	33.3
GAM	7.65	0.25	18.7
C32(S) hopane	32.7	1.28	30.3
C32(R) hopane	23.5	0.65	22.9
C33(S) hopane	23.5	0.44	21.8
C33(R) hopane	15.6	0.34	15.7
C34(S) hopane	13.7	0.25	18.1
C34(R) hopane	8.02	0.16	11.1
C35(S) hopane	10.1	0.12	15.4
C35(R) hopane	7.81	0.11	14.2
C27aßß steranes	563	39.4	96.4
C28aßß steranes	395	21.4	68.7
C29aßß steranes	446	22.1	101
Total	2057	128	853
Diagnostic Ratios			
C23/C24	0.81	1.27	1.89

C23/C30	0.14	1.27	0.18	
C24/C30	0.18	1.00	0.10	
C29/C30	0.66	0.78	0.92	
C31(S)/C31(R)	1.33	1.35	1.16	
C32(S)/C32(R)	1.40	1.96	1.32	
Ts/Tm	1.52	1.60	0.48	
C27abb/ C29abb	1.26	1.78	0.95	
C30/(C31+C32+C33+C34+C35)	0.69	0.97	0.49	
Ts/C30aß hopane	0.32	0.65	0.21	191
Tm/C30aß hopane	0.21	0.41	0.44	191
28aß/C30aß hopane	/	/	/	191 C28 17a(H),21ß(H)-28,30-biosnorhopane
C29aß hopane/C30aß hopane	0.66	0.78	0.92	191
30O/C30aß hopane	/	/	/	191 C30 18a(H)-oleanane
31aßS/C30aß hopane	0.31	0.25	0.32	191
27dbR/27dbS	/	/	/	217 S before, R after
27bb/29bb	1.26	1.78	0.95	218 R before, S after
TASC26/RC26+SC27				231
TASC28/RC26+SC27				231
TARC27/RC26+SC27				231
TARC28/RC26+SC27				231

Table B 7 PAH analysis results (Canada)

Laboratory		Canada	Canada	Canada
ESTD sample No.		2021-09-17-6081	2021-09-17-6082	2021-09-17-6083
Sample Location		SINTEF, 2021-5427,	SINTEF, 2021-5428,	SINTEF, 2021-5429,
Sample Description		S1-S3	S1-S3	S1-S3
Alkylated PAHs		WRG	MGO	VLSFO
		µg/g oil	µg/g oil	µg/g oil
Naphthalene	C0-N	22.7	1107	1730
	C1-N	75.0	3719	3128
	C2-N	165	6676	4924
	C3-N	223	6241	4433
	C4-N	190	3364	2271
	Sum	677	21108	16486
Phenanthrene	C0-P	50.6	581	612
	C1-P	321	2194	3091
	C2-P	542	2465	4686
	C3-P	634	1688	4213
	C4-P	560	770	2525
	Sum	2108	7698	15126
Dibenzothiophene	C0-D	0.00	55.8	78.8
	C1-D	27.9	254	388
	C2-D	97.2	397	785
	C3-D	117	246	809
	Sum	242	953	2061
Fluorene	C0-F	27.3	479	151
	C1-F	208	1856	758

Laboratory		Canada	Canada	Canada
ESTD sample No.		2021-09-17-6081	2021-09-17-6082	2021-09-17-6083
Sample Location		SINTEF, 2021-5427, S1-S3	SINTEF, 2021-5428, S1-S3	SINTEF, 2021-5429, S1-S3
Sample Description		WRG	MGO	VLSFO
Alkylated PAHs		µg/g oil	µg/g oil	µg/g oil
Fluoranthene	C2-F	468	2835	1458
	C3-F	663	2357	1640
	Sum	1366	7527	4007
	C0-FI	2.94	29.0	74.0
	C1-FI	63.3	380	1653
	C2-FI	109	236	2507
	C3-FI	133	115	2635
	C4-FI	106	50.9	1512
Benzonaphthothiophene	sum	414	811	8380
	C0-B	0.00	10.1	47.4
	C1-B	0.00	38.4	424
	C2-B	0.00	30.5	616
	C3-B	0.00	15.7	581
	C4-B	0.00	0.00	322
	Sum	0.00	94.6	1990
Chrysene	C0-C	17.2	24.7	337
	C1-C	29.1	28.5	1464
	C2-C	47.3	24.9	2304
	C3-C	63.8	8.97	1955
	Sum	157	87.1	6059
Total alkylated PAHs		4964	38278	54110
4-Methyldibenzothiophene		4-MD	23.0	148
2-/3-Methyldibenzothiophene		2/3-MD	4.96	65.7
1-Methyldibenzothiophene		1-MD	0.00	27.6
Other Priority PAHs				
Biphenyl (Bph)		Bph	57.6	569
Acenaphthylene (Acl)		Acl	1.66	38.0
Acenaphthene (Ace)		Ace	4.01	90.2
Anthracene (An)		An	12.2	95.2
Fluoranthene (FI)		FI	4.26	36.7
Pyrene (Py)		Py	22.6	255
Benz(a)anthracene (BaA)		BaA	2.20	7.04
Benzo(b)fluoranthene (BbF)		BbF	2.84	1.57
Benzo(k)fluoranthene (BkF)		BkF	0.00	0.00
Benzo(e)pyrene (BeP)		BeP	6.72	1.79
Benzo(a)pyrene (BaP)		BaP	0.67	0.52
Perylene (Pe)		Pe	1.09	0.43
Indeno(1,2,3-cd)pyrene (IP)		IP	0.29	0.06
Dibenzo(ah)anthracene (DA)		DA	0.25	0.09
Benzo(ghi)perylene (BgP)		BgP	1.69	0.10
Total EPA priority PAHs		118	1096	1926
Total aromatic compounds		5082	39374	56036
Diagnostic Ratios				
2-m-N:1-m-N		1.30	1.45	1.65
(3+2-)/(4-/9-+1-m-phen)		0.70	1.60	1.67
4-:2-/3-:1-m-DBT		1.00:0.22:0	1.00:0.44:0.19	1.00:0.95:0.18
(C2D/C2P):(C3D/C3P)		0.97	1.11	0.87
C0N:C1N:C2N:C3N:C4N		0.12:0.39:0.87:1.18:1.00	0.33:1.11:1.98:1.86:1.00	0.76:1.38:2.17:1.95:1.00

Laboratory	Canada	Canada	Canada
ESTD sample No.	2021-09-17-6081	2021-09-17-6082	2021-09-17-6083
Sample Location	SINTEF, 2021-5427, S1-S3	SINTEF, 2021-5428, S1-S3	SINTEF, 2021-5429, S1-S3
Sample Description	WRG	MGO	VLSFO
Alkylated PAHs	µg/g oil	µg/g oil	µg/g oil
Ci-N:Ci-P:Ci-D-Ci-F:Ci-Fl:Ci-B:Ci-C	0.32:1.00:0.11:0.65:0. 2:0:0.07	2.74:1.00:0.12:0.98:0. 11:0.01:0.01	1.09:1.00:0.14:0.26:0. 55:0.13:0.4
2MP/1MP	0.81	1.95	1.82
2MA/1MP	0.05	0.10	0.44
4MD/1MD	/	5.26	5.56
2MF/4MPy	0.06	0.31	0.20
B(a)F/4MPy	0.18	0.57	0.29
B(b+C)F/4MPy	0.09	0.26	0.20
2MPy/4MPy	0.41	1.55	0.85
1MPy/4MPy	0.58	0.66	0.77
Retene/TMPhe	/	/	/
BNT/TMPhe	0.00	0.01	0.02
Sulfur content			
1M-DBT/30ab	0.00	4.58	0.28
4M-DBT/30ab	0.14	24.5	1.54
BNT/30ab	0.00	1.67	0.40
If 30ab is small or not present (lighter products)			
1M-DBT/1MP	0.00	0.08	0.06
4M-DBT/1MP	0.28	0.42	0.35
BNT/TMPhe	0.00	0.01	0.02
Optional ratios sulfur content			
C2-DBT/C2-Phe	0.18	0.16	0.17
C3-DBT/C2-Phe	0.22	0.10	0.17
BNT/C2-Phe	0.00	0.00	0.01
C2-BT/C2-Phe	/	/	/

B3 Reported results chemistry of oils – China

Table B 8 Summary of the chemical composition of the oils (China)

Laboratory	China	China	China
Sample ID	2021-5427	2021-5428	2021-5429
Internal Lab ID			
Oil type	WRG	MGO	VLSFO
Sample description	OIL 1(WRG)	OIL 2(MGO)	OIL 3(VLSFO)
	mg/kg oil	mg/kg oil	mg/kg oil
Sum SVOC	2399	2838	4119
Sum VOC	2962	7129	1571
Decalins	26.8	29.9	19.2
Naphthalenes	2102	2350	3462
2-3 ring PAH	87.7	254	325
4-6 ring PAH	60.1	55.4	168
C0-C5 phenols	122	149	146
BTEX	1632	3632	981
C3-benzenes	882	2726	498
Other VOC (Sum VOC-(BTEX+C3-benzenes))	447	771	91.5

Table B 9 Semi volatiles in the oils (mg analyte/kg oil) (China)

Laboratory	China	China	China	
Sample ID	2021-5427	2021-5428	2021-5429	
Internal Lab ID				
Oil type	WRG	MGO	VLSFO	备注
	mg/kg oil	mg/kg oil	mg/kg oil	
Decalin	26.8	29.9	19.2	
C1-decalins				
C2-decalins				
C3-decalins				
C4-decalins				
Benzo(b)thiophene	2.64	23.0	38.5	
Naphthalene	12.2	167	166	
C1-naphthalenes	254	182	2720	
C2-naphthalenes	1836	2001	576	C2+C3-naphthalene
C3-naphthalenes				
C4-naphthalenes				
Biphenyl				
Acenaphthylene				
Acenaphthene				
Dibenzofuran				
Fluorene	21.5	111	57.6	
C1-fluorenes				

Laboratory	China	China	China	
Sample ID	2021-5427	2021-5428	2021-5429	
Internal Lab ID				
Oil type	WRG	MGO	VLSFO	备注
	mg/kg oil	mg/kg oil	mg/kg oil	
C2-fluorenes				
C3-fluorenes				
Phenanthrene	8.43	19.4	14.3	Phenanthrene/Anthracene
Anthracene				
C1-phenanthrenes/anthracenes	2.21	17.7	15.8	
C2-phenanthrenes/anthracenes	43.5	62.7	160	
C3-phenanthrenes/anthracenes				
C4-phenanthrenes/anthracenes				
Dibenzothiophene	6.37	16.9	18.5	
C1-dibenzothiophenes				
C2-dibenzothiophenes	2.98	2.7898	20.2	
C3-dibenzothiophenes				
C4-dibenzothiophenes				
Fluoranthene	26.6	20.7	69.1	Fluoranthene/Pyrene
Pyrene				
C1-fluoranthrenes/pyrenes	8.31	24.6	33.3	
C2-fluoranthrenes/pyrenes				
C3-fluoranthrenes/pyrenes				
Benz(a)anthracene	2.44	0.69	5.95	Benz[a]anthracene+Chrysene
Chrysene				
C1-chrysenes	13.8	3.38	15.1	
C2-chrysenes	0.61	0.66	6.76	
C3-chrysenes				
C4-chrysenes				
Benzo(b)fluoranthene	1.40	0.166	7.31	benzo(bk)fluoranthene
Benzo(k)fluoranthene				
Benzo(e)pyrene	4.59	5.25	12.2	
Benzo(a)pyrene	1.55	0.000	4.53	
Perylene				
Indeno(1,2,3-c,d)pyrene	0.777	0.000	13.8	Indeno[1,2,3-c,d]pyrene+ Dibenz[a,h]anthracene+ Benzo(g,h,i)perylene
Dibenz(a,h)anthracene				
Benzo(g,h,i)perylene				
Phenol	24.4	27.2	38.6	
C1-Phenols	57.9	67.2	69.8	C1+C2-phenol
C2-Phenols				
C3-Phenols				
C4-Phenols		54.9	37.2	
C5-Phenols				
30 ab hopane				

Laboratory	China	China	China	
Sample ID	2021-5427	2021-5428	2021-5429	
Internal Lab ID				
Oil type	WRG	MGO	VLSFO	备注
	mg/kg oil	mg/kg oil	mg/kg oil	
Sum all compounds (not hopane)				
Decalins	26.8	29.9	19.2	
Naphthalenes	2102	2350	3461	
2-3 ring PAHs	87.7	254	324	
4-6 ring PAHs	60.1	55.4	168	
C0-C5 Phenols	122	149	146	

Table B 10 Volatiles in the oils (mg analyte/kg oil) (China)

Laboratory	China	China	China
Internal Lab ID			
Sample ID	2021-5427	2021-5428	2021-5429
Sample description	OIL 1(WRG)	OIL 2(MGO)	OIL 3(VLSFO)
	mg/kg	mg/kg	mg/kg
Isopentane	0.000	0.000	0.000
n-C5 (Pentane)	0.000	0.000	0.000
Cyclopentane	0.000	0.000	0.000
2-methylpentane	1.16	5.42	0.000
3-Methylpentane	2.11	7.11	1.97
n-C6 (Hexane)	1.27	4.02	0.000
Methylcyclopentane	10.3	30.1	0.000
Benzene	280	405	68.6
Cyclohexane	36.8	27.0	0.000
2,3-Dimethylpentane	3.48	10.1	0.000
3-methylhexane	3.80	0.000	0.000
n-C7 (Heptane)	1.52	11.9	0.000
Methylcyclohexane	23.479	25.7	0.000
Toluene	548	1749	278
2,4 dimethylhexane	0.000	55.3	0.000
2-Methylheptane	0.000	0.000	0.000
n-C8 (Octane)	322	366	0.000
Ethylbenzene	290	399	99.2
m-Xylene	381	896	0.000
p-Xylene			536
o-Xylene	133	183	0.000
n-C9 (Nonane)	27.3	37.4	51.0
Propylbenzene	45.5	128	38.5
1-Methyl-3-ethylbenzene	184	1074	272
1-Methyl-4-ethylbenzene	66.2		
1,3,5-trimethylbenzene	73.8		0.000

Laboratory	China	China	China
Internal Lab ID			
Sample ID	2021-5427	2021-5428	2021-5429
Sample description	OIL 1(WRG)	OIL 2(MGO)	OIL 3(VLSFO)
	mg/kg	mg/kg	mg/kg
1-Methyl-2-ethylbenzene			
1,2,4-Trimethylbenzene	274	1524	0.000
n-C10 (Decane)			
1,2,3-Trimethylbenzene	240		188
n-Butylbenzene	12.4	12.1	30.7
1,2,4,5-Tetramethylbenzene	0.629	113	0.000
n-Pentylbenzene	1.21	65.5	7.77
Sum VOC	2962	7129	1571
BTEX	1632	3632	981
C3-benzenes	882	2726	498
Other VOC	447	770	91.5

B4 Reported results chemistry of oils – Sweden

Sweden has not reported the chemistry in the oils.

B5 Reported results chemistry of oils – Norway

Table B 11 *Summary of the chemical composition of the oils (Norway)*

Laboratory	Norway	Norway	Norway
Internal sample ID	2021-5427	2021-5428	2021-5429
Oil	WRG	MGO	VLSFO
Norway	g/kg	g/kg	g/kg
Sum SVOC	7.12	52.1	56.5
Sum VOC	1.14	49.3	1.46
Decalins	1.53	11.8	0.28
Naphthalenes	0.86	23.6	18.1
2-3 ring PAH	4.05	15.6	21.4
4-6 ring PAH	0.68	1.05	16.8
C0-C5 phenols	0.004	0.010	0.009
BTEX	0.18	5.28	0.27
C3-benzenes	0.22	16.6	0.69
Other VOC	0.73	27.4	0.49

Table B 12 *Semi-volatile components in the oils (in g analyte/kg oil) (Norway)*

Laboratory		Norway	Norway	Norway
Internal sample ID		2021-5427	2021-5428	2021-5429
Oil category		WRG	MGO	VLSFO
	RRF	g/kg oil	g/kg oil	g/kg oil
Decalin	0.307	0.232	1.554	0.022
C1-decalins	0.307	0.369	2.847	0.046
C2-decalins	0.307	0.371	3.002	0.074
C3-decalins	0.307	0.337	2.783	0.078
C4-decalins	0.307	0.219	1.642	0.057
Benzo(b)thiophene	1.181	0.002	0.028	0.048
Naphthalene	1.234	0.061	2.193	2.503
C1-naphthalenes	1.234	0.120	5.246	3.820
C2-naphthalenes	1.234	0.191	7.515	5.604
C3-naphthalenes	1.234	0.237	5.590	4.037
C4-naphthalenes	1.234	0.247	3.072	2.099
Biphenyl	1.288	0.078	0.886	0.151
Acenaphthylene	1.016	0.002	0.031	0.033
Acenaphthene	0.751	ND	0.108	0.154
Dibenzofuran	1.321	0.010	0.249	0.056
Fluorene	0.960	0.030	0.583	0.203
C1-fluorenes	0.960	0.158	1.427	0.637

Laboratory		Norway	Norway	Norway
Internal sample ID		2021-5427	2021-5428	2021-5429
Oil category		WRG	MGO	VLSFO
	RRF	g/kg oil	g/kg oil	g/kg oil
C2-fluorenes	0.960	0.459	2.309	1.373
C3-fluorenes	0.960	0.601	1.816	1.481
Phenanthrene	1.416	0.071	0.789	0.925
Anthracene	1.232	0.011	0.092	0.025
C1-phenanthrenes/anthracenes	1.416	0.317	2.071	2.929
C2-phenanthrenes/anthracenes	1.416	0.578	2.288	4.611
C3-phenanthrenes/anthracenes	1.416	0.645	1.403	4.359
C4-phenanthrenes/anthracenes	1.416	0.688	0.688	2.541
Dibenzothiophene	1.725	0.001	0.052	0.085
C1-dibenzothiophenes	1.725	0.041	0.178	0.319
C2-dibenzothiophenes	1.725	0.108	0.254	0.570
C3-dibenzothiophenes	1.725	0.117	0.211	0.517
C4-dibenzothiophenes	1.725	0.133	0.128	0.414
Fluoranthene	1.482	0.005	0.033	0.086
Pyrene	1.562	0.021	0.267	0.589
C1-fluoranthrenes/pyrenes	1.482	0.106	0.403	1.825
C2-fluoranthrenes/pyrenes	1.482	0.087	0.055	0.697
C3-fluoranthrenes/pyrenes	1.482	0.211	0.157	4.030
Benz(a)anthracene	1.556	0.002	0.008	0.283
Chrysene	1.672	0.031	0.041	0.578
C1-chrysenes	1.672	0.049	0.039	1.962
C2-chrysenes	1.672	0.060	0.025	2.754
C3-chrysenes	1.672	0.045	0.012	2.124
C4-chrysenes	1.672	0.032	0.003	0.923
Benzo(b)fluoranthene	1.833	0.011	0.002	0.114
Benzo(k)fluoranthene	1.804	ND	ND	ND
Benzo(e)pyrene	1.861	0.009	0.002	0.224
Benzo(a)pyrene	1.668	0.009	0.001	0.171
Perylene	0.939	0.001	0.001	0.177
Indeno(1,2,3-c,d)pyrene	1.770	ND	ND	0.028
Dibenz(a,h)anthracene	1.763	ND	ND	0.055
Benzo(g,h,i)perylene	1.871	0.002	ND	0.143
Phenol	0.464	0.004	0.010	0.009
C1-Phenols	0.464	ND	ND	ND
C2-Phenols	0.464	ND	ND	ND
C3-Phenols	0.464	ND	ND	ND
C4-Phenols	0.464	ND	ND	ND
C5-Phenols	0.464	ND	ND	ND
30 ab hopane	1.013	0.251	0.007	0.193
Sum all compounds (not hopane)		7.12	52.1	56.5
Decalins		1.53	11.8	0.28

Laboratory	Norway	Norway	Norway
Internal sample ID	2021-5427	2021-5428	2021-5429
Oil category	WRG	MGO	VLSFO
RRF	g/kg oil	g/kg oil	g/kg oil
Naphthalenes	0.86	23.6	18.1
2-3 ring PAHs	4.05	15.6	21.4
4-6 ring PAHs	0.68	1.05	16.8
C0-C5 Phenols	0.004	0.010	0.009

Table B 13 *Volatile components in the oils (in g/kg oil) (Norway)*

Laboratory	Norway	Norway	Norway
Internal sample ID	2021-5427	2021-5428	2021-5429
Oil category	WRG	MGO	VLSFO
Norway	RRF	g/kg	g/kg
Isopentane	0.290	ND	ND
n-C5 (Pentane)	0.367	ND	ND
Cyclopentane	0.532	ND	ND
2-methylpentane	0.425	ND	ND
3-Methylpentane	0.457	ND	ND
n-C6 (Hexane)	0.405	ND	ND
Methylcyclopentane	0.583	ND	ND
Benzene	1.535	ND	ND
Cyclohexane	0.499	ND	ND
2,3-Dimethylpentane	0.343	ND	ND
3-methylhexane	0.274	ND	ND
n-C7 (Heptane)	0.350	ND	ND
Methylcyclohexane	0.443	0.076	ND
Toluene	1.403	0.048	0.042
2,4 dimethylhexane	0.797	ND	ND
2-Methylheptane	0.245	ND	ND
n-C8 (Octane)	0.168	ND	0.005
Ethylbenzene	0.868	0.020	0.031
m-Xylene	0.524	0.065	0.106
p-Xylene	0.621	0.021	0.040
o-Xylene	0.616	0.028	0.052
n-C9 (Nonane)	0.156	0.071	0.032
Propylbenzene	0.815	0.011	0.023
1-Methyl-3-ethylbenzene	0.565	0.041	0.131
1-Methyl-4-ethylbenzene	0.673	0.019	0.058
1,3,5-trimethylbenzene	0.580	0.022	0.060
1-Methyl-2-ethylbenzene	0.646	0.022	0.045
1,2,4-Trimethylbenzene	0.702	0.069	0.289
n-C10 (Decane)	0.226	0.511	0.101
1,2,3-Trimethylbenzene	0.702	0.040	0.089
n-Butylbenzene	0.742	0.019	0.034

1,2,4,5-Tetramethylbenzene	0.640	0.013	1.755	0.260
n-Pentylbenzene	0.671	0.040	0.606	0.061
Sum VOC		1.14	49.3	1.46
BTEX		0.18	5.28	0.27
C3-benzenes		0.22	16.6	0.69
Other VOC		0.73	27.4	0.49

Appendix C Reported result chemistry of the WAFs

C1 Reported results chemistry of WAFs – USA

Tabell C 1 Summary of the chemical composition of the WAFs (USA)

Laboratory	USA	USA	USA
Sample ID	WRG	MGO	VLSFO
Internal Lab ID	LSFO 1	LSFO 2	LSFO 3
Oil to water ratio	1:40	1:40	1:40
Sampling	18 hrs	18 hrs	18 hrs
	µg/L	µg/L	µg/L
Tot WAF			
TPH	981	5702	8787
Sum SVOC	25.0	554	615
Sum VOC			
UCM			
Decalins			
Naphthalenes	9.35	479	574
2-3 ring PAH	22.1	553	612
4-6 ring PAH	2.92	0.94	2.68
C0-C5 phenols			
BTEX	137	597	230
C3-benzenes			
Other VOC			

Tabell C 2 Semi-volatile components in the WAFs (in µg/L) (USA)

Laboratory	USA	USA	USA
Sample ID	WRG	MGO	VLSFO
Internal Lab ID	LSFO 1	LSFO 2	LSFO 3
Oil type	WRG	MGO	VLSFO
Oil to water ratio	1 to 40	1 to 40	1 to 40
Sample description	WAF 1	WAF 2	WAF 3
	µg/L	µg/L	µg/L
Decalin			
C1-decalins			
C2-decalins			
C3-decalins			
C4-decalins			
Benzo(b)thiophene			
Naphthalene	2.49	183	345
C1-naphthalenes	2.95	188	148
C2-naphthalenes	2.18	85.1	62.4
C3-naphthalenes	1.16	19.6	16.0

Laboratory	USA	USA	USA
Sample ID	WRG	MGO	VLSFO
Internal Lab ID	LSFO 1	LSFO 2	LSFO 3
Oil type	WRG	MGO	VLSFO
Oil to water ratio	1 to 40	1 to 40	1 to 40
Sample description	WAF 1	WAF 2	WAF 3
	µg/L	µg/L	µg/L
C4-naphthalenes	0.573	3.88	3.17
Biphenyl	1.68	19.9	3.72
Acenaphthylene	0.043	0.427	0.287
Acenaphthene	0.034	1.77	2.63
Dibenzofuran	0.283	5.50	1.26
Fluorene	0.566	9.96	2.83
C1-fluorenes	1.45	10.8	3.82
C2-fluorenes	1.18	3.93	2.14
C3-fluorenes	0.684	1.67	0.851
Phenanthrene	0.641	5.54	5.10
Anthracene	0.090	0.515	0.690
C1-phenanthrenes/anthracenes	1.47	6.23	6.69
C2-phenanthrenes/anthracenes	1.35	2.12	3.31
C3-phenanthrenes/anthracenes	1.01	0.445	0.958
C4-phenanthrenes/anthracenes	1.02	0.000	0.000
Dibenzothiophene	0.093	0.530	0.727
C1-dibenzothiophenes	0.307	1.85	2.04
C2-dibenzothiophenes	0.302	1.05	0.696
C3-dibenzothiophenes	0.301	0.854	0.000
C4-dibenzothiophenes	0.233	0.327	0.000
Fluoranthene	0.088	0.115	0.129
Pyrene	0.041	0.335	0.536
C1-fluoranthrenes/pyrenes	1.11	0.438	0.866
C2-fluoranthrenes/pyrenes	0.623	0.000	0.488
C3-fluoranthrenes/pyrenes	0.267	0.000	0.326
Benz(a)anthracene	0.016	0.016	0.063
Chrysene+Triphenylene	0.026	0.032	0.057
C1-chrysenes	0.199	0.000	0.120
C2-chrysenes	0.165	0.000	0.037
C3-chrysenes	0.000	0.000	0.000
C4-chrysenes	0.000	0.000	0.000
Benzo(b)fluoranthene	0.090	0.000	0.000
Benzo(k)fluoranthene	0.029	0.000	0.024
Benzo(e)pyrene	0.112	0.000	0.000
Benzo(a)pyrene	0.121	0.000	0.000
Perylene	0.027	0.000	0.000
Indeno(1,2,3-c,d)pyrene	0.000	0.000	0.039
Dibenz(a,h)anthracene	0.000	0.000	0.000
Benzo(g,h,i)perylene	0.000	0.000	0.000

3 ring

4 ring+

Laboratory	USA	USA	USA
Sample ID	WRG	MGO	VLSFO
Internal Lab ID	LSFO 1	LSFO 2	LSFO 3
Oil type	WRG	MGO	VLSFO
Oil to water ratio	1 to 40	1 to 40	1 to 40
Sample description	WAF 1	WAF 2	WAF 3
	µg/L	µg/L	µg/L
Phenol			
C1-Phenols			
C2-Phenols			
C3-Phenols			
C4-Phenols			
C5-Phenols			
30 ab hopane	0.004	0.000	0.005
Sum all SVOC (not hopane)	25.0	554	615
Decalins			
Naphthalenes	9.35	479	574
2-3 ring PAHs	22.1	553	612
4-6 ring PAHs	2.92	0.94	2.68
C0-C5 Phenols			
TPH (C10-C36, from GC/FID), mg/L	0.98	5.70	8.79
Surrogate Recovery (in %)			
D10-1-methylnaphthalene	74	98	85
D10-phenanthrene	117	128	115
D10-pyrene	113	110	109
5B-Cholestane	123	117	116

Tabell C 3 *Volatile components in the WAFs (in µg/L) (USA)*

Laboratory	USA	USA	USA
Sample ID	WRG	MGO	VLSFO
Internal Lab ID	LSFO 1	LSFO 2	LSFO 3
Oil type	WRG	MGO	VLSFO
Oil to water ratio	1 to 40	1 to 40	1 to 40
	µg/L	µg/L	µg/L
Isopentane			
n-C5 (Pentane)			
Cyclopentane			
2-methylpentane			
3-Methylpentane			
n-C6 (Hexane)			
Methylcyclopentane			
Benzene	16	45	34
Cyclohexane			
2,3-Dimethylpentane			
3-methylhexane			
n-C7 (Heptane)			
Methylcyclohexane			
Toluene	51	177	84
2,4 dimethylhexane			
2-Methylheptane			
n-C8 (Octane)			
Ethylbenzene	7	61	29
m-Xylene + p-Xylene	44	204	54
p-Xylene			
o-Xylene	20	111	29
n-C9 (Nonane)			
Propylbenzene			
1-Methyl-3-ethylbenzene			
1-Methyl-4-ethylbenzene			
1,3,5-trimethylbenzene			
1-Methyl-2-ethylbenzene			
1,2,4-Trimethylbenzene			
n-C10 (Decane)			
1,2,3-Trimethylbenzene			
n-Butylbenzene			
1,2,4,5-Tetramethylbenzene			
n-Pentylbenzene			
Sum VOC			
BTEX	137	597	230
C3-benzenes			
Other VOC			

C2 Reported results chemistry of WAFs – Canada

No volatiles reported from Canada. WAF of MGO was generated twice, as there in the first setup was much higher mortality in the control with only 40% survival. In the main report only one of the analyzed samples are given.

Tabell C 4 Summary of the WAF results, two samples from each system (Canada). "/" indicates not measured.

Laboratory	CAN	CAN	CAN	CAN	CAN	CAN	CAN	CAN	
Sample ID									
Internal Lab ID	WGO		MGO		VLSFO		MGO - repetition		Notes
Oil type	WRG	WRG	MGO	MGO	VLSFO	VLSFO	MGO	MGO	
Oil to water ratio	1:40	1:40	1:40	1:40	1:40	1:40	1:40	1:40	
Sample description	WAF 1	WAF 2	WAF 1	WAF 2	WAF 1	WAF 2	WAF 1	WAF 2	
	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	
Tot WAF	204	224	1582	1715	1705	1453	2197	1876	Sum of PAHs and alkanes C9 to C40
TPH	185	205	1304	1422	1396	1122	1894	1566	
Sum SVOC	19.3	19.1	278	293	309	331	303	310	
Sum VOC	/	/	/	/	/	/	/	/	
UCM (TPH-SVOC)	1.8	3.9	13.5	13.50	20.2	9.400	149	139	
Decalins	/	/	/	/	/	/	/	/	
Naphthalenes	10.1	9.5	228	239	263	303	247	255	
2-3 ring PAH	18.4	17.5	275	287	294	327	301	307	
4-6 ring PAH	0.89	1.59	1.13	1.18	7.29	2.50	1.29	1.29	
C0-C5 phenols	/	/	/	/	/	/	/	/	
BTEX	/	/	/	/	/	/	/	/	Added this row to calculate the sum of SVOC.
C3-benzenes	/	/	/	/	/	/	/	/	
Other VOC	/	/	/	/	/	/	/	/	
Sum alkanes	0.07	0.06	1.33	5.15	7.42	1.37	1.32	1.12	

Tabell C 5 *Semi-volatile components in the WAFs (in g analyte/L water). Two samples from each system. "/" indicates not measured, nd: not detectable. (Canada.)*

Laboratory	CAN	CAN	CAN	CAN	CAN	CAN	CAN	CAN	
Sample ID									
Internal Lab ID	WGO		MGO		VLSFO		MGO - repetition		
Oil type	WRG	WRG	MGO	MGO	VLSFO	VLSFO	MGO	MGO	
Oil to water ratio	01:40	01:40	01:40	01:40	01:40	01:40	01:40	01:40	
Sample description	WAF 1	WAF 2	WAF 1	WAF 2	WAF 1	WAF 2	WAF 1	WAF 2	Notes
	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	
Decalin	/	/	/	/	/	/	/	/	
C1-decalins	/	/	/	/	/	/	/	/	
C2-decalins	/	/	/	/	/	/	/	/	
C3-decalins	/	/	/	/	/	/	/	/	
C4-decalins	/	/	/	/	/	/	/	/	
Benzo(b)thiophene	/	/	/	/	/	/	/	/	
Naphthalene	2.88	2.77	56.1	60.9	94.7	149	65.1	73.0	
C1-naphthalenes	3.57	3.42	91.4	95.7	101	93.0	95.2	97.9	
C2-naphthalenes	2.20	2.01	57.7	59.7	48.6	45.8	60.1	59.0	
C3-naphthalenes	0.98	0.89	18.3	17.7	16.0	13.3	20.8	19.2	
C4-naphthalenes	0.44	0.38	4.66	4.68	2.71	2.46	6.19	5.95	
Biphenyl	1.97	1.94	11.4	11.6	3.08	2.69	11.3	11.6	
Acenaphthylene	0.01	0.01	0.28	0.30	0.50	0.45	0.31	0.30	
Acenaphthene	0.03	0.03	1.17	1.17	2.15	2.02	1.17	1.15	
Dibenzofuran	/	/	/	/	/	/	/	/	
Fluorene	0.45	0.42	5.23	5.37	1.95	1.67	5.13	5.07	
C1-fluorenes	1.07	0.96	6.24	6.25	2.79	2.42	5.97	5.82	
C2-fluorenes	0.64	0.65	3.25	3.33	1.92	1.48	3.01	3.00	
C3-fluorenes	0.30	0.28	1.23	1.19	1.02	0.59	0.89	1.15	
Phenanthrene	0.43	0.43	3.02	3.13	3.12	2.90	2.80	2.75	
Anthracene	0.06	0.06	2.43	2.46	0.49	0.46	4.15	3.97	
C1-phenanthrenes/anthracenes	0.96	0.97	7.39	7.82	5.19	4.06	10.6	10.2	
C2-phenanthrenes/anthracenes	1.13	1.13	3.63	3.61	3.74	2.34	5.59	5.31	
C3-phenanthrenes/anthracenes	0.74	0.71	0.74	0.85	2.12	0.97	1.24	1.21	
C4-phenanthrenes/anthracenes	0.31	0.30	0.16	0.22	1.22	0.27	0.24	0.21	
Dibenzothiophene	0.14	0.01	0.27	0.27	0.43	0.39	0.25	0.24	
C1-dibenzothiophenes	0.04	0.04	0.27	0.28	0.58	0.46	0.25	0.23	
C2-dibenzothiophenes	0.03	0.04	0.13	0.14	0.49	0.27	0.12	0.10	
C3-dibenzothiophenes	0.01	0.02	0.04	0.04	0.32	0.11	0.03	0.03	
C4-dibenzothiophenes	/	/	/	/	/	/	/	/	
Fluoranthene	0.10	0.25	0.27	0.27	0.11	0.07	0.34	0.33	
Pyrene	0.05	0.55	0.32	0.34	0.50	0.33	0.27	0.26	
C1-fluoranthrenes/pyrenes	0.33	0.33	0.41	0.43	0.84	0.42	0.51	0.54	
C2-fluoranthrenes/pyrenes	0.23	0.20	0.09	0.11	1.19	0.45	0.12	0.12	
C3-fluoranthrenes/pyrenes	0.10	0.09	0.02	0.03	1.16	0.35	0.02	0.02	
Benz(a)anthracene	0.02	0.03	0.01	0.00	0.69	0.19	0.01	0.00	



Laboratory	CAN	CAN	CAN	CAN	CAN	CAN	CAN	CAN	
Sample ID									
Internal Lab ID	WGO		MGO		VLSFO		MGO - repetition		
Oil type	WRG	WRG	MGO	MGO	VLSFO	VLSFO	MGO	MGO	
Oil to water ratio	01:40	01:40	01:40	01:40	01:40	01:40	01:40	01:40	
Sample description	WAF 1	WAF 2	WAF 1	WAF 2	WAF 1	WAF 2	WAF 1	WAF 2	Notes
	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	
Chrysene	0.01	0.04	0.01	0.01	0.18	0.07	0.01	0.01	
C1-chrysenes	0.01	0.02	0.01	0.01	0.64	0.16	0.01	0.01	
C2-chrysenes	0.01	0.01	0.00	0.00	0.92	0.21	0.01	0.01	
C3-chrysenes	0.01	0.01	0.00	0.00	0.80	0.18	0.00	0.00	
C4-chrysenes	/	/	/	/	/	/	/	/	
Benzo(b)fluoranthene	0.01	0.02	0.00	0.00	0.03	0.01	0.00	0.00	
Benzo(k)fluoranthene	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	
Benzo(e)pyrene	0.00	0.01	0.00	0.00	0.08	0.02	0.00	0.00	
Benzo(a)pyrene	0.00	0.01	0.00	0.00	0.06	0.01	0.00	0.00	
Perylene	0.00	0.00	0.00	0.00	0.02	0.01	0.00	0.00	
Indeno(1,2,3-c,d)pyrene	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	
Dibenz(a,h)anthracene	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	
Benzo(g,h,i)perylene	0.00	0.02	0.00	0.00	0.04	0.01	0.00	0.00	
Phenol	/	/	/	/	/	/	/	/	
C1-Phenols	/	/	/	/	/	/	/	/	
C2-Phenols	/	/	/	/	/	/	/	/	
C3-Phenols	/	/	/	/	/	/	/	/	
C4-Phenols	/	/	/	/	/	/	/	/	
C5-Phenols	/	/	/	/	/	/	/	/	
30 ab hopane	nd	nd	nd	nd	0.07	0.02	nd	nd	
	WGO		MGO		VLSFO		MGO - repetition		include alkanes and PAHs
Sample ID	WAF 1	WAF 2	WAF 1	WAF 2	WAF 1	WAF 2	WAF 1	WAF 2	
Sum all SVOC (not hopane)	19.3	19.1	278	293	309	331	303	310	
Decalins	/	/	/	/	/	/	/	/	
Naphthalenes	10.1	9.48	228	239	263	303	247	255	
2-3 ring PAHs	18.4	17.5	275	287	294	327	301	307	
4-6 ring PAHs	0.89	1.59	1.13	1.18	7.29	2.50	1.29	1.29	
C0-C5 Phenols	/	/	/	/	/	/	/	/	
TPH (C10-C36, from GC/FID)	185	205	1304	1422	1396	1122	1894	1566	Include all PAH congeners Include all PAH congeners

Surrogate recovery from ESTS analysis.

d8-naphthalene	67.7	67.9	58.2	62.9	53.3	53.5	64.3	59.5	
d10-Acenaphthene	81.2	81.0	96.2	99.9	83.9	81.4	100	97.3	
d10-Phenanthrene	82.3	81.3	86.1	89.2	85.6	86.9	91.7	89.4	
d12-Benz(a)anthracene	82.5	78.7	87.9	92.0	92.2	93.1	95.7	89.0	
d12-Perylene	83.0	80.5	93.7	98.2	103	101	93.9	86.8	

C3 Reported results chemistry of WAFs – China

Tabell C 6 Summary of the WAF results, both prepared in seawater and freshwater (China)

Laboratory	China	China	China	China	China	China
Sample ID	2021-5427	2021-5428	2021-5429	2021-5427	2021-5428	2021-5429
Internal Lab ID						
Oil type	WRG	MGO	VLSFO	WRG	MGO	VLSFO
Oil to water ratio	1:40	1:40	1:40	1:40	1:40	1:40
Sample description	WAF 1 (seawater)	WAF 2 (seawater)	WAF 3 (seawater)	WAF 1 (freshwater)	WAF 2 (freshwater)	WAF 3 (freshwater)
	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L
Tot WAF (Sum VOC+TPH)	1967	2582	1008	2426	2956	1251
TPH	1820	1440	693	1942	1685	952
Sum SVOC	464	523	420	371	538	577
Sum VOC	147	1142	315	484	1271	299
UCM (TPH-SVOC)	1356	917	273	1571	1147	375
Decalins	0.00	0.00	0.00	0.00	0.00	0.00
Naphthalenes	293	296	350	177	326	428
2-3 ring PAH	29.6	27.9	15.5	17.7	11.4	7.80
4-6 ring PAH	13.5	19.9	12.7	8.51	5.43	2.74
C0-C5 phenols	128	180	42.3	167	195	138
BTEX	102	656	155	232	592	163
C3-benzenes	42.8	471	139	134	480	91.2
Other VOC (Sum VOC- (BTEX+C3-benzenes))	2.00	14.9	20.8	117	200	44.6

Tabell C 7 Semi-volatile components in the WAFs (in g analyte/L water) (China)

Laboratory	China	China	China	China	China	China
Sample ID	2021-5427	2021-5428	2021-5429	2021-5427	2021-5428	2021-5429
Internal Lab ID						
Oil type	WRG	MGO	VLSFO	WRG	MGO	VLSFO
Oil to water ratio	1:40	1:40	1:40	1:40	1:40	1:40
Sample description	WAF 1 (seawater)	WAF 2 (seawater)	WAF 3 (seawater)	WAF 1 (freshwater)	WAF 2 (freshwater)	WAF 3 (freshwater)
	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L
Decalin	0.000	0.000	0.000	0.000	0.000	0.000
C1-decalins						
C2-decalins						
C3-decalins						
C4-decalins						
Benzo(b)thiophene	8.45	8.89	4.30	1.46	1.08	1.34
Naphthalene	198	221	210	7.28	27.3	95.3
C1-naphthalenes	43.1	28.5	88.4	31.0	154	280
C2-naphthalenes	51.9	46.1	51.2	139	145	53.1
C3-naphthalenes						

C2+C3-
naphthalene

Laboratory	China	China	China	China	China	China	
Sample ID	2021-5427	2021-5428	2021-5429	2021-5427	2021-5428	2021-5429	
Internal Lab ID							
Oil type	WRG	MGO	VLSFO	WRG	MGO	VLSFO	
Oil to water ratio	1:40	1:40	1:40	1:40	1:40	1:40	
Sample description	WAF 1 (seawater)	WAF 2 (seawater)	WAF 3 (seawater)	WAF 1 (freshwater)	WAF 2 (freshwater)	WAF 3 (freshwater)	
	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	
C4-naphthalenes							
Biphenyl							
Acenaphthylene							
Acenaphthene							
Dibenzofuran							
Fluorene				1.50	1.19	0.975	
C1-fluorenes							
C2-fluorenes							
C3-fluorenes							
Phenanthrene	2.79	2.79	2.79	1.86	1.78	1.15	Phenanthrene/A nthracene
Anthracene							
C1-phenanthrenes/anthracenes				2.00	1.00	0.25	
C2-phenanthrenes/anthracenes	12.30	13.10	5.99	7.54	4.29	3.51	
C3-phenanthrenes/anthracenes							
C4-phenanthrenes/anthracenes							
Dibenzothiophene	6.01	3.10	2.43	2.82	1.49	0.415	
C1-dibenzothiophenes							
C2-dibenzothiophenes				0.464	0.551	0.160	
C3-dibenzothiophenes							
C4-dibenzothiophenes							
Fluoranthene	2.45	4.94	4.02	0.910	0.493	0.143	Fluoranthene/Py rene
Pyrene							
C1-fluoranthrenes/pyrene	5.04	7.26	2.69	3.26	1.62	0.489	
C2-fluoranthenes/pyrenes							
C3-fluoranthenes/pyrenes							
Benz(a)anthracene	3.86	2.05	2.36	0.271	0.289	0.222	Benz[a]anthrace ne+Chrysene
Chrysene							
C1-chrysenes				0.069	0.069	0.161	
C2-chrysenes				0.339	0.232	0.292	
C3-chrysenes							
C4-chrysenes							
Benzo(b)fluoranthene							
Benzo(k)fluoranthene							
Benzo(e)pyrene				0.945	0.884	0.322	
Benzo(a)pyrene	2.12	5.61	3.58	2.71	1.85	1.12	
Perylene							
Indeno[1,2,3-c,d]pyrene							

Laboratory	China	China	China	China	China	China
Sample ID	2021-5427	2021-5428	2021-5429	2021-5427	2021-5428	2021-5429
Internal Lab ID						
Oil type	WRG	MGO	VLSFO	WRG	MGO	VLSFO
Oil to water ratio	1:40	1:40	1:40	1:40	1:40	1:40
Sample description	WAF 1 (seawater)	WAF 2 (seawater)	WAF 3 (seawater)	WAF 1 (freshwater)	WAF 2 (freshwater)	WAF 3 (freshwater)
	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L
Dibenz(a,h)anthracene						
Benzo(g,h,i)perylene						
Phenol	23.9	70.8	17.4	18.9	25.7	28.6
C1-Phenols	82.8	92.3	13.2	101	115	79.4
C2-Phenols						
C3-Phenols						
C4-Phenols	20.9	16.8	11.7	47.6	53.7	30.1
C5-Phenols						
30 ab hopane						
Sum all SVOC (not hopane)	464	523	420	371	538	577
Decalins						
Naphthalenes	293	296	350	177	326	428
2-3 ring PAHs	29.6	27.9	15.5	17.6	11.4	7.80
4-6 ring PAHs	13.5	19.9	12.7	8.51	5.43	2.74
C0-C5 Phenols	128	180	42.3	167	195	138
TPH (C10-C36, from GC/FID)	1820	1440	693	1942	1685	952

Tabell C 8 Volatile components in the WAFs (in g analyte/kg oil) (China)

Laboratory	China	China	China	China	China	China
Sample ID	2021-5427	2021-5428	2021-5429	2021-5427	2021-5428	2021-5429
Internal Lab ID						
Oil type	WRG	MGO	VLSFO	WRG	MGO	VLSFO
Oil to water ratio	1:40	1:40	1:40	1:40	1:40	1:40
Sample description	WAF 1 (seawater)	WAF 2 (seawater)	WAF 3 (seawater)	WAF 1 (freshwater)	WAF 2 (freshwater)	WAF 3 (freshwater)
	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L
Isopentane	0.03	0.02	1.78	3.19	0.000	0.000
n-C5 (Pentane)				25.6	0.000	0.034
Cyclopentane	0.23	0.21	0.05			
2-methylpentane	0.04	0.00	0.00			
3-Methylpentane	0.01	0.01	0.00	1.02	0.383	0.026
n-C6 (Hexane)	0.15	0.07	0.00	0.000	0.000	0.185
Methylcyclopentane	0.07	0.14	0.00	3.48	2.73	0.649
Benzene	13.53	31.02	13.58	60.6	86.0	14.4

Laboratory	China	China	China	China	China	China
Sample ID	2021-5427	2021-5428	2021-5429	2021-5427	2021-5428	2021-5429
Internal Lab ID						
Oil type	WRG	MGO	VLSFO	WRG	MGO	VLSFO
Oil to water ratio	1:40	1:40	1:40	1:40	1:40	1:40
Sample description	WAF 1 (seawater)	WAF 2 (seawater)	WAF 3 (seawater)	WAF 1 (freshwater)	WAF 2 (freshwater)	WAF 3 (freshwater)
	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L
Cyclohexane	0.01	0.00	0.00	13.4	2.24	2.34
2,3-Dimethylpentane				0.427	0.561	1.100
3-methylhexane	0.01	0.06	0.00	0.474	0.000	0.000
n-C7 (Heptane)	0.44	7.40	12.70	0.000	1.05	0.060
Methylcyclohexane	0.04	3.43	4.74	13.8	3.45	5.54
Toluene	40.74	171.06	43.95	81.2	269	65.0
2,4 dimethylhexane				0.000	10.1	0.012
2-Methylheptane	0.14	0.16	0.35			
n-C8 (Octane)	0.30	0.10	0.87	49.4	69.9	21.4
Ethylbenzene	7.11	84.39	16.29	26.9	79.0	30.9
m-Xylene	25.69	218.19	48.03	57.8	151	45.7
p-Xylene	15.00	150.11	33.43			
o-Xylene	0.09	1.35	0.00	6.02	6.35	6.87
n-C9 (Nonane)	0.00	2.75	0.01	3.25	19.0	7.60
Propylbenzene	1.68	26.99	4.22	7.60	20.1	9.74
1-Methyl-3-ethylbenzene	13.0	121	43.9	22.5	85.2	26.9
1-Methyl-4-ethylbenzene	2.72	31.7	8.07	11.0	34.4	14.2
1,3,5-trimethylbenzene	5.98	78.8	22.8	11.1	39.8	
1-Methyl-2-ethylbenzene	9.62	81.6	25.5			
1,2,4-Trimethylbenzene	5.98	78.8	22.8	45.6	188	40.4
n-C10 (Decane)						
1,2,3-Trimethylbenzene	3.92	52.4	11.7	36.0	113	
n-Butylbenzene	0.00	0.00	0.00	1.50	4.96	1.58
1,2,4,5-Tetramethylbenzene	0.04	0.58	0.03	1.21	50.9	2.25
n-Pentylbenzene	0.00	0.01	0.00	0.62	34.6	1.78
Sum VOC	147	1142	315	484	1271	299
BTEX	102	656	155	232	592	163
C3-benzenes	42.8	471	139	134	480	91.2
Other VOC	1.51	14.9	20.5	117	200	44.6

C4 Reported results chemistry of WAFs – Sweden

WAF and toxicity testing were reported by ALS Toxicon AB.

Tabell C 9 Summary of the chemical composition of the WAFs (Sweden). Table not reported, but prepared by SINTEF.

Laboratory	Sweden	Sweden	Sweden
Sample ID	ALS Global	ALS Global	ALS Global
Internal Lab ID	E21-055-1	E21-055-3	E21-055-2
Oil type	WRG	MGO	VLSFO
Oil to water ratio	1:40	1:40	1:40
Sample description	WAF 1	WAF 2	WAF 3
	µg/L	µg/L	µg/L
Tot WAF (Sum VOC+TPH)	4865	2276	1243
TPH	4670*	1120*	859*
Sum SVOC	16.0	925	1670**
Sum VOC	195	1156	384
UCM (TPH-SVOC)	4654*	195*	-811**
Decalins	NA	NA	NA
Naphthalenes	11.1	907	1653
2-3 ring PAH	4.30	18.0	16.8
4-6 ring PAH	0.551	0.500	0.519
C0-C5 phenols	NA	NA	NA
BTEX	164	922	296
C3-benzenes	30.3	226	86.5
Other VOC	0.00	26.0	1.60

* Are the samples for TPH analysis mixed up? If so, UCM is also mixed up.

** Higher SVOC cons than TPH in WAF 3

Tabell C 10 Semi-volatile components the WAFs (Sweden). *: Not analyzed

Laboratory	ALS Global	Sweden	Sweden	Sweden
Sample ID				
Internal Lab ID		E21-055-1	E21-055-3	E21-055-2
Oil type		WRG	MGO	VLSFO
Oil to water ratio				
Sample description		WAF 1 - WRG	WAF 2 - MGO	WAF 3 - VLSFO
	LOR	µg/L	µg/L	µg/L
Decalin	*	*	*	*
C1-decalins	*	*	*	*
C2-decalins	*	*	*	*
C3-decalins	*	*	*	*
C4-decalins	*	*	*	*
Benzo(b)thiophene	*	*	*	*
Naphthalene	0.015	4.00	380	1100
C1-naphthalenes	<1.00	7.14	501	529

Laboratory	ALS Global	Sweden	Sweden	Sweden
Sample ID				
Internal Lab ID		E21-055-1	E21-055-3	E21-055-2
Oil type		WRG	MGO	VLSFO
Oil to water ratio				
Sample description		WAF 1 - WRG	WAF 2 - MGO	WAF 3 - VLSFO
	LOR	µg/L	µg/L	µg/L
C2-naphthalenes	<1.00	<1.00	25.5	24
C3-naphthalenes	<1.00	<1.00	<1.00	<1.00
C4-naphthalenes	*	*	*	*
Biphenyl	*	*	*	*
Acenaphthylene	<0.010	<0.040	0.48	0.89
Acenaphthene	<0.010	<0.20	<2.5	3.5
Dibenzofuran	*	*	*	*
Fluorene	<0.010	0.56	9.5	3.3
C1-fluorenes	*	*	*	*
C2-fluorenes	*	*	*	*
C3-fluorenes	*	*	*	*
Phenanthrene	<0.010	0.88	3.9	3.9
Anthracene	<0.010	0.18	0.32	0.54
C1-phenanthrenes/anthracenes	<1.00	2.68	3.76	4.71
C2-phenanthrenes/anthracenes	<1.00	<1.50	<1.00	<1.00
C3-phenanthrenes/anthracenes	<1.00	<1.00	<1.00	<1.00
C4-phenanthrenes/anthracenes	*	*	*	*
Dibenzothiophene	<1.00	<1.00	<1.00	<1.00
C1-dibenzothiophenes	<1.00	<1.00	<1.00	<1.00
C2-dibenzothiophenes	<1.00	<1.00	<1.00	<1.00
C3-dibenzothiophenes	<1.00	<1.00	<1.00	<1.00
C4-dibenzothiophenes	*	*	*	*
Fluoranthene	<0.010	0.33	0.23	0.11
Pyrene	<0.010	0.17	0.27	0.35
C1-fluoranthrenes/pyrenes	*	*	*	*
C2-fluoranthrenes/pyrenes	*	*	*	*
C3-fluoranthrenes/pyrenes	*	*	*	*
Benz(a)anthracene	<0.010	<0.040	<0.010	0.024
Chrysene	<0.010	0.04	<0.010	0.035
C1-chrysenes	*	*	*	*
C2-chrysenes	*	*	*	*
C3-chrysenes	*	*	*	*
C4-chrysenes	*	*	*	*
Benzo(b)fluoranthene	<0.010	<0.030	<0.010	<0.010
Benzo(k)fluoranthene	<0.010	<0.020	<0.010	<0.010
Benzo(e)pyrene	*	*	*	*
Benzo(a)pyrene	<0.010	<0.020	<0.010	<0.010
Perylene	*	*	*	*
Indeno(1,2,3-c,d)pyrene	<0.010	<0.010	<0.010	<0.010

Laboratory	ALS Global	Sweden	Sweden	Sweden
Sample ID				
Internal Lab ID		E21-055-1	E21-055-3	E21-055-2
Oil type		WRG	MGO	VLSFO
Oil to water ratio				
Sample description		WAF 1 - WRG	WAF 2 - MGO	WAF 3 - VLSFO
	LOR	µg/L	µg/L	µg/L
Dibenz(a,h)anthracene	<0.010	<0.010	<0.010	<0.010
Benzo(g,h,i)perylene	<0.010	0.01	<0.010	<0.010
Phenol	*	*	*	*
C1-Phenols	*	*	*	*
C2-Phenols	*	*	*	*
C3-Phenols	*	*	*	*
C4-Phenols	*	*	*	*
C5-Phenols	*	*	*	*
30 ab hopane	*	*	*	*
Sample ID		WRG	MGO	VLSFO
Sum all SVOC (not hopane)		16.0	925	1670
Decalins		*	*	*
Naphthalenes		11.1	907	1653
2-3 ring PAHs		4.30	18.0	16.8
4-6 ring PAHs		0.55	0.50	0.52
C0-C5 Phenols		*	*	*
TPH (C10-C36, from GC/FID)		4670	1120	859

Tabell C 11 Volatile components the WAFs (Sweden). *: Not analyzed. As concentrations of VOC used in calculations of toxicity was not in accordance with the reported data in Appendix 2, components named in the right column were added by SINTEF. However, the results still were different.

Laboratory	ALS Global	Sweden	Sweden	Sweden
Sample ID				
Internal Lab ID		E21-055-1	E21-055-3	E21-055-2
Oil type		WRG	MGO	VLSFO
Oil to water ratio				
Sample description		WAF 1 - WRG	WAF 2 - MGO	WAF 3 - VLSFO
	LOR	µg/L	µg/L	µg/L
Isopentane	*	*	*	*
n-C5 (Pentane)	*	*	*	*
Cyclopentane	*	*	*	*
2-methylpentane	*	*	*	*
3-Methylpentane	*	*	*	*
n-C6 (Hexane)	*	*	*	*
Methylcyclopentane	*	*	*	*
Benzene	<0.20	19.8	60.4	24.7

Laboratory	ALS Global	Sweden	Sweden	Sweden
Sample ID				
Internal Lab ID		E21-055-1	E21-055-3	E21-055-2
Oil type		WRG	MGO	VLSFO
Oil to water ratio				
Sample description		WAF 1 - WRG	WAF 2 - MGO	WAF 3 - VLSFO
	LOR	µg/L	µg/L	µg/L
Cyclohexane	*	*	*	*
2,3-Dimethylpentane	*	*	*	*
3-methylhexane	*	*	*	*
n-C7 (Heptane)				
Methylcyclohexane	*	*	*	*
Toluene	<0.20	66.9	243	94.1
2,4 dimethylhexane	*	*	*	*
2-Methylheptane	*	*	*	*
n-C8 (Octane)	*	*	*	*
Ethylbenzene	<0.10	10.4	146	25.6
m-Xylene	*	*	*	*
p-Xylene	*	*	*	*
m,p-xylene	<0.20	45.9	308	99.6
o-Xylene	<0.10	21.3	165	51.9
n-C9 (Nonane)	*	*	*	*
Propylbenzene	<1.0	3.10	44.5	5.70
1-Methyl-3-ethylbenzene	*	*	*	*
1-Methyl-4-ethylbenzene	*	*	*	*
1,3,5-trimethylbenzene	<1.0	5.30	61.5	13.3
1-Methyl-2-ethylbenzene		1.60	29.7	1.00
1,2,4-Trimethylbenzene	<1.0	20.3	90.5	66.5
n-C10 (Decane)	*	*	*	*
1,2,3-Trimethylbenzene	*	*	*	*
n-Butylbenzene	<1.0	<1.0	7.00	1.60
1,2,4,5-Tetramethylbenzene	*	<1	<1	<1
n-Pentylbenzene	*	*	*	*
sek-butylbenzene		<1	9.90	<1
p-isopropyltoluene		<1	9.10	<1
Sum VOC		195	1175	384
BTEX		164	922	296
C3-benzenes		30.3	226	86.5
Other VOC		0.0	26.0	1.60

(isopropylbenzene)

(tert-methylbenzene)

C5 Reported results chemistry of WAFs – Norway

Tabell C 12 Summary of the chemical composition of the WAFs (Norway)

Laboratory	Norway	Norway	Norway
Internal sample ID	2021-5427	2021-5428	2021-5429
Sample name	WRG	MGO	VLSFO
Oil to water ratio	1:40	1:40	1:40
Sampling	72 hrs	72 hrs	72 hrs
Norway	µg/L	µg/L	µg/L
Tot WAF	392	7237	3127
TPH	187	4911	2250
Sum SVOC	18.2	702	540
Sum VOC	205	2326	877
UCM	169	4209	1710
Decalins	0.18	1.12	0.26
Naphthalenes	8.00	276	471
2-3 ring PAH	5.08	36.3	25.9
4-6 ring PAH	0.30	1.54	1.28
C0-C5 phenols	4.64	387	41.9
BTEX	140	1406	418
C3-benzenes	49.4	796	392
Other VOC	15.6	125	66.9

Tabell C 13 Semi-volatile components in the WAFs (in µg/L) (Norway)

Laboratory		Norway	Norway	Norway
Internal sample ID		2021-5427	2021-5428	2021-5429
Oil category		WRG	MGO	VLSFO
Oil to water ratio		1:40	1:40	1:40
Norway	RRF	µg/L	µg/L	µg/L
Decalin	0.393	0.05	0.40	0.01
C1-decalins	0.393	0.02	0.16	0.01
C2-decalins	0.393	0.02	0.13	0.06
C3-decalins	0.393	0.03	0.18	0.09
C4-decalins	0.393	0.05	0.26	0.09
Benzo(b)thiophene	1.416	ND	0.06	3.87
Naphthalene	1.451	3.43	130	296
C1-naphthalenes	1.451	2.18	102	120
C2-naphthalenes	1.451	1.38	32.7	43.4
C3-naphthalenes	1.451	0.84	8.69	9.34
C4-naphthalenes	1.451	0.17	3.21	1.63
Biphenyl	1.414	2.23	10.60	3.59
Acenaphthylene	0.776	0.03	0.64	1.22
Acenaphthene	0.726	0.02	1.11	2.84
Dibenzofuran	1.446	0.22	2.49	0.89
Fluorene	0.913	0.44	5.05	2.50

Laboratory		Norway	Norway	Norway
Internal sample ID		2021-5427	2021-5428	2021-5429
Oil category		WRG	MGO	VLSFO
Oil to water ratio		1:40	1:40	1:40
Norway	RRF	µg/L	µg/L	µg/L
C1-fluorenes	0.913	0.51	3.45	1.35
C2-fluorenes	0.913	0.35	1.97	0.80
C3-fluorenes	0.913	0.14	0.56	0.67
Phenanthrene	1.475	0.38	2.66	3.19
Anthracene	0.946	0.02	0.58	0.40
C1-phenanthrenes/anthracenes	1.475	0.31	2.45	2.29
C2-phenanthrenes/anthracenes	1.475	0.21	0.89	1.05
C3-phenanthrenes/anthracenes	1.475	0.05	0.34	0.23
C4-phenanthrenes/anthracenes	1.475	0.02	0.23	0.05
Dibenzothiophene	1.694	0.01	0.28	0.38
C1-dibenzothiophenes	1.694	0.03	0.76	0.34
C2-dibenzothiophenes	1.694	0.04	1.10	0.16
C3-dibenzothiophenes	1.694	0.03	0.79	0.04
C4-dibenzothiophenes	1.694	0.03	0.30	0.02
Fluoranthene	1.245	0.01	0.25	0.10
Pyrene	1.211	0.02	0.27	0.43
C1-fluoranthrenes/pyrenes	1.245	0.04	0.28	0.30
C2-fluoranthrenes/pyrenes	1.245	0.05	0.49	0.07
C3-fluoranthrenes/pyrenes	1.245	0.05	0.17	0.22
Benz(a)anthracene	1.862	0.02	0.01	0.03
Chrysene	3.042	ND	ND	0.02
C1-chrysenes	3.042	0.01	0.02	0.03
C2-chrysenes	3.042	0.01	0.01	0.01
C3-chrysenes	3.042	0.03	0.01	0.03
C4-chrysenes	3.042	ND	ND	ND
Benzo(b)fluoranthene	2.546	0.01	ND	ND
Benzo(k)fluoranthene	2.459	ND	ND	ND
Benzo(e)pyrene	2.693	0.01	ND	0.01
Benzo(a)pyrene	1.743	ND	ND	ND
Perylene	1.358	ND	ND	ND
Indeno(1,2,3-c,d)pyrene	1.516	0.01	ND	ND
Dibenz(a,h)anthracene	1.498	0.01	ND	ND
Benzo(g,h,i)perylene	2.165	0.01	ND	ND
Phenol	0.573	0.92	63.1	6.05
C1-Phenols	0.573	0.93	111	5.30
C2-Phenols	0.573	0.44	112	10.3
C3-Phenols	0.573	1.20	62.3	12.1
C4-Phenols	0.573	0.45	30.9	6.10
C5-Phenols	0.573	0.69	7.47	2.06
30 ab hopane	1.222	ND	ND	ND

Laboratory		Norway	Norway	Norway
Internal sample ID		2021-5427	2021-5428	2021-5429
Oil category		WRG	MGO	VLSFO
Oil to water ratio		1:40	1:40	1:40
Norway	RRF	µg/L	µg/L	µg/L
Sum all SVOC (not hopane)		18.2	702	540
Decalins		0.18	1.12	0.26
Naphthalenes		8.00	276	471
2-3 ring PAHs		5.08	36.3	25.9
4-6 ring PAHs		0.30	1.54	1.28
C0-C5 Phenols		4.64	387	41.9

Tabell C 14 *Volatile components in the WAFs (in µg/L) (Norway)*

Laboratory		Norway	Norway	Norway
Internal sample ID		2021-5427	2021-5428	2021-5429
Oil category		WRG	MGO	VLSFO
Oil to water ratio		1:40	1:40	1:40
Norway	RRF	µg/L	µg/L	µg/L
Isopentane	0.29	ND	ND	ND
n-C5 (Pentane)	0.367	ND	ND	ND
Cyclopentane	0.532	ND	ND	ND
2-methylpentane	0.425	ND	ND	ND
3-Methylpentane	0.457	ND	ND	ND
n-C6 (Hexane)	0.405	ND	ND	ND
Methylcyclopentane	0.583	1.19	1.58	2.38
Benzene	1.535	9.72	62.7	24.9
Cyclohexane	0.499	6.51	8.41	1.06
2,3-Dimethylpentane	0.343	ND	ND	ND
3-methylhexane	0.274	ND	ND	ND
n-C7 (Heptane)	0.350	ND	ND	ND
Methylcyclohexane	0.443	3.43	10.1	0.92
Toluene	1.403	49.8	358	112
2,4 dimethylhexane	0.797	ND	ND	ND
2-Methylheptane	0.245	ND	ND	ND
n-C8 (Octane)	0.168	ND	ND	ND
Ethylbenzene	0.868	9.10	128	34.6
m-Xylene	0.524	39.6	463	124
p-Xylene	0.621	11.1	126	38.1
o-Xylene	0.616	20.9	268	83.7
n-C9 (Nonane)	0.156	ND	ND	ND
Propylbenzene	0.815	1.71	58.1	10.7
1-Methyl-3-ethylbenzene	0.565	9.22	235	76.7
1-Methyl-4-ethylbenzene	0.673	3.49	79.4	26.5
1,3,5-trimethylbenzene	0.58	4.11	98.6	30.2

Laboratory		Norway	Norway	Norway
Internal sample ID		2021-5427	2021-5428	2021-5429
Oil category		WRG	MGO	VLSFO
Oil to water ratio		1:40	1:40	1:40
Norway	RRF	µg/L	µg/L	µg/L
1-Methyl-2-ethylbenzene	0.646	4.66	130	32.7
1,2,4-Trimethylbenzene	0.702	16.4	ND	147
n-C10 (Decane)	0.226	ND	ND	ND
1,2,3-Trimethylbenzene	0.702	9.81	195	68.1
n-Butylbenzene	0.742	0.41	11.8	4.18
1,2,4,5-Tetramethylbenzene	0.640	0.42	27.0	57.0
n-Pentylbenzene	0.671	3.63	65.9	1.38
Sum VOC		205	2326	877
BTEX		140	1406	418
C3-benzenes		49.4	796	392
Other VOC		15.6	125	66.9

Appendix D Reported results toxicity

D1 Toxicity results – USA

Table D 1 *Lethal immobilization following 48 hours exposure of A. bahia and 96 hours exposure of M. beryllina to the WAFs. Specific toxicity is normalized to total SVOC concentration and are given as LC50. Observed mortality at test endpoint in 100% WAF is also given (USA).*

Laboratory	USA	USA	USA	USA	USA	USA
Internal Lab ID	LSFO-1	LSFO-2	LSFO-3	LSFO-1	LSFO-2	LSFO-3
Sample ID	WRG	MGO	VLSFO	WRG	MGO	VLSFO
Specie	48-hour <i>A. bahia</i>	48-hour <i>A. bahia</i>	48-hour <i>A. bahia</i>	96-hour <i>M. beryllina</i>	96-hour <i>M. beryllina</i>	96-hour <i>M. beryllina</i>
Sample description	WAF 1	WAF 2	WAF 3	WAF 1	WAF 2	WAF 3
WAF cons (mg PAH/L)						
Control	0.000	0.000	0.000	0.000	0.000	0.000
Treatment 1	0.002	0.035	0.038	0.002	0.035	0.038
Treatment 2	0.003	0.069	0.077	0.003	0.069	0.077
Treatment 3	0.006	0.138	0.154	0.006	0.138	0.154
Treatment 4	0.013	0.277	0.307	0.013	0.277	0.307
Treatment 5	0.025	0.554	0.615	0.025	0.554	0.615
LC ₅₀ (%)	>100%	51.45 %	51.60 %	>100%	56.34 %	>100%
(CI _{95%})	--	(47.68 - 55.23)	(48.02 - 55.19)	--	(18.28 - 94.41)	--
LC ₅₀ (mg/L)	--	0.28*	0.32*	--	0.31*	--
(CI _{95%})	--	(0.26 - 0.30)	(0.30 - 0.34)	--	(0.10 - 0.52)	--
Observed mortality at endpoint in 100% WAF	0% mortality	100% mortality	93% mortality	13% mortality	100% mortality	0% mortality
		*LC50: Used tot SVOC				

Table D 2 *Calculated toxic units in the WAFs. Input data to the calculations are also given (mole weight (Mw), the octanol-water coefficient ($\log K_{ow}$), and the predicted LC_{50} for each component). TU was not reported, table is prepared by SINTEF.*

Laboratory				USA	USA	USA
Sample ID				WRG	MGO	VLSFO
Internal Lab ID				LSFO 1	LSFO 2	LSFO 3
Oil type				WRG	MGO	VLSFO
Oil to water ratio						
Sample description				WAF 1	WAF 2	WAF 3
Compound	Mw	log Kow	LC_{50} (mg/L)	TU	TU	TU
Benzene	78	1.94	71.8	0.00022	0.00062	0.00048
Toluene	92	2.51	26.0	0.00195	0.00681	0.00321
Ethylbenzene	106	3.01	10.6	0.00064	0.00574	0.00275
m-xylene	106	3.04	9.98	0.00443	0.02043	0.00540
p-xylene	106	3.04	9.98			
o-xylene	106	2.95	12.0	0.00164	0.00921	0.00244
C3-benzenes	120	3.58	3.69			
Decalin	138	4.20	0.57			
C1-decalins	152	4.61	0.21			
C2-decalins	166	5.11	0.06			
C3-decalins	180	5.60	0.02			
C4-decalins	194	6.09	0.01			
Benzo(b)thiophene	134	3.13	9.68			
Naphthalene	128	3.30	5.87	0.00042	0.03110	0.05874
C1-naphthalenes	142	3.79	1.76	0.00168	0.10702	0.08399
C2-naphthalenes	156	4.24	0.58	0.00375	0.14673	0.10758
C3-naphthalenes	170	4.73	0.17	0.00680	0.11512	0.09401
C4-naphthalenes	184	5.22	0.05	0.01147	0.07753	0.06345
Biphenyl	154	3.94	1.27	0.00132	0.01564	0.00293
Acenaphthylene	152	3.44	4.79	0.00001	0.00009	0.00006
Acenaphthene	154	3.88	1.50	0.00002	0.00118	0.00176
Dibenzofuran	168	3.95	1.35	0.00021	0.00407	0.00093
Fluorene	166	3.93	1.41	0.00040	0.00706	0.00201
C1-fluorenes	180	4.37	0.47	0.00308	0.02301	0.00812
C2-fluorenes	194	4.82	0.15	0.00788	0.02620	0.01427
C3-fluorenes	208	5.32	0.04	0.01709	0.04184	0.02127
Phenanthrene	178	4.58	0.27	0.00238	0.02051	0.01888
Anthracene	178	4.55	0.29	0.00031	0.00178	0.00238
C1-phenanthrenes	192	5.04	0.08	0.01836	0.07790	0.08363
C2-phenanthrenes	206	5.45	0.03	0.04505	0.07056	0.11024
C3-phenanthrenes	220	5.91	0.01	0.10101	0.04449	0.09580
C4-phenanthrenes	234	6.36	0.003	0.34028	0.00000	0.00000
Dibenzothiophene	184	4.37	0.48	0.00019	0.00110	0.00151
C1-dibenzothiophenes	198	4.86	0.14	0.00220	0.01323	0.01456
C2-dibenzothiophenes	212	5.33	0.043	0.00702	0.02450	0.01620
C3-dibenzothiophenes	226	5.81	0.013	0.02319	0.06568	0.00000

Laboratory				USA	USA	USA
Sample ID				WRG	MGO	VLSFO
Internal Lab ID				LSFO 1	LSFO 2	LSFO 3
Oil type				WRG	MGO	VLSFO
Oil to water ratio						
Sample description				WAF 1	WAF 2	WAF 3
Compound	Mw	log Kow	LC ₅₀ (mg/L)	TU	TU	TU
C4-dibenzothiophene	240	6.43	0.003	0.09312	0.13075	0.00000
Fluoranthene	202	5.19	0.059	0.00150	0.00196	0.00218
Pyrene	202	5.13	0.069	0.00059	0.00485	0.00776
C1-fluoranthenes/pyrene	216	5.26	0.052	0.02140	0.00843	0.01665
C2-fluoranthenes/pyrene	230	5.56	0.025	0.02492	0.00000	0.01953
C3-fluoranthenes/pyrene	244	6.38	0.003	0.08898	0.00000	0.10874
Benz(a)anthracene	228	5.74	0.015	0.00107	0.00107	0.00417
Chrysene	228	5.78	0.014	0.00188	0.00232	0.00404
C1-chrysenes	242	6.19	0.0049	0.04054	0.00000	0.02458
C2-chrysenes	256	6.59	0.0018	0.09162	0.00000	0.02062
C3-chrysenes	270	5.97	0.0098	0.00000	0.00000	0.00000
C4-chrysenes	284	7.42	0.0002	0.00000	0.00000	0.00000
Benzo(b)fluoranthene	252	5.57	0.0270	0.00332	0.00000	0.00000
Benzo(k)fluoranthene	252	6.40	0.0029	0.00999	0.00000	0.00813
Benzo(e)pyrene	252	6.45	0.0025	0.04497	0.00000	0.00000
Benzo(a)pyrene	252	6.41	0.0028	0.04309	0.00000	0.00000
Perylene	252	6.45	0.0025	0.01071	0.00000	0.00000
Indeno(1,2,3-c,d)pyrene	276	6.16	0.006	0.00000	0.00000	0.00645
Dibenz(a,h)anthracene	278	7.13	0.0005	0.00000	0.00000	0.00000
Benzo(g,h,i)perylene	276	7.47	0.0002	0.00000	0.00000	0.00000
Phenol	94	1.50	16.3			
C1-Phenols	108	1.98	10.2			
C2-Phenols	122	2.35	7.21			
C3-Phenols	136	2.70	5.16			
C4-Phenols	150	3.31	2.63			
C5-phenols	164	3.50	2.26			
BTEX				0.00887	0.04281	0.01428
C3-benzenes				0.00000	0.00000	0.00000
Decalin				0.00000	0.00000	0.00000
Naphthalenes				0.01266	0.39997	0.34432
2-3 ring PAH				0.66313	0.56958	0.39454
4-6 ring PAH				0.38458	0.01863	0.22286
C0-C5 phenols				0.00000	0.00000	0.00000
Total TU				1.08	1.11	1.04

D2 Toxicity results – Canada

Table D 3 Toxicity testing of *A. tonsa* (Canada). *: Total WAF concentration is in this project used to calculate specific toxicity, and as volatiles are not analyzed, TPH is used.

Laboratory	Canada	Canada	Canada
Internal Lab ID	MGO repetition		
Sample ID	WAF 1 (Wide Range Gas Oil)	WAF 2 (Marine Gas Oil)	WAF 3 (Very Low Sulfur Fuel Oil)
Specie	<i>A. tonsa</i>	<i>A. tonsa</i>	<i>A. tonsa</i>
Sample description	WRG	MGO	VLSFO
WAF cons (mg/L)	25.0 mg/L	25.0 mg/L	25.0 mg/L
LC ₅₀ (%)	63.3	28.3	41.9
(Cl _{95%})	47.5-81.4	25.5-31.4	36.7-47.8
LC ₅₀ (mg/L)	15 825	7 075	10 475
(Cl _{95%})	11.875-20.350	6.375-7.850	9.175-11.950
Observed mortality at endpoint in 100% WAF	85 %	100 %	95 %
WAF conc (TPH)*	0.185	1.894	1.122
LC50 (mg/L)*	0.117	0.536	0.470

Table D 4 Calculated toxic units in the WAFs. Input data to the calculations are also given (mole weight (Mw), the octanol-water coefficient (logK_{ow}), and the predicted LC₅₀ for each component). "/" indicates not measured. MGO rep (repetition) is used in tables and figures in the main report. TU was not reported, table is prepared by SINTEF.

Laboratory				CAN	CAN	CAN	CAN	CAN	CAN	CAN	CAN
Sample ID											
Internal Lab ID				WGO	WGO	MGO-rep	MGO rep	VLSFO	VLSFO	MGO	MGO
Oil type				WRG	WRG	MGO	MGO	VLSFO	VLSFO	MGO	MGO
Oil to water ratio				1:40	1:40	1:40	1:40	1:40	1:40	1:40	1:40
				WAF1	WAF2	WAF1	WAF2	WAF1	WAF2	WAF1	WAF2
Compound	Mw	log K _{ow}	LC ₅₀ (mg/L)	WRG	WRG	MGO	MGO	VLSFO	VLSFO	MGO	MGO
Benzene	78	1.94	71.8	/	/	/	/	/	/	/	/
Toluene	92	2.51	26.0	/	/	/	/	/	/	/	/
Ethylbenzene	106	3.01	10.6	/	/	/	/	/	/	/	/
m-xylene	106	3.04	9.98	/	/	/	/	/	/	/	/
p-xylene	106	3.04	9.98	/	/	/	/	/	/	/	/
o-xylene	106	2.95	12.0	/	/	/	/	/	/	/	/
C3-benzenes	120	3.58	3.69	/	/	/	/	/	/	/	/
Decalin	138	4.20	0.57	/	/	/	/	/	/	/	/
C1-decalins	152	4.61	0.21	/	/	/	/	/	/	/	/



Laboratory				CAN	CAN	CAN	CAN	CAN	CAN	CAN	CAN
Sample ID											
Internal Lab ID				WGO	WGO	MGO-rep	MGO rep	VLSFO	VLSFO	MGO	MGO
Oil type				WRG	WRG	MGO	MGO	VLSFO	VLSFO	MGO	MGO
Oil to water ratio				1:40	1:40	1:40	1:40	1:40	1:40	1:40	1:40
				WAF1	WAF2	WAF1	WAF2	WAF1	WAF2	WAF1	WAF2
Compound	Mw	log K _{OW}	LC ₅₀ (mg/L)	WRG	WRG	MGO	MGO	VLSFO	VLSFO	MGO	MGO
C2-decalins	166	5.11	0.06	/	/	/	/	/	/	/	/
C3-decalins	180	5.60	0.02	/	/	/	/	/	/	/	/
C4-decalins	194	6.09	0.01	/	/	/	/	/	/	/	/
Benzo(b)thiophene	134	3.13	9.68	/	/	/	/	/	/	/	/
Naphthalene	128	3.30	5.87	0.0005	0.0005	0.0111	0.0124	0.0161	0.0253	0.0096	0.0104
C1-naphthalenes	142	3.79	1.76	0.0020	0.0019	0.0541	0.0556	0.0575	0.0528	0.0520	0.0544
C2-naphthalenes	156	4.24	0.58	0.0038	0.0035	0.1036	0.1017	0.0839	0.0790	0.0995	0.1029
C3-naphthalenes	170	4.73	0.17	0.0057	0.0053	0.1226	0.1127	0.0940	0.0781	0.1077	0.1041
C4-naphthalenes	184	5.22	0.05	0.0089	0.0077	0.1238	0.1190	0.0542	0.0492	0.0931	0.0936
Biphenyl	154	3.94	1.27	0.0016	0.0015	0.0089	0.0091	0.0024	0.0021	0.0090	0.0091
Acenaphthylene	152	3.44	4.79	0.0000	0.0000	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
Acenaphthene	154	3.88	1.50	0.0000	0.0000	0.0008	0.0008	0.0014	0.0013	0.0008	0.0008
Dibenzofuran	168	3.95	1.35	/	/	/	/	/	/	/	/
Fluorene	166	3.93	1.41	0.0003	0.0003	0.0036	0.0036	0.0014	0.0012	0.0037	0.0038
C1-fluorenes	180	4.37	0.47	0.0023	0.0020	0.0127	0.0124	0.0059	0.0052	0.0133	0.0133
C2-fluorenes	194	4.82	0.15	0.0043	0.0043	0.0201	0.0200	0.0128	0.0098	0.0217	0.0222
C3-fluorenes	208	5.32	0.04	0.0076	0.0070	0.0224	0.0288	0.0254	0.0147	0.0307	0.0296
Phenanthrene	178	4.58	0.27	0.0016	0.0016	0.0104	0.0102	0.0116	0.0108	0.0112	0.0116
Anthracene	178	4.55	0.29	0.0002	0.0002	0.0143	0.0137	0.0017	0.0016	0.0084	0.0085
C1-phenanthrenes	192	5.04	0.08	0.0120	0.0122	0.1322	0.1271	0.0649	0.0507	0.0924	0.0977
C2-phenanthrenes	206	5.45	0.03	0.0376	0.0376	0.1863	0.1769	0.1246	0.0779	0.1211	0.1202
C3-phenanthrenes	220	5.91	0.01	0.0743	0.0712	0.1244	0.1214	0.2117	0.0968	0.0739	0.0845
C4-phenanthrenes	234	6.36	0.003	0.1027	0.0996	0.0808	0.0712	0.4054	0.0896	0.0544	0.0748
Dibenzothiophene	184	4.37	0.48	0.0003	0.0000	0.0005	0.0005	0.0009	0.0008	0.0006	0.0006
C1-dibenzothiophenes	198	4.86	0.14	0.0003	0.0003	0.0018	0.0016	0.0041	0.0033	0.0019	0.0020
C2-dibenzothiophenes	212	5.33	0.043	0.0008	0.0008	0.0027	0.0023	0.0113	0.0063	0.0030	0.0032
C3-dibenzothiophenes	226	5.81	0.013	0.0006	0.0016	0.0021	0.0021	0.0248	0.0083	0.0027	0.0032
C4-dibenzothiophene	240	6.43	0.0025	/	/	/	/	/	/	/	/
Fluoranthene	202	5.19	0.059	0.0018	0.0043	0.0058	0.0055	0.0019	0.0013	0.0045	0.0046
Pyrene	202	5.13	0.069	0.0007	0.0079	0.0039	0.0038	0.0073	0.0048	0.0046	0.0049
C1-fluoranthenes/pyrene	216	5.26	0.052	0.0064	0.0063	0.0098	0.0103	0.0162	0.0082	0.0079	0.0082
C2-fluoranthenes/pyrene	230	5.56	0.025	0.0091	0.0080	0.0048	0.0046	0.0477	0.0178	0.0037	0.0043
C3-fluoranthenes/pyrene	244	6.38	0.003	0.0347	0.0310	0.0080	0.0076	0.3870	0.1179	0.0070	0.0088
Benz(a)anthracene	228	5.74	0.015	0.0016	0.0021	0.0004	0.0003	0.0459	0.0125	0.0005	0.0000
Chrysene	228	5.78	0.014	0.0007	0.0032	0.0004	0.0004	0.0131	0.0053	0.0006	0.0006
C1-chrysenes	242	6.19	0.0049	0.0030	0.0032	0.0026	0.0022	0.1299	0.0324	0.0013	0.0020
C2-chrysenes	256	6.59	0.0018	0.0062	0.0066	0.0039	0.0031	0.5113	0.1179	-0.0006	-0.0008
C3-chrysenes	270	5.97	0.0098	0.0006	0.0006	-0.0001	0.0000	0.0813	0.0180	0.0000	-0.0001
C4-chrysenes	284	7.42	0.0002	/	/	/	/	/	/	/	/
Benzo(b)fluoranthene	252	5.57	0.0270	0.0003	0.0009	0.0000	0.0000	0.0012	0.0003	0.0000	0.0000
Benzo(k)fluoranthene	252	6.40	0.0029	0.0007	0.0024	0.0001	0.0001	0.0022	0.0007	0.0002	0.0001
Benzo(e)pyrene	252	6.45	0.0025	0.0002	0.0028	0.0001	0.0001	0.0324	0.0068	0.0001	0.0001
Benzo(a)pyrene	252	6.41	0.0028	0.0001	0.0018	0.0000	0.0000	0.0200	0.0043	0.0000	0.0000

Laboratory				CAN	CAN	CAN	CAN	CAN	CAN	CAN	CAN
Sample ID											
Internal Lab ID				WGO	WGO	MGO-rep	MGO rep	VLSFO	VLSFO	MGO	MGO
Oil type				WRG	WRG	MGO	MGO	VLSFO	VLSFO	MGO	MGO
Oil to water ratio				1:40	1:40	1:40	1:40	1:40	1:40	1:40	1:40
				WAF1	WAF2	WAF1	WAF2	WAF1	WAF2	WAF1	WAF2
Compound	Mw	log K _{OW}	LC ₅₀ (mg/L)	WRG	WRG	MGO	MGO	VLSFO	VLSFO	MGO	MGO
Perylene	252	6.45	0.0025	0.0000	0.0011	0.0000	0.0000	0.0097	0.0022	0.0000	0.0000
Indeno(1,2,3-c,d)pyrene	276	6.16	0.006	0.0000	0.0008	0.0000	0.0000	0.0014	0.0003	0.0000	0.0000
Dibenz(a,h)anthracene	278	7.13	0.0005	0.0000	0.0000	0.0000	0.0000	0.0221	0.0057	0.0000	0.0000
Benzo(g,h,i)perylene	276	7.47	0.0002	0.0000	0.0790	0.0000	0.0000	0.2003	0.0428	0.0000	0.0000
Phenol	94	1.50	16.3	/	/	/	/	/	/	/	/
C1-Phenols	108	1.98	10.2	/	/	/	/	/	/	/	/
C2-Phenols	122	2.35	7.21	/	/	/	/	/	/	/	/
C3-Phenols	136	2.70	5.16	/	/	/	/	/	/	/	/
C4-Phenols	150	3.31	2.63	/	/	/	/	/	/	/	/
C5-phenols	164	3.50	2.26	/	/	/	/	/	/	/	/
BTEX				/	/	/	/	/	/	/	/
C3-benzenes				/	/	/	/	/	/	/	/
Decalin				/	/	/	/	/	/	/	/
Naphthalenes				0.021	0.019	0.415	0.401	0.306	0.284	0.362	0.365
2-3 ring PAH				0.246	0.240	0.624	0.602	0.911	0.380	0.449	0.485
4-6 ring PAH				0.066	0.162	0.040	0.038	1.531	0.399	0.030	0.033
C0-C5 phenols				/	/	/	/	/	/	/	/
Total TU				0.33	0.42	1.08	1.04	2.75	1.06	0.84	0.88

D3 Toxicity results – China

Table D 5 Toxicity testing of zebrafish and *M. mongolica* (China)

Laboratory	China	China	China	China	China	China
Sample ID	2021-5427	2021-5428	2021-5429	2021-5427	2021-5428	2021-5429
Internal Lab ID						
Oil type	WRG	MGO	VLSFO	WRG	MGO	VLSFO
Sample description	1:40	1:40	1:40	1:40	1:40	1:40
	WAF 1	WAF 2	WAF 3	WAF 1	WAF 2	WAF 3
	(seawater)	(seawater)	(seawater)	(freshwater)	(freshwater)	(freshwater)
Tot WAF conc (mg/L)	1.967	2.582	1.008	2.426	2.956	1.251
LC50 (%) (zebrafish)				>100%	87.09	94.63
LC50 (mg/L)				>2.43	2.57	1.18
Observed toxicity at end point in 100% WAF				6%	70%	58%
TU				2.28	1.92	1.21
LC50 (%) (<i>M. mongolica</i>)	>100	42.35	48.23			
LC50 (mg/L)	>1.97	1.1	0.49			
Observed toxicity at end point in 100% WAF	32%	87%	87%			
TU	1.77	3.15	2.00			

Table D 6 Calculated toxic units in the WAFs. Input data to the calculations are also given (mole weight (Mw), the octanol-water coefficient ($\log K_{ow}$), and the predicted LC_{50} for each component). (China)

Laboratory				China	China	China	China	China	China
Sample ID				2021-5427	2021-5428	2021-5429	2021-5427	2021-5428	2021-5429
Internal Lab ID									
Oil type				WRG	MGO	VLSFO	WRG	MGO	VLSFO
Oil to water ratio				1:40	1:40	1:40	1:40	1:40	1:40
Compound	Mw	log Kow	LC ₅₀ (mg/L)	WAF 1 (seawater)	WAF 2 (seawater)	WAF 3 (seawater)	WAF 1 (freshwater)	WAF 2 (freshwater)	WAF 3 (freshwater)
Benzene	78	1.94	71.8				0.000844	0.001197	0.000200
Toluene	92	2.51	26.0				0.003122	0.010363	0.002500
Ethylbenzene	106	3.01	10.6				0.002538	0.007449	0.002916
m-xylene	106	3.04	9.98				0.000729	0.002738	0.009551
p-xylene	106	3.04	9.98				0	0	0
o-xylene	106	2.95	12.0	0.000007	0.000113	0.000000	0.000501	0.000530	0.000573
C3-benzenes	120	3.58	3.69	0.011610	0.127627	0.037649	0.036249	0.130050	0.024720
Decalin	138	4.20	0.57	0	0	0	0	0	0
C1-decalins	152	4.61	0.21	0	0	0	0	0	0
C2-decalins	166	5.11	0.06	0	0	0	0	0	0
C3-decalins	180	5.60	0.02	0	0	0	0	0	0
C4-decalins	194	6.09	0.01	0	0	0	0	0	0
Benzo(b)thiophene	134	3.13	9.68	0.000873	0.000918	0.000444	0.000151	0.000112	0.000138
Naphthalene	128	3.30	5.87	0.033731	0.037649	0.035775	0.001240	0.004655	0.016238
C1-naphthalenes	142	3.79	1.76	0.024489	0.016193	0.050227	0.017595	0.087400	0.158889
C2-naphthalenes	156	4.24	0.58	0.089483	0.079483	0.088276	0.239381	0.250398	0.091563
C3-naphthalenes	170	4.73	0.17	0	0	0	0	0	0



Laboratory				China	China	China	China	China	China
Sample ID				2021-5427	2021-5428	2021-5429	2021-5427	2021-5428	2021-5429
Internal Lab ID									
Oil type				WRG	MGO	VLSFO	WRG	MGO	VLSFO
Oil to water ratio				1:40	1:40	1:40	1:40	1:40	1:40
Compound	Mw	log Kow	LC ₅₀ (mg/L)	WAF 1	WAF 2	WAF 3	WAF 1	WAF 2	WAF 3
				(seawater)	(seawater)	(seawater)	(freshwater)	(freshwater)	(freshwater)
C4-naphthalenes	184	5.22	0.05	0	0	0	0	0	0
Biphenyl	154	3.94	1.27	0	0	0	0	0	0
Acenaphthylene	152	3.44	4.79	0	0	0	0	0	0
Acenaphthene	154	3.88	1.50	0	0	0	0	0	0
Dibenzofuran	168	3.95	1.35	0	0	0	0	0	0
Fluorene	166	3.93	1.41	0	0	0	0.001061	0.000842	0.000691
C1-fluorenes	180	4.37	0.47	0	0	0	0	0	0
C2-fluorenes	194	4.82	0.15	0	0	0	0	0	0
C3-fluorenes	208	5.32	0.04	0	0	0	0	0	0
Phenanthrene	178	4.58	0.27	0.010333	0.010333	0.010333	0.006899	0.006585	0.004275
Anthracene	178	4.55	0.29	0	0	0	0	0	0
C1-phenanthrenes	192	5.04	0.08	0	0	0	0.025031	0.012524	0.003127
C2-phenanthrenes	206	5.45	0.03	0.410000	0.436667	0.199667	0.251195	0.143020	0.116922
C3-phenanthrenes	220	5.91	0.01	0	0	0	0	0	0
C4-phenanthrenes	234	6.36	0.003	0	0	0	0	0	0
Dibenzothiophene	184	4.37	0.48	0.012521	0.006458	0.005063	0.005881	0.003105	0.000865
C1-dibenzothiophenes	198	4.86	0.14	0	0	0	0	0	0
C2-dibenzothiophenes	212	5.33	0.043	0	0	0	0.010794	0.012826	0.003717
C3-dibenzothiophenes	226	5.81	0.013	0	0	0	0	0	0
C4-dibenzothiophene	240	6.43	0.0025	0	0	0	0	0	0
Fluoranthene	202	5.19	0.059	0.041525	0.083729	0.068136	0.015431	0.008363	0.002417
Pyrene	202	5.13	0.069	0	0	0	0	0	0
C1-fluoranthenes/pyrene	216	5.26	0.052	0.096923	0.139615	0.051731	0.062634	0.031101	0.009402
C2-fluoranthenes/pyrene	230	5.56	0.025	0	0	0	0	0	0
C3-fluoranthenes/pyrene	244	6.38	0.003	0	0	0	0	0	0
Benz(a)anthracene	228	5.74	0.015	0.257333	0.136667	0.157333	0.018071	0.019285	0.014831
Chrysene	228	5.78	0.014	0	0	0	0	0	0
C1-chrysenes	242	6.19	0.0049	0	0	0	0.014016	0.014022	0.032805
C2-chrysenes	256	6.59	0.0018	0	0	0	0.188393	0.128816	0.162020
C3-chrysenes	270	5.97	0.0098	0	0	0	0	0	0
C4-chrysenes	284	7.42	0.0002	0	0	0	0	0	0
Benzo(b)fluoranthene	252	5.57	0.0270	0	0	0	0	0	0
Benzo(k)fluoranthene	252	6.40	0.0029	0	0	0	0	0	0
Benzo(e)pyrene	252	6.45	0.0025	0	0	0	0.378118	0.353672	0.128652
Benzo(a)pyrene	252	6.41	0.0028	0.757143	2.003571	1.278571	0.969421	0.659807	0.398860
Perylene	252	6.45	0.0025	0	0	0	0	0	0
Indeno(1,2,3-c,d)pyrene	276	6.16	0.006	0	0	0	0	0	0
Dibenz(a,h)anthracene	278	7.13	0.0005	0	0	0	0	0	0
Benzo(g,h,i)perylene	276	7.47	0.0002	0	0	0	0	0	0
Phenol	94	1.50	16.3	0.001466	0.004344	0.001067	0.001162	0.001577	0.001756
C1-Phenols	108	1.98	10.2	0.008118	0.009049	0.001294	0.009891	0.011311	0.007786
C2-Phenols	122	2.35	7.21	0	0	0	0	0	0
C3-Phenols	136	2.70	5.16	0	0	0	0	0	0
C4-Phenols	150	3.31	2.63	0.007947	0.006388	0.004449	0.018105	0.020419	0.011451

Laboratory				China	China	China	China	China	China
Sample ID				2021-5427	2021-5428	2021-5429	2021-5427	2021-5428	2021-5429
Internal Lab ID									
Oil type				WRG	MGO	VLSFO	WRG	MGO	VLSFO
Oil to water ratio				1:40	1:40	1:40	1:40	1:40	1:40
Compound	Mw	log Kow	LC ₅₀ (mg/L)	WAF 1	WAF 2	WAF 3	WAF 1	WAF 2	WAF 3
				(seawater)	(seawater)	(seawater)	(freshwater)	(freshwater)	(freshwater)
C5-phenols	164	3.50	2.26	0	0	0	0	0	0
BTEX				0.006510	0.051989	0.011579	0.007735	0.022276	0.015740
C3-benzenes				0.011610	0.127627	0.037649	0.036249	0.130050	0.024720
Decalin				0	0	0	0	0	0
Naphthalenes				0.147702	0.133325	0.174278	0.258216	0.342453	0.266690
2-3 ring PAH				0.433727	0.454377	0.215507	0.301011	0.179013	0.129736
4-6 ring PAH				1.152925	2.363582	1.555771	1.646084	1.215066	0.748988
C0-C5 phenols				0.017531	0.019780	0.006810	0.029158	0.033307	0.020992
Total TU				1.77	3.15	2.00	2.28	1.92	1.21

D4 Toxicity results – Sweden

Methodology and more detailed results described in the report E21-055 from ALS Toxicon AB, May 2, 2022 (not included in the report).

Table D 7 *LC50-values for Nitocra spinipes determined after 48 hours of exposure to the WAFs. As no data reported in the template file, the table is prepared by SINTEF.*

Laboratory	Sweden	Sweden	Sweden
	TOXICON ALS Global	TOXICON ALS Global	TOXICON ALS Global
Internal Lab ID	E21-055-1	E21-055-3	E21-053-2
Sample ID	12669825	12670165	1267191
Specie	<i>N. spinipes</i>	<i>N. spinipes</i>	<i>N. spinipes</i>
Sample description	WAF 1 - WRG	WAF 2 - MGO	WAF 3 - VLSFO
WAF cons (mg/L)	4.865	2.276	1.243
LC ₅₀ (%)	75.3	80.9	17.4
(CI _{95%})			
LC ₅₀ (mg/L)	3.67	1.86	0.22
(CI _{95%})			
Observed mortality at endpoint in 100% WAF	90	60	100

Table D 8 *Calculated toxic units in the WAFs. Input data to the calculations are also given (mole weight (Mw), the octanol-water coefficient (logK_{ow}), and the predicted LC₅₀ for each component). TU was not reported, table is prepared by SINTEF.*

Laboratory	Sweden			Sweden	Sweden	Sweden
Sample ID						
Internal Lab ID				E21-055-1	E21-055-3	E21-055-2
Oil type				WRG	MGO	VLSFO
Oil to water ratio						
Compound	Mw	log Kow	LC ₅₀ (mg/L)	WRG	MGO	VLSFO
Benzene	78	1.94	71.8	0.00028	0.00084	0.00034
Toluene	92	2.51	26.0	0.00257	0.00935	0.00362
Ethylbenzene	106	3.01	10.6	0.00098	0.01377	0.00242
m-xylene	106	3.04	9.98	0.00000	0.00000	0.00000
p-xylene	106	3.04	9.98	0.00460	0.03086	0.00998
o-xylene	106	2.95	12.0	0.00178	0.01375	0.00433
C3-benzenes	120	3.58	3.69	0.00821	0.06130	0.02344
Decalin	138	4.20	0.57	0.00000	0.00000	0.00000
C1-decalins	152	4.61	0.21	0.00000	0.00000	0.00000
C2-decalins	166	5.11	0.06	0.00000	0.00000	0.00000
C3-decalins	180	5.60	0.02	0.00000	0.00000	0.00000
C4-decalins	194	6.09	0.01	0.00000	0.00000	0.00000
Benzo(b)thiophene	134	3.13	9.68	0.00000	0.00000	0.00000

Laboratory				Sweden	Sweden	Sweden
Sample ID						
Internal Lab ID				E21-055-1	E21-055-3	E21-055-2
Oil type				WRG	MGO	VLSFO
Oil to water ratio						
Compound	Mw	log Kow	LC ₅₀ (mg/L)	WRG	MGO	VLSFO
Naphthalene	128	3.30	5.87	0.00068	0.06474	0.18739
C1-naphthalenes	142	3.79	1.76	0.00406	0.28466	0.30057
C2-naphthalenes	156	4.24	0.58		0.04397	0.04138
C3-naphthalenes	170	4.73	0.17			
C4-naphthalenes	184	5.22	0.05	0.00000	0.00000	0.00000
Biphenyl	154	3.94	1.27	0.00000	0.00000	0.00000
Acenaphthylene	152	3.44	4.79		0.00010	0.00019
Acenaphthene	154	3.88	1.50			
Dibenzofuran	168	3.95	1.35	0.00000	0.00000	0.00000
Fluorene	166	3.93	1.41	0.00040	0.00674	0.00234
C1-fluorenes	180	4.37	0.47	0.00000	0.00000	0.00000
C2-fluorenes	194	4.82	0.15	0.00000	0.00000	0.00000
C3-fluorenes	208	5.32	0.04	0.00000	0.00000	0.00000
Phenanthrene	178	4.58	0.27	0.00326	0.01444	0.01444
Anthracene	178	4.55	0.29	0.00062	0.00110	0.00186
C1-phenanthrenes	192	5.04	0.08	0.03350	0.04700	0.05888
C2-phenanthrenes	206	5.45	0.03			
C3-phenanthrenes	220	5.91	0.01			
C4-phenanthrenes	234	6.36	0.003	0.00000	0.00000	0.00000
Dibenzothiophene	184	4.37	0.48			
C1-dibenzothiophenes	198	4.86	0.14			
C2-dibenzothiophenes	212	5.33	0.043			
C3-dibenzothiophenes	226	5.81	0.013			
C4-dibenzothiophene	240	6.43	0.0025	0.00000	0.00000	0.00000
Fluoranthene	202	5.19	0.059	0.00559	0.00390	0.00186
Pyrene	202	5.13	0.069	0.00246	0.00391	0.00507
C1-fluoranthenes/pyrene	216	5.26	0.052	0.00000	0.00000	0.00000
C2-fluoranthenes/pyrene	230	5.56	0.025	0.00000	0.00000	0.00000
C3-fluoranthenes/pyrene	244	6.38	0.003	0.00000	0.00000	0.00000
Benz(a)anthracene	228	5.74	0.015			0.00160
Chrysene	228	5.78	0.014	0.00271		0.00250
C1-chrysenes	242	6.19	0.0049	0.00000	0.00000	0.00000
C2-chrysenes	256	6.59	0.0018	0.00000	0.00000	0.00000
C3-chrysenes	270	5.97	0.0098	0.00000	0.00000	0.00000
C4-chrysenes	284	7.42	0.0002	0.00000	0.00000	0.00000
Benzo(b)fluoranthene	252	5.57	0.0270			
Benzo(k)fluoranthene	252	6.40	0.0029			
Benzo(e)pyrene	252	6.45	0.0025	0.00000	0.00000	0.00000
Benzo(a)pyrene	252	6.41	0.0028			
Perylene	252	6.45	0.0025	0.00000	0.00000	0.00000

Laboratory				Sweden	Sweden	Sweden
Sample ID						
Internal Lab ID				E21-055-1	E21-055-3	E21-055-2
Oil type				WRG	MGO	VLSFO
Oil to water ratio						
Compound	Mw	log Kow	LC ₅₀ (mg/L)	WRG	MGO	VLSFO
Indeno(1,2,3-c,d)pyrene	276	6.16	0.006			
Dibenz(a,h)anthracene	278	7.13	0.0005			
Benzo(g,h,i)perylene	276	7.47	0.0002	0.06500		
Phenol	94	1.50	16.3	0.00000	0.00000	0.00000
C1-Phenols	108	1.98	10.2	0.00000	0.00000	0.00000
C2-Phenols	122	2.35	7.21	0.00000	0.00000	0.00000
C3-Phenols	136	2.70	5.16	0.00000	0.00000	0.00000
C4-Phenols	150	3.31	2.63	0.00000	0.00000	0.00000
C5-phenols	164	3.50	2.26	0.00000	0.00000	0.00000
BTEX				0.010	0.069	0.021
C3-benzenes				0.008	0.061	0.023
Decalin				0.000	0.000	0.000
Naphthalenes				0.00	0.39	0.53
2-3 ring PAH				0.038	0.069	0.078
4-6 ring PAH				0.08	0.01	0.01
C0-C5 phenols				0.000	0.000	0.000
Total TU				0.14	0.60	0.66

D5 Toxicity results – Norway

Table D 9 *Lethal immobilization following 48 hours exposure of A. tonsa (stage CVI) to the WAFs. Specific toxicity is normalized to total WAF concentration, and are given as LC10, LC50 and LC 90. Lethal mortality at test endpoint in 100% WAF is also given (Norway).*

Norway WAF-system/-concentration:	LC-value (% WAF)	95%CI	LC-value (mg/L)	95%CI	% Lethal immobilization in 100% WAF at end of exposure:
2021-5427 WRG/0.392 mg/L					
LC ₁₀	> 100	NC	> 0.392	NC	
LC₅₀	> 100	NC	> 0.392	NC	2.5
LC ₉₀	> 100	NC	> 0.392	NC	
2021-5428 MGO/7.237 mg/L					
LC ₁₀	31.1	28.8 – 33.5	2.25	2.09 – 2.43	
LC₅₀	45.5	43.6 – 47.5	3.30	3.16 – 3.44	100
LC ₉₀	66.7	62.0 – 71.7	4.82	4.48 – 5.18	
2021-5429 VLSFO/3.127 mg/L					
LC ₁₀	22.4	17.8 – 28.3	0.697	0.553 – 0.878	
LC₅₀	43.3	38.9 – 48.3	1.35	1.21 – 1.51	100
LC ₉₀	83.7	66.3 – 106	2.63	2.08 – 3.32	

Table D 10 *Lethal immobilization following 96 hours exposure of C. finmarchicus (stage CV) to the WAFs. Specific toxicity is normalized to total WAF concentration, and are given as LC10, LC50 and LC 90. Lethal mortality at test endpoint in 100% WAF is also given. (Norway)*

Norway WAF-system/-concentration:	LC-value (% WAF)	95%CI	LC-value (mg/L)	95%CI	% Lethal immobilization in 100% WAF at end of exposure:
2021-5427 WRG/0.392 mg/L					
LC ₁₀	> 100	NC	> 0.392	NC	
LC₅₀	> 100	NC	> 0.392	NC	0
LC ₉₀	> 100	NC	> 0.392	NC	
2021-5428 MGO/7.237 mg/L					
LC ₁₀	23.0	19.5 – 27.1	1.67	1.41 – 1.97	
LC₅₀	37.2	34.6 – 40.0	2.70	2.50 – 2.90	100
LC ₉₀	60.1	49.9 – 72.4	4.36	3.62 – 5.25	
2021-5429 VLSFO/3.127 mg/L					
LC ₁₀	14.6	10.4 – 20.4	0.455	0.325 – 0.637	
LC₅₀	54.2	46.7 – 62.8	1.70	1.46 – 1.97	81
LC ₉₀	> 100	NC	> 3.127	NC	

Table D 11 *Lethal immobilization following 72 hours exposure of C. finmarchicus (stage NM3/N4 (nauplii)) to the WAFs. Specific toxicity is normalized to total WAF concentration, and are given as LC10, LC50 and LC 90. Lethal mortality at test endpoint in 100% WAF is also given. (Norway)*

Norway WAF-system/-concentration:	LC-value (% WAF)	95%CI	LC-value (mg/L)	95%CI	% Lethal immobilization in 100% WAF at end of exposure:
2021-5427 WRG/0.392 mg/L					
LC ₁₀	25.0	20.7 – 30.2	0.098	0.088 – 0.118	
LC₅₀	> 100	NC	> 0.392	NC	29.5
LC ₉₀	> 100	NC	> 0.392	NC	
2021-5428 MGO/7.237 mg/L					
LC ₁₀	9.8	8.6 – 11.0	0.706	0.624 – 0.798	
LC₅₀	20.1	19.0 – 21.2	1.45	1.37 – 1.54	100
LC ₉₀	41.3	36.5 – 46.8	2.99	2.64 – 3.38	
2021-5429 VLSFO/3.127 mg/L					
LC ₁₀	6.5	5.7 – 7.4	0.202	0.176 – 0.232	
LC₅₀	18.8	17.7 – 20.0	0.588	0.553 - 0.626	100
LC ₉₀	54.5	47.5 – 62.5	1.71	1.49 – 1.96	

Table D 12 *Summary of the calculated toxic units. Total TUs are calculated both with and without decalins (Norway).*

Norway	2021-5427	2021-5428	2021-5429
	WRG	MGO	VLSFO
BTEX	0.010	0.108	0.031
C3-benzenes	0.019	0.306	0.151
Decalins	0.013	0.065	0.024
Naphthalenes	0.013	0.252	0.282
2-3 ring PAH	0.049	0.445	0.166
4-6 ring PAH	0.122	0.125	0.147
C0-C5 phenols	0.001	0.058	0.008
Total TU	0.23	1.36	0.81
TU without decalins	0.21	1.29	0.78

Table D 13 *Calculated toxic units in the WAFs. Input data to the calculations are also given (mole weight (Mw), the octanol-water coefficient (logK_{ow}), and the predicted LC₅₀ for each component).*

Laboratory	Norway			Norway	Norway	Norway
Sample name	WRG			MGO	VLSFO	
Internal sample ID	2021-5427			2021-5428	2021-5429	
Oil category	WRG			MGO	VLSFO	
Oil to water ratio	1:40			1:40	1:40	
Sample description	Mw	log K _{ow}	LC ₅₀ (mg/L)	WAF 1	WAF 2	WAF 3
Benzene	78	1.94	71.8	0.0001	0.0009	0.0003
Toluene	92	2.51	26.0	0.0019	0.0138	0.0043
Ethylbenzene	106	3.01	10.6	0.0009	0.0121	0.0033
m-xylene	106	3.04	9.98	0.0040	0.0464	0.0125
p-xylene	106	3.04	9.98	0.0011	0.0126	0.0038

Laboratory				Norway	Norway	Norway
Sample name				WRG	MGO	VLSFO
Internal sample ID				2021-5427	2021-5428	2021-5429
Oil category				WRG	MGO	VLSFO
Oil to water ratio				1:40	1:40	1:40
Sample description	Mw	log K _{ow}	LC ₅₀ (mg/L)	WAF 1	WAF 2	WAF 3
o-xylene	106	2.95	12.0	0.0017	0.0223	0.0070
C3-benzenes	120	3.58	3.69	0.0190	0.3058	0.1505
Decalin	138	4.20	0.57	0.0001	0.0007	0.0000
C1-decalins	152	4.61	0.21	0.0001	0.0008	0.0001
C2-decalins	166	5.11	0.06	0.0004	0.0021	0.0009
C3-decalins	180	5.60	0.02	0.0016	0.0103	0.0050
C4-decalins	194	6.09	0.01	0.0107	0.0516	0.0180
Benzo(b)thiophene	134	3.13	9.68	0.0000	0.0000	0.0004
Naphthalene	128	3.30	5.87	0.0006	0.0221	0.0505
C1-naphthalenes	142	3.79	1.76	0.0012	0.0579	0.0686
C2-naphthalenes	156	4.24	0.58	0.0024	0.0566	0.0751
C3-naphthalenes	170	4.73	0.17	0.0050	0.0512	0.0550
C4-naphthalenes	184	5.22	0.05	0.0034	0.0648	0.0328
Biphenyl	154	3.94	1.27	0.0017	0.0083	0.0028
Acenaphthylene	152	3.44	4.79	0.0000	0.0001	0.0003
Acenaphthene	154	3.88	1.50	0.0000	0.0007	0.0019
Dibenzofuran	168	3.95	1.35	0.0002	0.0018	0.0007
Fluorene	166	3.93	1.41	0.0003	0.0036	0.0018
C1-fluorenes	180	4.37	0.47	0.0011	0.0073	0.0029
C2-fluorenes	194	4.82	0.15	0.0023	0.0129	0.0052
C3-fluorenes	208	5.32	0.04	0.0032	0.0131	0.0156
Phenanthrene	178	4.58	0.27	0.0014	0.0100	0.0120
Anthracene	178	4.55	0.29	0.0001	0.0020	0.0014
C1-phenanthrenes	192	5.04	0.08	0.0037	0.0293	0.0273
C2-phenanthrenes	206	5.45	0.03	0.0070	0.0298	0.0350
C3-phenanthrenes	220	5.91	0.01	0.0059	0.0368	0.0251
C4-phenanthrenes	234	6.36	0.003	0.0069	0.0767	0.0158
Dibenzothiophene	184	4.37	0.48	0.0000	0.0006	0.0008
C1-dibenzothiophenes	198	4.86	0.14	0.0002	0.0054	0.0025
C2-dibenzothiophenes	212	5.33	0.043	0.0008	0.0258	0.0039
C3-dibenzothiophenes	226	5.81	0.013	0.0023	0.0631	0.0033
C4-dibenzothiophene	240	6.43	0.0025	0.0117	0.1177	0.0072
Fluoranthene	202	5.19	0.059	0.0001	0.0043	0.0017
Pyrene	202	5.13	0.069	0.0004	0.0039	0.0063
C1-fluoranthenes/pyrene	216	5.26	0.052	0.0007	0.0054	0.0057
C2-fluoranthenes/pyrene	230	5.56	0.025	0.0020	0.0197	0.0029
C3-fluoranthenes/pyrene	244	6.38	0.003	0.0168	0.0584	0.0759
Benz(a)anthracene	228	5.74	0.015	0.0014	0.0008	0.0020
Chrysene	228	5.78	0.014	0.0003	0.0003	0.0017
C1-chrysenes	242	6.19	0.0049	0.0016	0.0040	0.0068

Laboratory				Norway	Norway	Norway
Sample name				WRG	MGO	VLSFO
Internal sample ID				2021-5427	2021-5428	2021-5429
Oil category				WRG	MGO	VLSFO
Oil to water ratio				1:40	1:40	1:40
Sample description	Mw	log K _{ow}	LC ₅₀ (mg/L)	WAF 1	WAF 2	WAF 3
C2-chrysenes	256	6.59	0.0018	0.0039	0.0044	0.0061
C3-chrysenes	270	5.97	0.0098	0.0028	0.0012	0.0028
C4-chrysenes	284	7.42	0.0002	0.0000	0.0000	0.0000
Benzo(b)fluoranthene	252	5.57	0.0270	0.0003	0.0001	0.0001
Benzo(k)fluoranthene	252	6.40	0.0029	0.0017	0.0006	0.0004
Benzo(e)pyrene	252	6.45	0.0025	0.0022	0.0008	0.0020
Benzo(a)pyrene	252	6.41	0.0028	0.0017	0.0006	0.0009
Perylene	252	6.45	0.0025	0.0012	0.0007	0.0009
Indeno(1,2,3-c,d)pyrene	276	6.16	0.006	0.0020	0.0004	0.0007
Dibenz(a,h)anthracene	278	7.13	0.0005	0.0176	0.0043	0.0059
Benzo(g,h,i)perylene	276	7.47	0.0002	0.0651	0.0150	0.0239
Phenol	94	1.50	16.3	0.0001	0.0039	0.0004
C1-Phenols	108	1.98	10.2	0.0001	0.0109	0.0005
C2-Phenols	122	2.35	7.21	0.0001	0.0156	0.0014
C3-Phenols	136	2.70	5.16	0.0002	0.0121	0.0023
C4-Phenols	150	3.31	2.63	0.0002	0.0117	0.0023
C5-phenols	164	3.50	2.26	0.0003	0.0033	0.0009
BTEX				0.010	0.108	0.031
C3-benzenes				0.019	0.306	0.151
Decalins				0.013	0.065	0.024
Naphthalenes				0.013	0.252	0.282
2-3 ring PAH				0.049	0.445	0.166
4-6 ring PAH				0.122	0.125	0.147
C0-C5 phenols				0.001	0.057	0.008
Total TU				0.23	1.36	0.81

Appendix E Calculated diagnostic ratios for oil fingerprinting

E1 Calculated diagnostic ratios for oil fingerprinting – USA

No results reported.

E2 Calculated diagnostic ratios for oil fingerprinting – Canada

Table E 1 Calculated diagnostic ratios for screening fingerprinting analysis using GC/MS (Canada)

Laboratory		Canada	Canada	Canada	Notes
ESTS code		2021-09-17-6081	2021-09-17-6082	2021-09-17-6083	
Sample Location		2021-5427, S1-S3	2021-5428, S1-S3	2021-5429, S1-S3	
Sample Description		WRG	MGO	VLSFO	
m/z	Ratios				
	Alkanes				
85	n-C17/Pristane	1.76	2.21	4.01	Concentration ratios
85	n-C18/Phytane	1.26	1.44	3.06	Concentration ratios
85	Pr/Ph	0.63	0.82	0.68	Concentration ratios
	Biomarkers				
191	Ts/C30a β hopane	0.32	0.65	0.21	Concentration ratios
191	Tm/C30a β hopane	0.21	0.41	0.44	Concentration ratios
191	28a β /C30a β hopane	/	/	/	
191	C29a β hopane/C30a β hopane	0.66	0.78	0.92	Concentration ratios
191	30O/C30a β hopane	/	/	/	
191	31a β S/C30a β hopane	0.31	0.25	0.32	Concentration ratios
217	27dbR/27dbS	/	/	/	
218	27bb/29bb	1.26	1.78	0.95	Concentration ratios
231	TASC26/RC26+SC27	0.30	0.35	0.38	Area ratios
231	TASC28/RC26+SC27	0.64	0.58	0.73	Area ratios
231	TARC27/RC26+SC27	0.51	0.44	0.54	Area ratios
231	TARC28/RC26+SC27	0.49	0.37	0.62	Area ratios
	APAHs				
192	2MP/1MP	0.81	1.95	1.82	Concentration ratios
192	MA/1MP	0.05	0.10	0.44	Concentration ratios
198	4MD/1MD	/	5.26	5.56	Concentration ratios
216	2MF/4MPy	0.06	0.31	0.20	Concentration ratios
216	B(a)F/4MPy	0.18	0.57	0.29	Concentration ratios
216	B(b+C)F/4MPy	0.09	0.26	0.20	Concentration ratios
216	2MPy/4MPy	0.41	1.55	0.85	Concentration ratios
216	1MPy/4MPy	0.58	0.66	0.77	Concentration ratios
234	Retene/TMPhe	/	/	/	
234	BNT/TMPhe	0.00	0.01	0.02	Concentration ratios

Laboratory		Canada	Canada	Canada	Notes
ESTS code		2021-09-17-6081	2021-09-17-6082	2021-09-17-6083	
Sample Location		2021-5427, S1-S3	2021-5428, S1-S3	2021-5429, S1-S3	
Sample Description		WRG	MGO	VLSFO	
m/z	Ratios				
	Sulfur content				
198/191	1M-DBT/30ab	0.00	4.58	0.28	Concentration ratios
198/191	4M-DBT/30ab	0.14	24.5	1.54	Concentration ratios
234/191	BNT/30ab	0.00	1.67	0.40	Concentration ratios
	If 30ab is small or not present				
198/192	1M-DBT/1MP	0.00	0.08	0.06	Concentration ratios
198/192	4M-DBT/1MP	0.28	0.42	0.35	Concentration ratios
234/192	BNT/TMPhe	0.00	0.01	0.02	Concentration ratios
	Optional ratios sulfur content				
212/206	C2-DBT/C2-Phe	0.18	0.16	0.17	Concentration ratios
226/206	C3-DBT/C2-Phe	0.22	0.10	0.17	Concentration ratios
234/206	BNT/C2-Phe	0.00	0.00	0.01	Concentration ratios
162/206	C2-BT/C2-Phe	/	/	/	

E3 Calculated diagnostic ratios for oil fingerprinting – China

No results reported.

E4 Calculated diagnostic ratios for oil fingerprinting – Sweden

Table E 2 Calculated diagnostic ratios for screening fingerprinting analysis (Sweden). Source indicates if the data is from COSI or manual integration. *: GC/MS used for oil 3.

Laboratory		National Forensic Centre, Swe		Sweden	Sweden	Sweden
Sample ID						
Internal						
Lab ID				12669825	12670165	12670191
Oil type				Product WRG	Product MGO	Product VLSFO
	m/z	Ratios	Source	OIL 1	OIL 2	OIL 3
GC/FID		C17/pristane	Manual	1.47	1.41	4.09*
		C18/phytane	Manual	1.86	1.90	4.15*
		Pristane/phytane	Manual	1.07	1.69	0.79*
GC/MS	191	Ts/30ab	Manual	0.30	0.75	0.17
	191	Tm/30ab	Manual	0.22	0.45	0.44
	191	28ab/30ab	Manual	0.26	0.00	0.04
	191	29ab/30ab	Manual	0.50	0.68	0.69
	191	30O/30ab	Manual	0.06	<LOD (300)	0.09
	191	31abS/30ab	Manual	0.34	<LOD (31abS)	0.32

Laboratory	National Forensic Centre, Swe			Sweden	Sweden	Sweden
Sample ID				12669825	12670165	12670191
Internal						
Lab ID						
Oil type				Product WRG	Product MGO	Product VLSFO
	m/z	Ratios	Source	OIL 1	OIL 2	OIL 3
	191	30G/30ab	Manual	0.05	<LOD (30G)	0.06
	217	27dbR/27dbS	Manual	0.62	0.57	0.85
	218	27bb/29bb	Manual	1.56	2.16	1.04
	231	TASC26/RC26+SC27	Manual	0.31	0.40	0.51
	231	TASC28/RC26+SC27	Manual	0.54	0.51	0.59
	231	TARC27/RC26+SC27	Manual	0.55	0.42	0.59
	231	TARC28/RC26+SC27	Manual	0.39	0.27	0.55
	192	2MP/1MP	Manual	0.66	1.93	2.17
	192	MA/1MP	Manual	<LOD (MA)	0.03	0.39
	198	4MD/1MD	Manual	<LOD (1-MD)	4.62	4.18
	216	2MF/4MPy	Manual	<LOD (2MF)	0.22	0.14
	216	B(a)F/4MPy	Manual	0.20	0.37	0.21
	216	B(b+c)F/4MPy	Manual	<LOD (B(b+c)F)	0.12	0.11
	216	2MPy/4MPy	Manual	0.32	1.43	0.83
	216	1MPy/4MPy	Manual	0.50	0.63	0.81
	234	Retene/TMPhe	Manual	2.12	1.93	0.00
	234	BNT/TMPhe	Manual	<LOD (BNT)	0.15	0.19
	Sulfur content					
	198/191	1M-DBT/30ab	Manual	<LOD(1M-DBT)	5.56	0.26
	198/191	4M-DBT/30ab	Manual	0.07	25.65	1.09
GC/MS	234/191	BNT/30ab	Manual	<LOD (BNT)	0.98	0.68
	If 30ab is small or not present					
	198/192	1M-DBT/1MP	Manual	<LOD(1M-DBT)	0.07	0.07
	198/192	4M-DBT/1MP	Manual	0.20	0.32	0.30
	234/192	BNT/TMPhe	Manual	<LOD (BNT)	0.15	0.14
	Optional ratios sulfur content					
	212/206	C2-DBT/C2-Phe	Manual	0.19	0.14	0.15
	212/206	C3-DBT/C2-Phe	Manual	0.24	0.11	0.14
	234/206	BNT/C2-Phe	Manual	<LOD (BNT)	0.0005	0.0024
	162/206	C2-BT/C2-Phe	Manual	No pattern recognition C2-BT	No pattern recognition C2-BT	0.022

E5 Calculated diagnostic ratios for oil fingerprinting – Norway

Table E 3 Calculated diagnostic ratios for screening fingerprinting analysis. Source indicates if the data is from COSI or manual integration. ND: At least one of the peaks are not present.

Laboratory				Norway	Norway	Norway
Sample name			COSI no.	no-1-41.1	no-1-41.2	no-1-41.3
Internal sample ID				2021-5427	2021-5428	2021-5429
Oil category				WRG	MGO	VLSFO
Sample description	m/z	Ratios	Source*	OIL 1	OIL 2	OIL 3
GC/FID		C17/pristane	COSI	1.56	1.47	1.77
		C18/phytane	COSI	1.97	2.14	2.28
		Pristane/phytane	COSI	1.02	1.72	1.12
		C17/pristane	Manual int	1.60	1.48	1.92
		C18/phytane	Manual int	2.03	2.18	2.43
		Pristane/phytane	Manual int	0.98	1.73	1.04
GC/MS	191	Ts/30ab	COSI	0.31	0.57	0.18
	191	Tm/30ab	COSI	0.20	0.35	0.43
	191	28ab/30ab	COSI	0.28	0.30	ND
	191	29ab/30ab	COSI	0.50	0.59	0.71
	191	30O/30ab	COSI	ND	ND	0.20
	191	31abS/30ab	COSI	0.34	0.31	0.33
	191	30G/30ab	COSI	0.05	0.06	0.09
	217	27dbR/27dbS	COSI	0.62	0.57	0.06
	218	27bb/29bb	COSI	1.43	1.91	1.03
	231	TASC26/RC26+SC27	COSI	0.18	0.36	0.67
	231	TASC28/RC26+SC27	COSI	0.51	0.44	0.58
	231	TARC27/RC26+SC27	COSI	0.50	0.42	0.55
	231	TARC28/RC26+SC27	COSI	0.43	0.31	0.58
	192	2MP/1MP	COSI	0.68	1.74	1.99
	192	MA/1MP	COSI	ND	0.06	0.48
	198	4MD/1MD	COSI	3.65	5.63	4.87
	216	2MF/4MPy	COSI	0.09	0.19	0.14
	216	B(a)F/4MPy	COSI	0.21	0.45	0.26
	216	B(b+c)F/4MPy	COSI	0.09	0.17	0.15
	216	2MPy/4MPy	COSI	0.41	1.59	0.94
	216	1MPy/4MPy	COSI	0.60	0.67	0.89
	234	Retene/TMPhe	COSI	1.91	1.66	0.00
	234	BNT/TMPhe	COSI	ND	0.39	0.30
		Sulfur content				
GC/MS	198/191	1M-DBT/30ab	Manual int	0.05	6.09	0.34
	198/191	4M-DBT/30ab	Manual int	0.17	35.9	1.70
	234/191	BNT/30ab	Manual int	0.04	3.64	0.70
		If 30ab is small or not present				
	198/192	1M-DBT/1MP	Manual int	0.07	0.06	0.07
	198/192	4M-DBT/1MP	Manual int	0.26	0.38	0.33
	234/192	BNT/TMPhe	Manual int	0.15	0.41	0.31
		Optional ratios sulfur content				
	212/206	C2-DBT/C2-Phe	Manual int	0.19	0.12	0.14
	212/206	C3-DBT/C2-Phe	Manual int	0.22	0.11	0.15
	234/206	BNT/C2-Phe	Manual int	0.003	0.002	0.004
	162/206	C2-BT/C2-Phe	Manual int	0.023	0.11	0.15

Appendix F Overview chemical component groups

Table F 1 Target organic analytes (SVOC: Semi volatile organic compounds, VOC: Volatile organic compounds, TPH: Total petroleum hydrocarbons, UCM: Unresolved organic materials).

Group	Compound	Abb	Group	Compound	Abb
Decalins	Decalin	DE	C0-C5 phenols	Phenol	PH
	C1-decalins	DE1		C1-phenols	PH1
	C2-decalins	DE2		C2-phenols	PH2
	C3-decalins	DE3		C3-phenols	PH3
	C4-decalins	DE4		C4-phenols	PH4
Naphthalenes	Naphthalene	N		C5-phenols	PH5
	C1-naphthalenes	N1	Other VOC	Isopentane	
	C2-naphthalenes	N2		n-C5 (Pentane)	
	C3-naphthalenes	N3		Cyclopentane	
2-3 ring PAHs	C4-naphthalenes	N4		2-methylpentane	
	Benzo(b)thiophene	BT		3-methylpentane	
	Biphenyl	B		n-C6 (Hexane)	
	Acenaphthylene	ANY		Methylcyclopentane	
	Acenaphthene	ANA		Cyclohexane	
	Dibenzofuran	DBF		2,3-dimethylpentane	
	Fluorene	F		3-methylhexane	
	C1-fluorenes	F1		n-C7 (Heptane)	
	C2-fluorenes	F2		Methylcyclohexane	
	C3-fluorenes	F3		2,4-dimethylhexane	
	Phenanthrene	P		2-methylheptane	
	Anthracene	A		n-C8 (Octane)	
	C1-phenanthrenes/anthracenes	P1		n-C9 (Nonane)	
	C2-phenanthrenes/anthracenes	P2		n-C10 (Decane)	
	C3-phenanthrenes/anthracenes	P3		n-Butylbenzene	
	C4-phenanthrenes/anthracenes	P4		1,2,4,5-tetramethylbenzene	
	Dibenzothiophene	D		n-pentylbenzene	
	C1-dibenzothiophenes	D1	BTX	Benzene	
	C2-dibenzothiophenes	D2		Toluene	
	C3-dibenzothiophenes	D3		Ethylbenzene	
	C4-dibenzothiophenes	D4		m-xylene	
4-6 ring PAHs	Fluoranthene	FL		p-xylene	
	Pyrene	PY		o-xylene	
	C1-fluoranthenes/pyrenes	FL1	C3-benzenes	Propylbenzene	
	C2-fluoranthenes/pyrenes	FL2		1-methyl-3-ethylbenzene	
	C3-fluoranthenes/pyrenes	FL3		1-methyl-4-ethylbenzene	
	Benz[a]anthracene	BA		1,3,5-Trimethylbenzene	
	Chrysene	C		1-methyl-2-ethylbenzene	
	C1-chrysenes	C1		1,2,4-trimethylbenzene	
	C2-chrysenes	C2		1,2,3-trimethylbenzene	
	C3-chrysenes	C3	TPH		
	C4-chrysenes	C4			
	Benzo[b]fluoranthene	BBF			
	Benzo[k]fluoranthene	BKF		C10-C36	
	Benzo[e]pyrene	BEP		Sum of VOC and TPH	
	Benzo[a]pyrene	BAP		TPH - SVOC	
	Perylene	PE			
	Indeno[1,2,3-c,d]pyrene	IN			
	Dibenz[a,h]anthracene	DBA			
	Benzo(g,h,i)perylene	BPE			