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Enhanced emission of intermediate-volatility/semi-volatile organic matter in gas and particle phases from ship exhausts with low-sulfur fuels

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Table S1 Abbreviations used in this article and their definitions

Abbreviations	Full name
IMO	International Maritime Organization
MARPOL	International Convention for the Prevention of Pollution from Ships
SECA	Sulfur Emission Control Area
STEAM	Ship Traffic Emissions Assessment Model
SOA	secondary organic aerosol
POA	primary organic aerosol
VOC	volatile organic compound
IVOC	intermediate organic compound
SVOC	intermediate organic compound
OGV	ocean-going vessel
ICS	inland cargo ship
HSF	high-sulfur fuel
LSF	low-sulfur fuel
HFO	heavy fuel oil
MGO	marine gas oil
WCO	waste cooking oil
ME	main engine
AE	auxiliary engine
LSE	low-speed engine
MSE	medium-speed engine
SOAFP	secondary organic aerosol formation potential
UCM	unresolved complex mixture
PAH	polycyclic aromatic hydrocarbon
OPAH	oxygenated polycyclic aromatic hydrocarbon
b-alkane	branched alkane

Table S2 Detailed parameters of the test three ocean-going vessels (OGVs) and four inland cargo ships (ICSs)

Ship ID	Type	Tonnage (kt)	Main engine	Auxiliary engine	Ship age (year)
OGV1	Ocean going vessel	180.0	2-stroke, 15748 kW, 75 rpm	4-stroke, 1280 kW, 900 rpm	0
OGV2	Ocean going vessel	110.0	2-stroke, 13500 kW, 91.1 rpm	4-stroke, 900 kW, 900 rpm	0
OGV3	Ocean going vessel	210.0	2-stroke, 15745 kW, 75rpm	4-stroke, 1180 kW, 900 rpm	0
ICS1	Inland cargo ship	0.90	4-stroke, 255 kW, 1000 rpm	-	14
ICS2	Inland cargo ship	0.98	4-stroke, 300 kW, 1000 rpm	-	12
ICS3	Inland cargo ship	0.80	4-stroke, 145 kW, 1000 rpm	-	6
ICS4	Inland cargo ship	0.39	4-stroke, 138 kW, 1500 rpm	-	10

Table S3 Engine type, operating mode, and fuel type of each ship for each measurement

Ship ID	Engine type	Operating mode	Sampling duration	Ship ID	Engine type	Operating mode	Sampling duration
OGV1	Main engine	20%_MGO[a]	20 min	OGV3	Auxiliary engine	50%_MGO	20 min
		75%_MGO	20 min			50%_HFO	20 min
	Auxiliary engine	75%_MGO (NCR)	27 min			75%_HFO	20 min
OGV2	Main engine	25%_HFO	20 min	ICS1	Main engine	Maneuvering_No.0 diesel	20 min
		50%_HFO	20 min			Cruise_No.0 diesel	20 min
		75%_HFO	20 min	ICS2	Main engine	Maneuvering_No.0 diesel	20 min
	Auxiliary engine	85%_HFO	20 min			Cruise_No.0diesel	20 min
		100%_HFO	20 min	ICS3	Main engine	Maneuvering_No.0 diesel	20 min
		50%_MGO	25 min			Cruise_No.0 diesel	20 min
		50%_HFO	70 min	ICS4	Main engine	Maneuvering_No.0 diesel	20 min
OGV3	Main engine	75%_MGO	40 min			Cruise_No.0 diesel	20 min
		25%_HFO	20 min				
		50%_HFO	10 min				
		75%_HFO	40 min				
		95%_HFO	40 min				

[a], means percentage of engine load under what type of fuel

Table S4 The identified I/SVOC species in this study

Compounds	Abbreviation	M/Z	Detection limit (ng/m^3)	Recovery (%)	classification
(I) n-Alkanes					
Dodecane	C_{12}	170	0.11	86	IVOC
Tridecane	C_{13}	184	0.12	84	IVOC
Tetradecane	C_{14}	198	0.12	91	IVOC
Pentadecane	C_{15}	212	0.12	90	IVOC
Hexadecane	C_{16}	226	0.12	83	IVOC
Heptadecane	C_{17}	240	0.12	81	IVOC
Octadecane	C_{18}	254	0.26	83	IVOC
Nonadecane	C_{19}	268	0.25	85	IVOC
Icosane	C_{20}	282	0.26	82	IVOC
Henicosane	C_{21}	296	0.20	89	IVOC
Docosane	C_{22}	310	0.15	92	IVOC
Tricosane	C_{23}	324	0.56	93	SVOC
Tetracosane	C_{24}	338	0.29	95	SVOC
Pentacosane	C_{25}	352	0.11	80	SVOC
Hexacosane	C_{26}	366	0.45	88	SVOC
Heptacosane	C_{27}	380	0.24	96	SVOC
Octacosane	C_{28}	394	0.61	98	SVOC
Nonacosane	C_{29}	408	0.65	84	SVOC
Triacontane	C_{30}	422	0.56	96	SVOC
Hentriacontane	C_{31}	436	0.76	92	SVOC
Dotriacontane	C_{32}	450	0.37	90	SVOC
Tritriacontane	C_{33}	464	0.11	84	SVOC
Tetratriacontane	C_{34}	478	0.20	86	SVOC
Pentatriacontane	C_{35}	492	0.21	93	SVOC
Hexatriacontane	C_{36}	506	0.12	92	SVOC
(II)PAHs					
Phenanthrene	Phe	178	0.11	79	IVOC
Anthracene	Ant	178	0.02	80	IVOC
Fluoranthene	Flu	202	0.13	86	IVOC
Pyrene	Pyr	202	0.10	84	IVOC
Benz(a)anthracene	BaA	228	0.04	83	IVOC
Chrysene / Triphenylene	Chr/TP	228	0.25	85	IVOC
Benzo(b)fluoranthene	BbF	252	0.34	89	IVOC
Benzo(k)fluoranthene	BkF	252	0.11	93	IVOC
Benzo(a)pyrene	BaP	252	0.28	92	IVOC
Benzo(e)pyrene	BeP	252	0.09	95	IVOC
Perylene	Pery	252	0.02	83	IVOC
Indeno[123-cd]pyrene	IP	276	0.14	86	SVOC
Dibenz(a,h)anthracene	DBA	278	0.02	88	SVOC
Benzo(ghi)perylene	BghiP	276	0.10	89	SVOC
(III) OPAHs					
1-Naphthaldehyde	1-Nap	156	0.01	80	IVOC
9-Fluorenone	9-FO	180	0.01	97	IVOC
Anthraquinone	ATQ	208	0.01	98	IVOC
Benzanthrone	BZA	230	0.01	93	IVOC

Benzo(a)anthracene-7,12-dione	7,12-BaAQ	304	0.02	91	IVOC
1,4-Chrysenequione	1,4-CQ	258	0.01	99	SVOC
5,12-Naphthacenequione	5,12-NAQ	318	0.04	93	SVOC
6H-Benzo(cd)pyrene-6-one	BPYRone	254	0.01	97	SVOC
(IV) Fatty acids					
Capric Acid	$C_{10:0}$	172	0.32	93	IVOC
Undecanoic Acid	$C_{11:0}$	186	0.48	94	IVOC
Dodecanoic	$C_{12:0}$	200	0.75	93	IVOC
Tridecanoic	$C_{13:0}$	214	0.58	91	IVOC
Tetradecanoic	$C_{14:0}$	228	0.17	91	IVOC
Pentadecanoic	$C_{15:0}$	242	4.20	88	IVOC
Hexadecanoic	$C_{16:0}$	256	0.30	84	IVOC
Heptadecanoic	$C_{17:0}$	270	0.16	86	IVOC
Octadecanoic	$C_{18:0}$	284	0.56	91	IVOC
Octadecenoic	$C_{18:1}$	282	0.22	91	IVOC
Nonadecanoic	$C_{19:0}$	298	0.31	95	IVOC
Eicosanoic	$C_{20:0}$	312	0.95	92	IVOC
Heneicosanoic	$C_{21:0}$	326	0.95	93	IVOC
Docosanoic	$C_{22:0}$	340	0.93	88	IVOC
(V) Aromatic acids					
o-Phthalic acid	O-Ph	166	0.11	95	IVOC
m-Phthalic acid	M-Ph	166	0.05	92	IVOC
p-Phthalic acid	P-Ph	166	0.11	96	IVOC
(VI) Hopanes					
17α(H)-22,29,30-trisnorhopane	C_{27a}	191	0.08	86	SVOC
17β(H)-22,29,30-trisnorhopane	C_{27b}	191	0.03	86	SVOC
17α(H),21β(H)-30-norhopane	C_{29ab}	191	0.26	93	SVOC
17β(H),21α(H)-30-norhopane	C_{29ba}	191	0.04	89	SVOC
17α(H),21β(H)-hopane	C_{30ab}	191	0.19	94	SVOC
17β(H),21α(H)-hopane	C_{30ba}	191	0.01	86	SVOC
17α(H),21β(H)-22S-homohopane	$C_{31ab\ S}$	191	0.01	88	SVOC
17α(H),21β(H)-22R-homohopane	$C_{31ba\ S}$	191	0.01	84	SVOC
17β(H),21α(H)-homohopane	C_{31ba}	191	0.01	82	SVOC
17α(H),21β(H)-22S-bishomohopane	$C_{32ab\ S}$	191	0.01	86	SVOC
17α(H),21β(H)-22R-bishomohopane	$C_{32ab\ R}$	191	0.01	82	SVOC

M/Z: Mass-to-charge ratio

Table S5 SOA yields used in this study

Carbon Number	N-alkanes	B-alkanes	PAHs	UCM	Data sources
12	0.01	0.0017	0.28	0.01	N-alkanes and B-alkanes from Gentner et al. (2012); PAHs from Zhao et al. (2014).
13	0.019	0.0035	0.40	0.019	
14	0.033	0.007	0.49	0.033	
15	0.055	0.013	0.62	0.055	
16	0.089	0.024	0.70	0.089	
17	0.14	0.042	0.75	0.14	
18	0.23	0.073	0.79	0.23	
19	0.37	0.12	0.82	0.37	
20	0.56	0.20	0.82	0.56	
21	0.77	0.32	0.82	0.77	
22	0.96	0.47	0.82	0.96	
23	1.08	0.61	0.82	1.08	
24	1.14	0.70	0.82	1.14	
25	1.16	0.75	0.82	1.16	
26	1.16	0.75	0.82	1.16	
27	1.16	0.75	0.82	1.16	
28	1.16	0.75	0.82	1.16	
29	1.16	0.75	0.82	1.16	
30	1.16	0.75	0.82	1.16	
31	1.16	0.75	0.82	1.16	
32	1.16	0.75	0.82	1.16	
33	1.16	0.75	0.82	1.16	
34	1.16	0.75	0.82	1.16	
35	1.16	0.75	0.82	1.16	
36	1.16	0.75	0.82	1.16	

Note: The yield of $SOA_{n\text{-}alkane}$ after carbon number 25 was estimated by pentacosane, while yield of $SOA_{b\text{-}alkane}$ after carbon number 25 was also estimated by 25th b-alkane, yield of SOA_{UCM} was replaced with data from n-alkane, and other substances were replaced with corresponding data from n-alkanes based on their volatility distribution.(Gentner et al., 2012; Zhao et al., 2014) And the OH reaction rate constants (cm^3 $molec^{-1}$ s^{-1}) and SOA yields used in this study were reacted (Δt) after 48 h photo-oxidation at the OA concentration of 9 $\mu g/m^3$

Table S6 Reaction constant of OH radicals used in this study

Carbon Number	N-alkanes	B-alkanes	PAHs	UCM	Data sources
12	1.32E-11	1.32E-11	2.30E-11	1.32E-11	Zhao et al. (2014)
13	1.51E-11	1.51E-11	4.86E-11	1.51E-11	
14	1.68E-11	1.68E-11	6.00E-11	1.68E-11	
15	1.82E-11	1.82E-11	8.00E-11	1.82E-11	
16	1.96E-11	1.96E-11	8.00E-11	1.96E-11	
17	2.10E-11	2.10E-11	2.10E-11	2.10E-11	
18	2.24E-11	2.24E-11	2.24E-11	2.24E-11	
19	2.38E-11	2.38E-11	2.38E-11	2.38E-11	
20	2.52E-11	2.52E-11	2.52E-11	2.52E-11	
21	2.67E-11	2.67E-11	2.67E-11	2.67E-11	
22	2.81E-11	2.81E-11	2.81E-11	2.81E-11	

Table S7 Profiles of I/SVOCs in ship exhausts under different fuels(%)

Compounds	HFO	MGO	No.0 diesel
(I) Acids			
O-Ph	0.54±0.13	0.89±0.67	0.55±0.99
M-Ph	0.12±0.01	0.19±0.12	0.18±0.40
P-Ph	0.58±0.24	1.02±0.85	0.34±0.48
$C_{10:0}$	0.40±0.15	0.61±0.38	0.95±1.54
$C_{11:0}$	2.07±0.11	3.05±0.25	3.09±0.97
$C_{12:0}$	0.71±0.13	5.89±0.46	4.50±2.60
$C_{13:0}$	0.25±0.12	0.43±0.10	0.66±0.47
$C_{14:0}$	1.31±0.03	10.1±0.36	5.31±1.52
$C_{15:0}$	0.86±0.06	3.60±0.20	2.17±1.02
$C_{16:0}$	0.39±0.02	0.67±1.58	0.52±4.79
$C_{17:0}$	0.30±0.10	0.91±0.05	0.99±0.38
$C_{18:0}$	4.39±0.04	2.39±1.09	5.16±4.92
$C_{18:1}$	4.84±0.03	3.39±0.43	0.54±2.20
$C_{19:0}$	0.28±0.02	0.70±0.04	0.61±0.18
$C_{20:0}$	0.41±0.05	1.92±0.13	0.80±0.24
$C_{21:0}$	0.14±0.17	0.67±0.02	0.70±0.11
$C_{22:0}$	0.34±0.17	2.09±0.03	0.74±0.28
(II) n-Alkanes			
C_{12}	0.12±0.07	0.16±0.03	0.12±0.12
C_{14}	0.14±0.06	0.28±0.06	0.52±0.69
C_{15}	0.38±0.37	0.63±0.14	1.18±2.46
C_{16}	0.88±1.35	0.72±0.15	2.38±5.48
C_{17}	2.41±3.62	3.04±2.24	4.56±8.84
C_{18}	3.45±4.36	3.04±3.55	3.00±7.08
C_{19}	4.95±0.42	3.31±2.83	3.34±7.61
C_{20}	4.83±0.09	2.28±1.98	2.43±6.08
C_{21}	4.21±2.22	2.20±1.51	2.13±5.05
C_{22}	3.48±0.17	1.94±1.55	1.54±3.62
C_{23}	3.06±1.67	1.61±1.51	1.21±2.88
C_{24}	2.85±0.16	1.74±1.35	0.98±2.19
C_{25}	2.87±4.80	1.46±0.86	2.94±5.83
C_{26}	2.43±0.38	1.02±0.60	1.55±3.66
C_{27}	2.20±0.11	0.92±0.52	2.23±5.31
C_{28}	1.79±0.48	0.70±0.32	1.50±3.48
C_{29}	1.57±0.08	0.61±0.26	0.83±1.37
C_{30}	1.14±2.11	0.36±0.16	0.65±1.26
C_{31}	1.02±1.90	0.29±0.17	0.46±0.79
C_{32}	0.70±1.43	0.19±0.12	0.47±1.06
C_{33}	0.54±1.15	0.17±0.11	0.49±1.35
C_{34}	0.35±0.76	0.18±0.08	0.33±0.89
C_{35}	0.30±0.37	0.11±0.02	0.21±0.05
C_{36}	0.10±0.02	0.11±0.01	0.15±0.04
(III) PAHs			
Phe	0.81±0.13	0.72±0.10	0.77±0.23

Ant	0.06±0.01	0.04±0.01	0.09±0.01
Flu	0.29±0.24	0.18±0.12	0.22±0.28
Pyr	0.18±0.15	0.10±0.04	0.22±0.32
BaA	0.07±0.11	0.06±0.03	0.05±0.05
Chr/TP	0.10±0.13	0.06±0.09	0.03±0.05
BbF	0.10±0.12	0.07±0.06	0.10±0.11
BkF	0.03±0.03	0.04±0.01	0.08±0.03
BaP	0.04±0.06	0.01±0.02	0.02±0.04
BeP	0.08±0.02	0.12±0.01	0.03±0.01
Pery	0.02±0.01	0.04±0.01	0.00±0.01
IP	0.03±0.04	0.04±0.01	0.05±0.01
DBA	0.02±0.02	0.03±0.01	0.03±0.02
BghiP	0.02±0.01	0.02±0.01	0.02±0.00
(IV)OPAHs			
1-Nap	3.66±0.17	3.96±0.47	7.46±6.30
9-FO	0.17±0.17	0.26±0.36	0.17±0.23
ATQ	1.21±0.97	1.22±0.41	0.92±0.42
BZA	0.08±0.07	0.08±0.05	0.16±0.08
7,12-BaAQ	3.66±0.17	3.96±0.47	7.46±6.30
1,4-CQ	0.00±0.00	0.00±0.00	0.00±0.00
5,12-NAQ	0.00±0.00	0.00±0.00	0.00±0.00
BPYRone	0.00±0.00	0.00±0.00	0.00±0.00
(V)Hopanes			
C_{27a}	0.24±0.42	0.13±0.06	0.09±0.13
C_{27b}	0.05±0.09	0.07±0.09	0.02±0.01
C_{29ab}	1.07±2.22	0.49±0.54	0.25±0.66
C_{29ba}	0.09±0.17	0.05±0.04	0.03±0.08
C_{30ab}	0.85±1.67	0.37±0.37	0.25±0.63
C_{30ba}	0.10±0.16	0.05±0.04	0.05±0.12
$C_{31ab\ S}$	0.39±0.80	0.17±0.18	0.06±0.15
$C_{31ba\ S}$	0.21±0.38	0.10±0.09	0.09±0.23
C_{31ba}	0.05±0.11	0.04±0.05	0.02±0.05
$C_{32ab\ S}$	0.24±0.48	0.10±0.11	0.06±0.14
$C_{32ab\ R}$	0.03±0.08	0.04±0.05	0.01±0.01

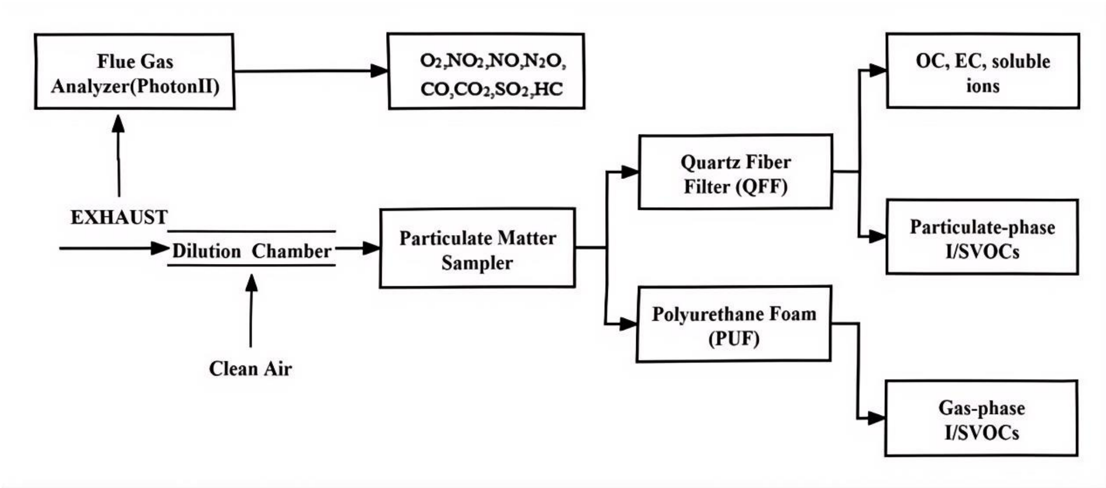

Figure S1 Schematic diagram of on-board measurement system

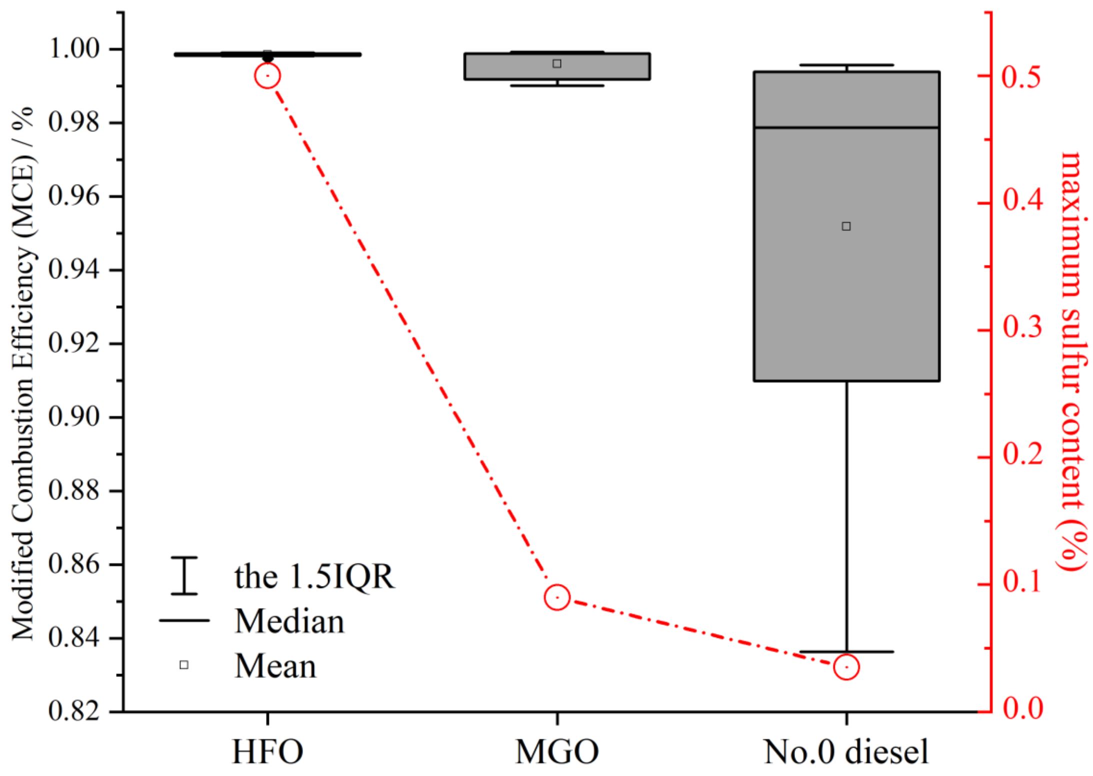

Figure S2 Box-whisker plot of the Modified Combustion Efficiency (MCE) with different fuel types

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