Supporting information

The influence of spatiality on shipping emissions, air quality and potential human exposure in Yangtze River Delta/Shanghai, China

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Additional Material and Methods

S.1 Estimation of ship emissions

Marine vessel emissions were calculated based on a bottom-up activity-based method.

The main engine load factor, LF_m, was calculated as

$$LF_m = (ActSpeed / MaxSpeed)^3 \quad (1)$$

where ActSpeed is the actual speed when ship is cruising and MaxSpeed is the maximum design speed for the ship.

Main engine emissions in grams, E_m, were calculated as

$$E_m = P_m \times LF_m \times LLAM \times T_m \times EF_m \times FCF_m \times CF_m \quad (2)$$

where P_m is the installed power of ME (kw), LLAM is the low load adjustment multiplier for the main engine, T_m is operation time of the main engine (h), EF_m is the main engine emissions factor (g/kwh), FCF_m is the main engine fuel correction factor, and CF_m is the main engine control factor.

Auxiliary engine emissions in grams, E_a, were calculated as

$$E_a = P_a \times LF_a \times T_a \times EF_a \times CF_a \quad (3)$$

where P_a is the installed power of the auxiliary engine (kw), LF_a is auxiliary engine load factors, T_a is operation time of the auxiliary engine (h), EF_a is auxiliary engine emissions factors (g/kwh), and CF_a is auxiliary engine control factors.

Auxiliary boiler emissions in grams, E_b, were calculated as

$$E_b = P_b \times LF_b \times T_b \times EF_b \times CF_b \quad (4)$$

where P_b is the installed power of the auxiliary boiler (kw), LF_b is AB load factors, T_b is operation time of the auxiliary boiler (h), EF_b is auxiliary boiler emissions factors (g/kwh), and CF_b is auxiliary boiler control factors.

The total emissions of the ship in grams, E, was

$$E = E_m + E_a + E_b \quad (5).$$

For ships available in Lloyd's register (Lloyds, 2009), the following data were derived from the Lloyd's database including: ship name, ship type, date of construction, flag name, revolutions per minute (RPM) of the main engine, speed, maximum design power of the main engine, maximum design power of the auxiliary engines and gross tonnage. For some domestic ships unavailable in Lloyd's database, the main engine power was assumed to be 7000 kw by default, based on the East China Sea-going ships in Lloyd's register (with main engine power mainly ranging from 11000 kw to 14000 kw) and domestic ships from the Chinese Classification Society

(CCS) (with main engine power mainly ranging from 4000 kw to 6000 kw).

S.2 Emission Factors, Low load adjustment multipliers, and Control factors

The sulfur content of residual oil was about 2.7 %, and the sulfur content of marine distillate was 0.5 %. The emission factors for SO_2, NO_x, CO, $NMVOC_s$, PM_{10}, $PM_{2.5}$ come primarily from the data published in Cooper (2004), ICF International (2009), and Goldsworthy and Goldsworthy (2015). Emissions factors for OC and EC were obtained from published data in Agrawal et al. (2008a), Agrawal et al. (2008b), Petzold et al. (2011), and Moldanová et al. (2013). Table S1 lists emission factors used in the present study.

Emission factors are adjusted for loads below 20 % using tables from studies conducted in other countries (ICF International, 2009; Starcrest Consulting Group, 2009). Because adjustment multipliers were not available for organic carbon (OC) and elemental carbon (EC), these pollutants were assigned the same low load adjustment multiplier (LLAM) as PM in the present study. Table S2 represents LLAMs for main engine emission factors.

For all marine engines over 130 kilowatts (kW) for engines built on or after January 1, 2000, NO_x limits in Annex VI applied. We used a control factor of 0.9024 for main engines and a factor of 0.906 for auxiliary engines to adjust the NO_x emissions. For vessels built after 2010, and thus complying with "IMO Tier 2", we used a main engine control factor of 0.875 and an auxiliary engine control factor of 0.8767 to adjust main engine emissions from ships with emission controls. The control factors were from ICF International (2009).

The detailed emission factors and low load adjustment multipliers and control factors were listed in Fan et al. (2016).

S.3 Calculation of Statistical metrics in the model evaluation

The statistical metrics in the model evaluation include Normalized Mean Bias (NMB), Normalized Mean Error (NME), Root Mean-square Error (RMSE), and Pearson's correlation coefficient (r). The statistical metrics are calculated as follows:

$$\text{NMB} = \frac{\sum_{i=1}^{n}(S_i - O_i)}{\sum_{i=1}^{n} O_i} \times 100\% \quad (6)$$

$$\text{NME} = \frac{\sum_{i=1}^{n}|S_i - O_i|}{\sum_{i=1}^{n} O_i} \times 100\% \quad (7)$$

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(S_i - O_i)^2}{n}} \quad (8)$$

$$r = \frac{\sum_{i=1}^{n}(S_i - \bar{S})(O_i - \bar{O})}{\sqrt{\sum_{i=1}^{n}(S_i - \bar{S})^2 \sum_{i=1}^{n}(O_i - \bar{O})^2}} \quad (9)$$

Where:

S_i = the daily-average simulated data at a certain monitoring station, day i

O_i = the daily-average observation data at a certain monitoring station, day i

$\bar{S}$ = the average simulated data at a certain monitoring station of all days

$\bar{O}$ = the average observation data at a certain monitoring station of all days

n = the total numbers of days of the monitoring stations for which the simulated results are compared with the observed ones

References:

Agrawal, H., Malloy, Q. G. J., Welch, W. A., Miller, J. W., and Iii, D. R. C.: In-use gaseous and particulate matter emissions from a modern ocean going container vessel, Atmos. Environ., 42, 5504-5510, 10.1016/j.atmosenv.2008.02.053, 2008a.

Agrawal, H., Welch, W. A., Miller, J. W., and Cocker, D. R.: Emission Measurements from a Crude Oil Tanker at Sea, Environ. Sci. Technol., 42, 7098, 10.1021/es703102y, 2008b.

Cooper, D.: Methodology for calculating emissions from ships: 1. Update of emission factors, Swedish Methodology for Environmental Data (SMED), 2004.

Goldsworthy, L., and Goldsworthy, B.: Modelling of ship engine exhaust emissions in ports and extensive coastal waters based on terrestrial AIS data - An Australian case study, Elsevier Science Publishers B. V., 45-60 pp., 2015.

Moldanová, J., Fridell, E., Winnes, H., and Holminfridell, S.: Physical and chemical characterisation of PM emissions from two ships operating in European Emission Control Areas, Atmos. Meas. Tech., 6, 3577-3596, 10.5194/amt-6-3577-2013, 2013.

Petzold, A., Lauer, P., Fritsche, U., Hasselbach, J., Lichtenstern, M., Schlager, H., and Fleischer, F.: Operation of marine diesel engines on biogenic fuels: modification of emissions and resulting climate effects, Environ. Sci. Technol., 45, 10394-10400, 10.1021/es2021439, 2011.

Starcrest Consulting Group: Port of Los Angeles Inventory of Air Emissions 2008, Technical Report Revision, 2009.

Additional Figures and Tables

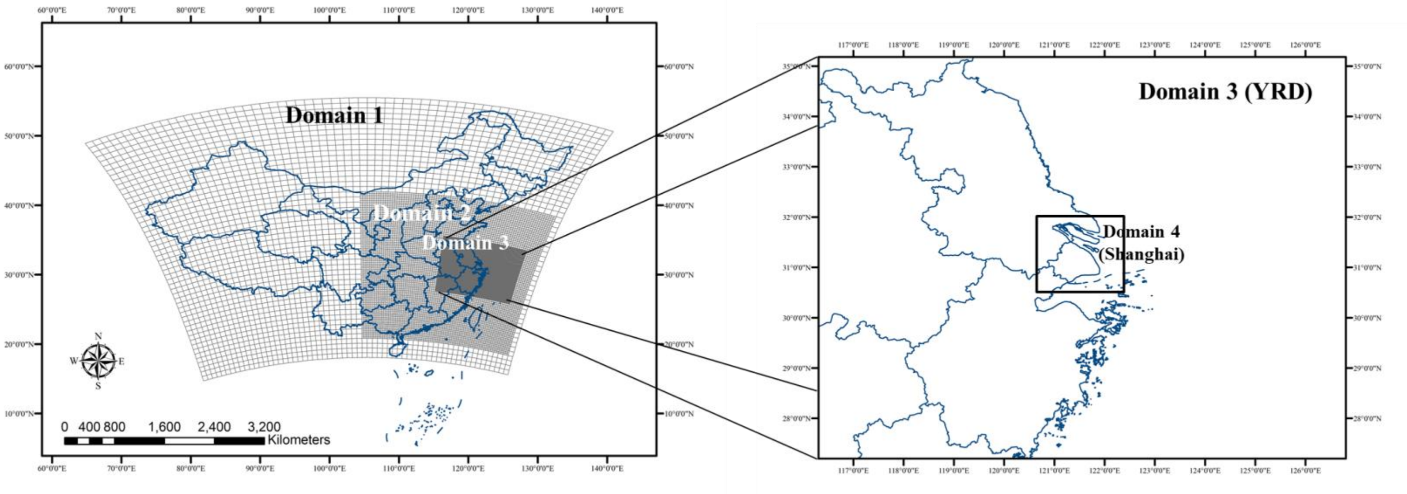

Figure S1. Nested simulation domains 1 to 4 in this study

Table S1 Pollution sources and pollutant types in national-scale non-shipping emission inventories

Domain	Pollution source	Pollutant type
Domain 1 (China) and Domain 2	Power plant, steel, cement	SO_2, NO_x, $PM_{2.5}$, PM_{10}, CO, NH_3
	Industrial point source	SO_2, $PM_{2.5}$, PM_{10}
	Industrial combustion, industrial process, domestic fuel combustion, domestic biomass combustion, on-road traffic, non-road traffic, open combustion	SO_2, NO_x, $PM_{2.5}$, PM_{10}, VOC_s, CO, NH_3
	Residential solvent, industrial solvent	VOC_s
	Agriculture, residential and commercial, waste	CO, NH_3

Table S2 Pollution sources and pollutant types in local-scale non-shipping emission inventories

Domain	Pollution source	Pollutant type
Domain 3 (YRD), and Domain 4 (Shanghai)	Power plant, industrial boiler, industrial process, domestic source	SO_2, NO_x, $PM_{2.5}$, PM_{10}, CO, NH_3, VOC_s
	On-road traffic	NO_x, $PM_{2.5}$, PM_{10}, CO, NH_3, VOC_s
	Non-road traffic	SO_2, NO_x, $PM_{2.5}$, PM_{10}, CO, VOC_s
	Dust	$PM_{2.5}$, PM_{10}
	Agriculture	NH_3

Table S3 Inputs for each run of the simulations

Run #	**Run name**	**Land-Based Emissions**	**Shipping and port-related emissions**
	Domain 1 (D1), 81-km		
1	D1 baseline	National-scale land-based emission inventory	National scale shipping inventory based on AIS
	Domain 2 (D2), 27-km		
2	D2 baseline	National-scale land-based emission inventory	National scale shipping inventory based on AIS
	Domain 3 (D3), 9-km		
3	D3 baseline	Local YRD land-based emission inventory	Shipping emission inventory based on AIS
4	Remove all coastal ships, ocean-going ships and inland ships	Local YRD land-based emission inventory	Container trucks and port machineries
5	Remove 12-200Nm shipping sources	Local YRD land-based emission inventory	Shipping emissions inside 12 Nm
6	Remove 24-200Nm shipping sources	Local YRD land-based emission inventory	Shipping emissions inside 24 Nm
7	Remove 48-200nm shipping sources	Local YRD land-based emission inventory	Shipping emissions inside 48 Nm
8	Remove 96-200nm shipping sources	Local YRD land-based emission inventory	Shipping emissions inside 96 Nm
	Domain 4 (D4), 1 km		
10	D4 baseline	Local land-based emission inventory	Local shipping inventory for inland-water ships and coastal ships, and container-cargo trucks and port terminal equipment

11	Remove cargo trucks and port terminal equipment	Local land-based emission inventory	Inland-water ships, and coastal ships
12	Remove inland-water ships (including international ships going on the rivers)	Local land-based emission inventory	Coastal ships, and container-cargo trucks and port terminal equipment
13	Remove coastal ships	Local land-based emission inventory	Inland-water ships, and container-cargo trucks and port terminal equipment

Table S4 Average and peak contributions from ship emissions in different offshore coastal areas to the land ambient $PM_{2.5}$ concentrations in January and June

Offshore distance	Average contribution to the land ambient $PM_{2.5}$ ($\mu g/m^3$)		Maximum contribution to the land ambient $PM_{2.5}$ ($\mu g/m^3$)	
	January	June	January	June
Inland and within 12 NM	0.24	0.56	1.62	4.02
12-24 NM	0.01	0.04	0.05	0.2
24-48 NM	0.04	0.07	0.11	0.34
48-96 NM	0.07	0.07	0.14	0.3
96-200 NM	0.003	0.01	0.02	0.05