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The impact of ship emissions on air quality and human health in the Gothenburg area – Part 1: 2012 emissions

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S1 Statistical indicators and model performance indicators

In the statistical analysis of the model performance, the following statistical indicators are used: normalized mean bias (NMB), standard deviation (STD), root mean square error (RMSE), correlation coefficient (r), index of agreement (IOA) and the fraction of predictions within a factor of two of observations (FAC2). The overall bias captures the average deviations between the model and observed data and the NMB is given by:

$$NMB = \frac{\overline{M} - \overline{O}}{\overline{O}}$$

where $\overline{M}$ and $\overline{O}$ stand for the averaged model and observation results, respectively. The RMSE combines the magnitudes of the errors in predictions for various times into a single measure and is defined as

$$RMSE = \sqrt{\frac{1}{N} * \sum_{i=1}^{N} (M_i - O_i)^2}$$

where subscript *i* indicates the time step and *N* the number of observations. RMSE is a measure of accuracy, to compare prediction errors of different models for a particular data and not between datasets, as it is scale-dependent. The correlation coefficient (Pearson r) for the temporal correlation is defined as:

$$r = \frac{\sum_{i=1}^{n}(O_i - \bar{O}) \cdot (M_i - \bar{M})}{\sqrt{\sum_{i=1}^{n}(O_i - \bar{O})^2 \cdot \sum_{i=1}^{n}(M - \bar{M})^2}}$$

The index of agreement is defined as:

$$IOA = 1 - \frac{\sum_{i=1}^{N}(O_i - M_i)^2}{\sum_{i=1}^{N}(|M_i - \bar{M}| + |O_i - \bar{O}|)^2}$$

An IOA value close to 1 indicates agreement between modelled and observed data. The fraction of modelled values within a factor of two (FAC2) of the observed values are the fraction of model predictions that satisfy is defined as:

$$0.5 \leq \frac{M_i}{O_i} \leq 2.0 \qquad (9)$$

For evaluation of modelled values in rural areas, the acceptance criteria is FAC2 ≥ 0.5, while in urban areas it is FAC2 ≥ 0.3.

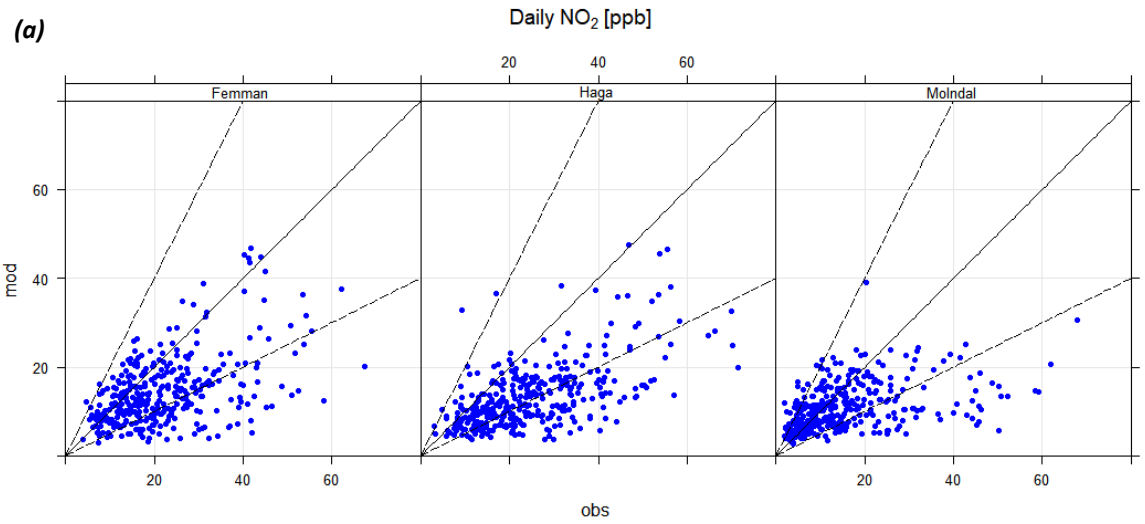
Table S1: Evaluation of modelled versus measured hourly meteorological parameters

parameter	site	n	MB	NMB	RMSE	r	IOA
Temp	all sites	34261	-0.46	-0.06	2.09	0.96	0.87
Temp	Femman	8003	-1.14	-0.12	2.15	0.97	0.85
Temp	GbgA	8784	-0.53	-0.06	2.09	0.97	0.87
Temp	Landvetter	8783	-0.03	0.00	2.27	0.96	0.86
Temp	VingaA	8691	-0.20	-0.02	1.81	0.97	0.88
ws	all sites	34004	-0.18	-0.04	0.51	0.99	0.93
ws	Femman	7772	-0.17	-0.05	0.26	0.99	0.93
ws	GbgA	8780	-0.26	-0.09	0.76	0.93	0.80
ws	Landvetter	8779	0.06	0.01	0.11	1.00	0.97
ws	VingaA	8673	-0.35	-0.05	0.61	0.99	0.92
wd	all sites	34008	2.35	0.01	46.31	0.87	0.93
wd	Femman	7776	1.18	0.01	24.63	0.96	0.97
wd	GbgA	8780	2.40	0.01	66.18	0.76	0.85
wd	Landvetter	8779	5.02	0.03	46.14	0.87	0.94
wd	VingaA	8673	0.66	0.003	35.72	0.92	0.96
rh	all sites	25457	2.73	0.04	12.49	0.64	0.59
rh	Femman	8003	6.02	0.08	13.70	0.67	0.57
rh	GbgA	8781	1.30	0.02	13.12	0.64	0.59
rh	VingaA	8673	1.15	0.01	10.51	0.65	0.61
rain	all sites	24935	0.32	3.37	0.87	0.29	-0.15
rain	Femman	7772	0.39	4.00	0.99	0.29	-0.26
rain	GbgA	8551	0.37	3.13	0.97	0.30	-0.11
rain	VingaA	8612	0.22	2.98	0.62	0.26	-0.06
tsr	Femman	7941	21.48	0.18	125.95	0.82	0.77

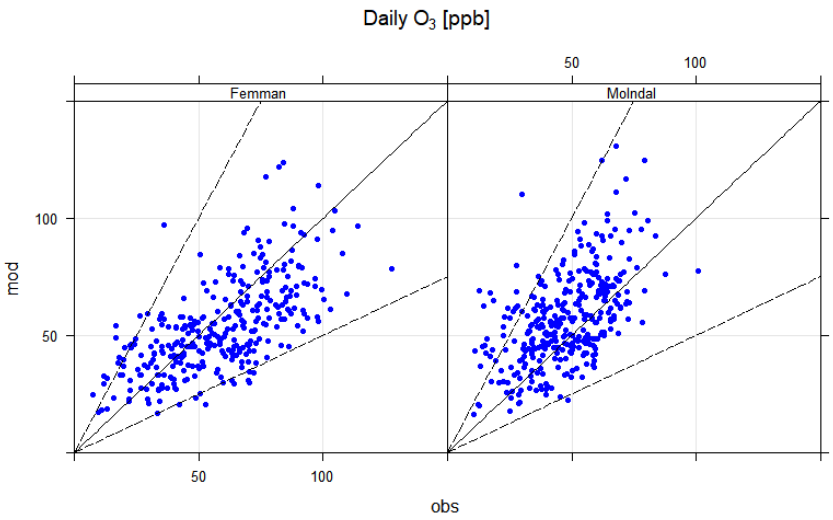
Table S2: Evaluation of modelled versus measured daily concentrations of NO_2, O_3, PM_{10} and $PM_{2.5}$

NO_2											
site	period	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r	COE	IOA
Femman	annual	346	0.71	-7.58	9.24	-0.34	0.42	12.68	0.50	-0.03	0.48
Femman	summer	92	0.96	-0.16	4.02	-0.01	0.27	5.14	0.65	0.22	0.61
Femman	winter	90	0.43	-15.35	15.88	-0.53	0.55	19.27	0.46	-0.46	0.27
Haga	annual	366	0.58	-11.93	12.62	-0.47	0.50	16.44	0.59	-0.18	0.41
Haga	summer	92	0.76	-8.06	8.15	-0.39	0.39	9.93	0.76	-0.12	0.44
Haga	winter	91	0.40	-18.59	18.78	-0.58	0.59	23.63	0.62	-0.32	0.34
Molndal	annual	338	0.68	-5.72	8.41	-0.34	0.50	14.39	0.37	0.14	0.57
Molndal	summer	88	0.73	2.38	4.01	0.25	0.42	5.10	0.53	0.02	0.51
Molndal	winter	74	0.38	-17.44	18.23	-0.64	0.67	26.47	0.54	-0.06	0.47
O_3											
Femman	annual	326	0.92	-4.95	14.82	-0.08	0.25	18.40	0.66	0.22	0.61
Femman	summer	92	0.95	-12.26	16.44	-0.19	0.26	19.89	0.53	-0.23	0.38
Femman	winter	52	0.87	3.50	11.25	0.09	0.28	13.79	0.76	0.34	0.67
Molndal	annual	338	0.91	9.58	15.27	0.20	0.32	19.51	0.55	-0.17	0.42
Molndal	summer	88	0.98	0.97	10.88	0.02	0.20	13.30	0.53	-0.18	0.41
Molndal	winter	74	0.78	11.66	17.14	0.32	0.47	21.31	0.33	-0.44	0.28
PM_{10}											
Femman	annual	324	0.56	-6.80	7.96	-0.43	0.51	10.39	0.24	-0.45	0.28
Femman	summer	91	0.52	-7.73	7.91	-0.53	0.54	9.71	0.17	-0.84	0.08
Femman	winter	59	0.63	-4.25	7.25	-0.27	0.45	9.13	0.28	-0.12	0.44
Haga	annual	343	0.42	-12.15	12.92	-0.58	0.62	17.55	0.10	-0.43	0.28
Haga	summer	79	0.23	-16.36	16.40	-0.72	0.72	21.40	0.17	-0.69	0.15
Haga	winter	81	0.65	-6.07	7.74	-0.36	0.46	11.37	0.25	-0.08	0.46
$PM_{2.5}$											
Haga	annual	343	0.42	-3.31	4.09	-0.44	0.54	4.96	0.59	-0.59	0.21
Haga	summer	79	0.24	-4.63	4.63	-0.63	0.63	5.03	0.47	-1.54	-0.21
Haga	winter	81	0.53	-3.14	4.26	-0.36	0.49	5.29	0.50	-0.41	0.30

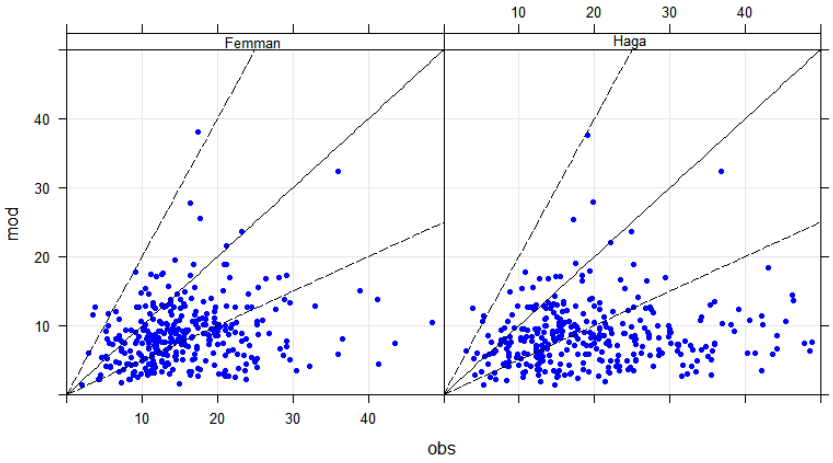
(a)


Daily NO2 [ppb]
Femman
Haga
Molndal
mod
obs
20
40
60

(b)


Daily O3 [ppb]
Femman
Molndal
mod
obs
50
100

(c)


Daily PM10 [µg m−3]
Femman
Haga
mod
obs
10
20
30
40

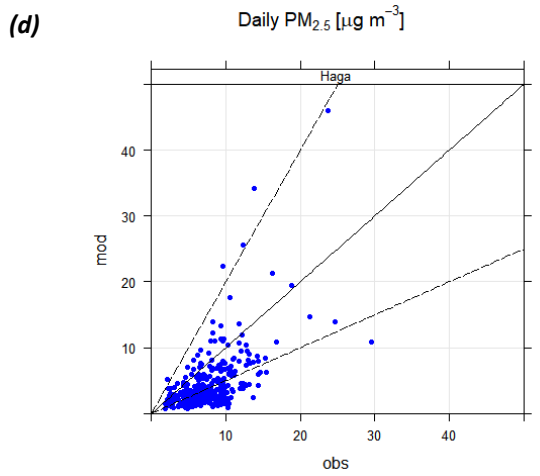


Figure S1: Scatter plots of measured versus observed daily (a) NO_2, (b) O_3, (c) PM_{10} and (d) $PM_{2.5}$ concentrations.

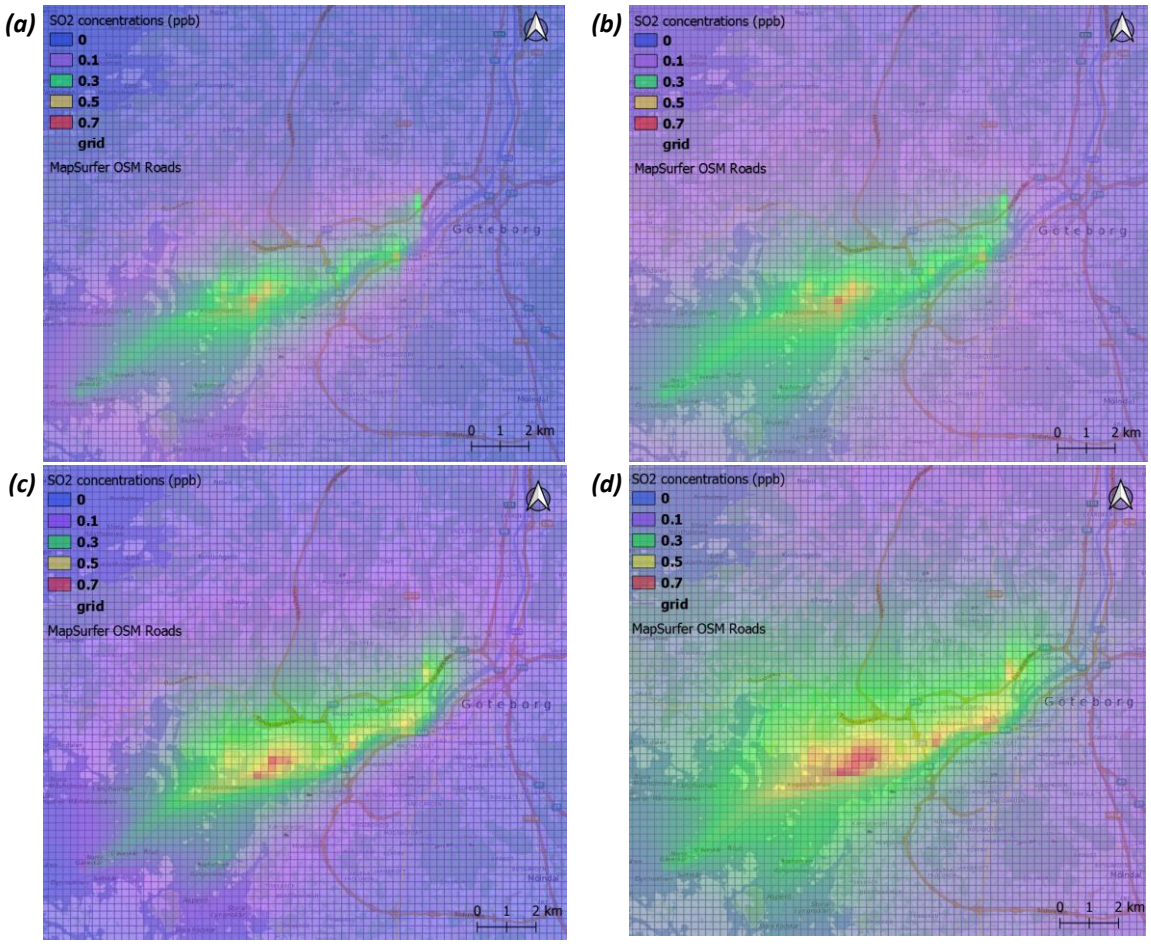


Figure S2: Contributions of shipping to concentrations of SO_2 (in ppb) as mean of winter months (DJF) and summer months (JJA) in year 2012: (a) Local shipping contribution in winter; (b) Local and regional shipping contributions in winter; (c) Local shipping contribution in summer; (d) Local and regional shipping contributions in summer. Base map credits: © OpenStreetMap contributors (openstreetmap.org). Distributed under a Creative Commons BY-SA License.

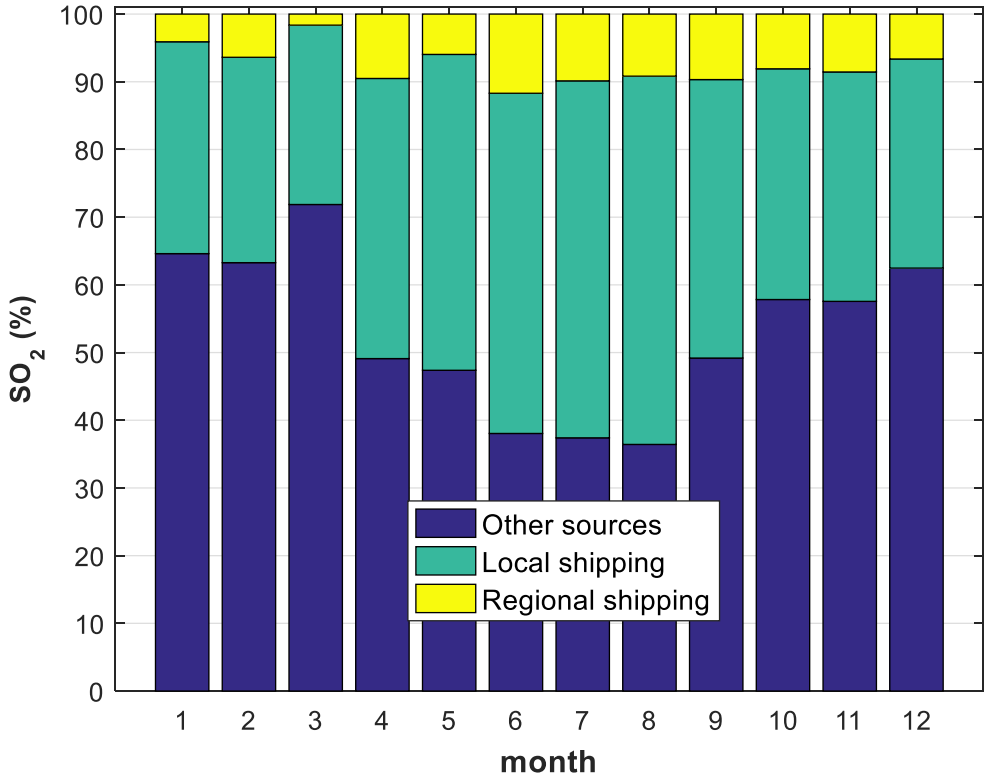


Figure S3: Modelled monthly mean relative contributions from local shipping, regional shipping and all other emission sources (road traffic, industry etc.) to SO_2 concentrations at Eriksberg in year 2012.

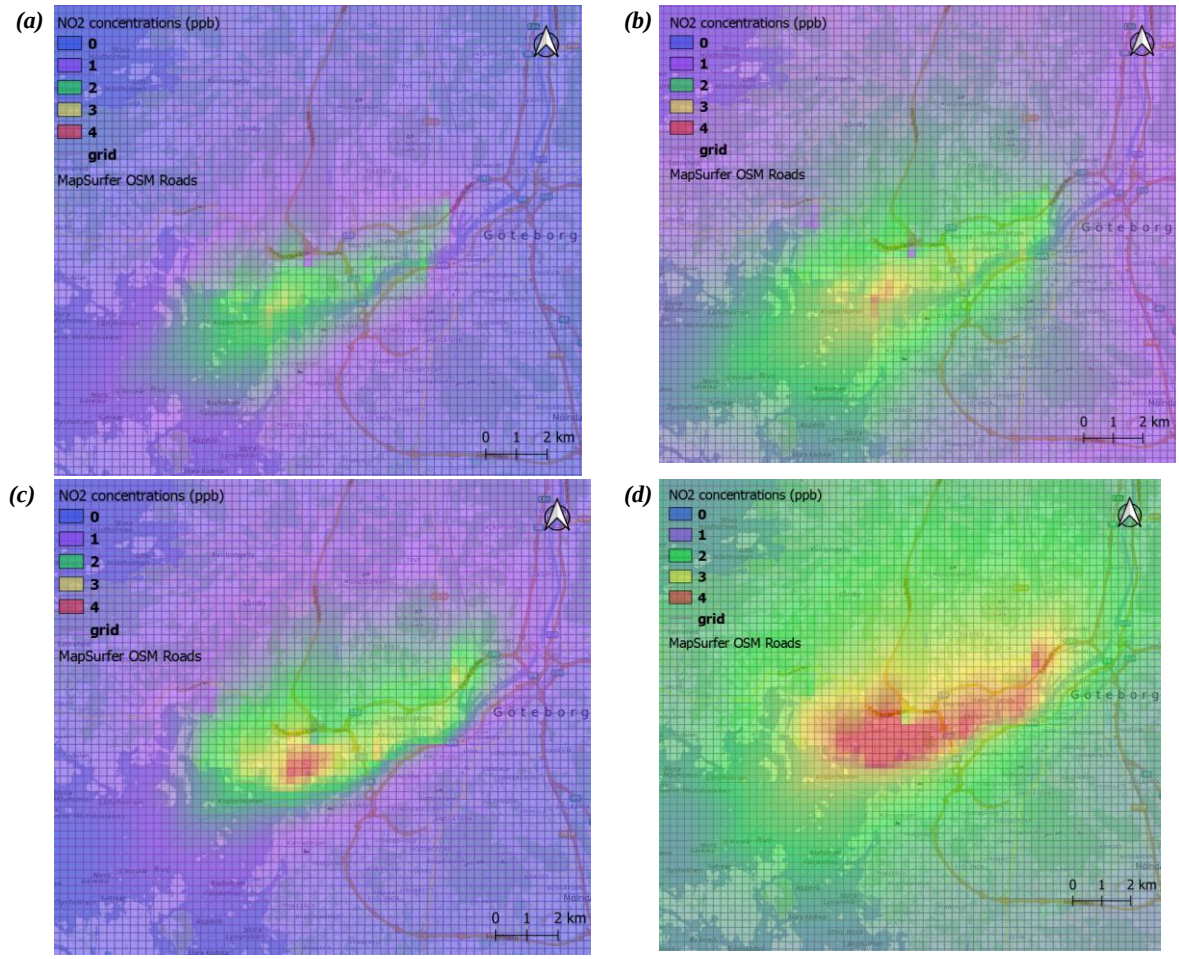


Figure S4: Contributions of shipping to air concentration of NO_2 (ppb) as mean of winter months (DJF) and summer months (JJA) in year 2012: (a) Local shipping contribution in winter; (b) Local and regional shipping contributions in winter; (c) Local shipping contribution in summer; (d) Local and regional shipping contributions in summer. Base map credits: © OpenStreetMap contributors (openstreetmap.org). Distributed under a Creative Commons BY-SA License.

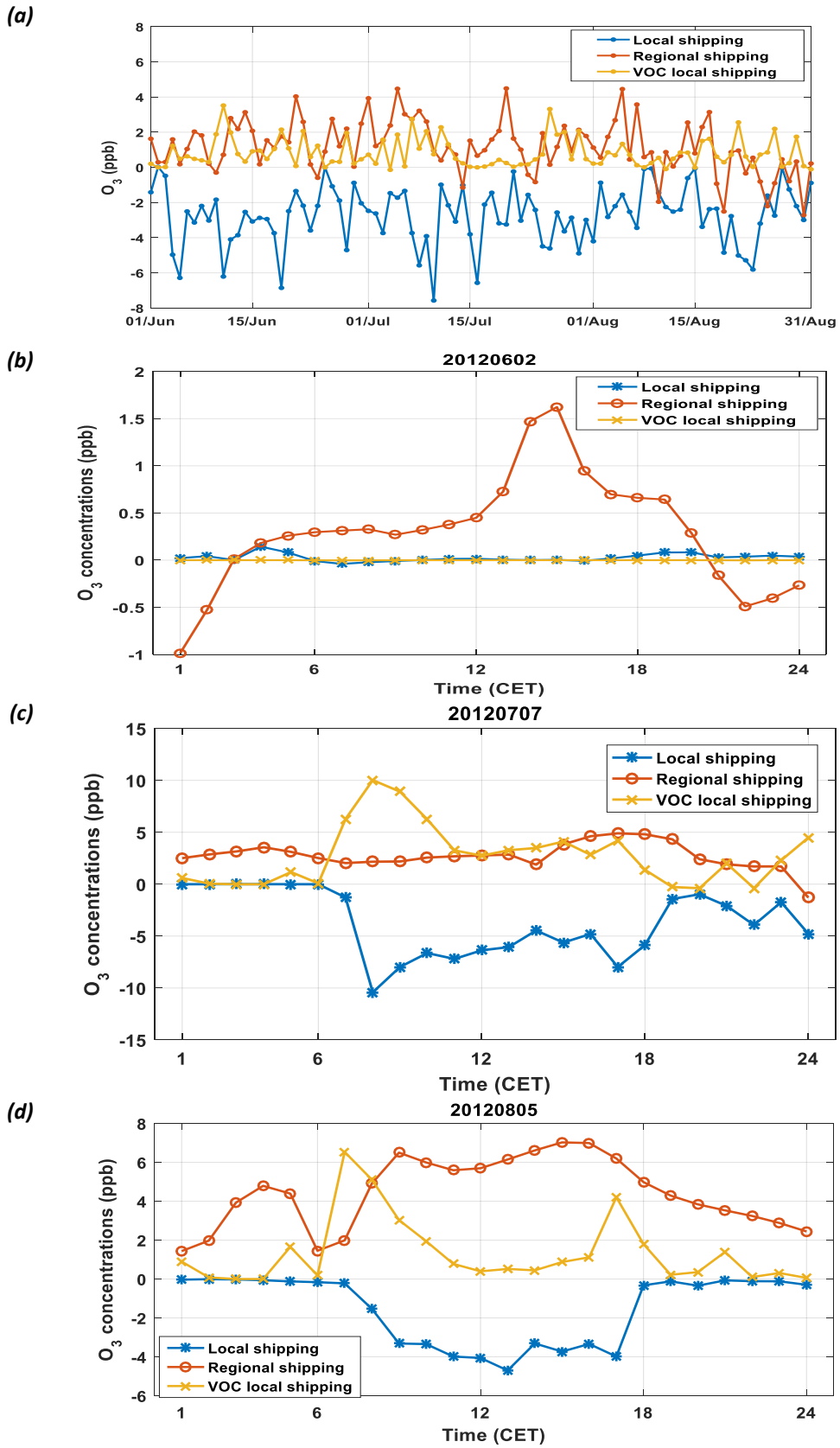


Figure S5: (a) Modelled daily mean contributions to ozone concentrations from local shipping, regional shipping and VOCs emissions from local shipping at Eriksberg in summer (JJA) 2012. (b)–(d) Diurnal variation of the contributions to ozone concentration in panel (a) on selected days: (b) 2 June 2012; (c) 7 July 2012 and (d) 5 August 2012.

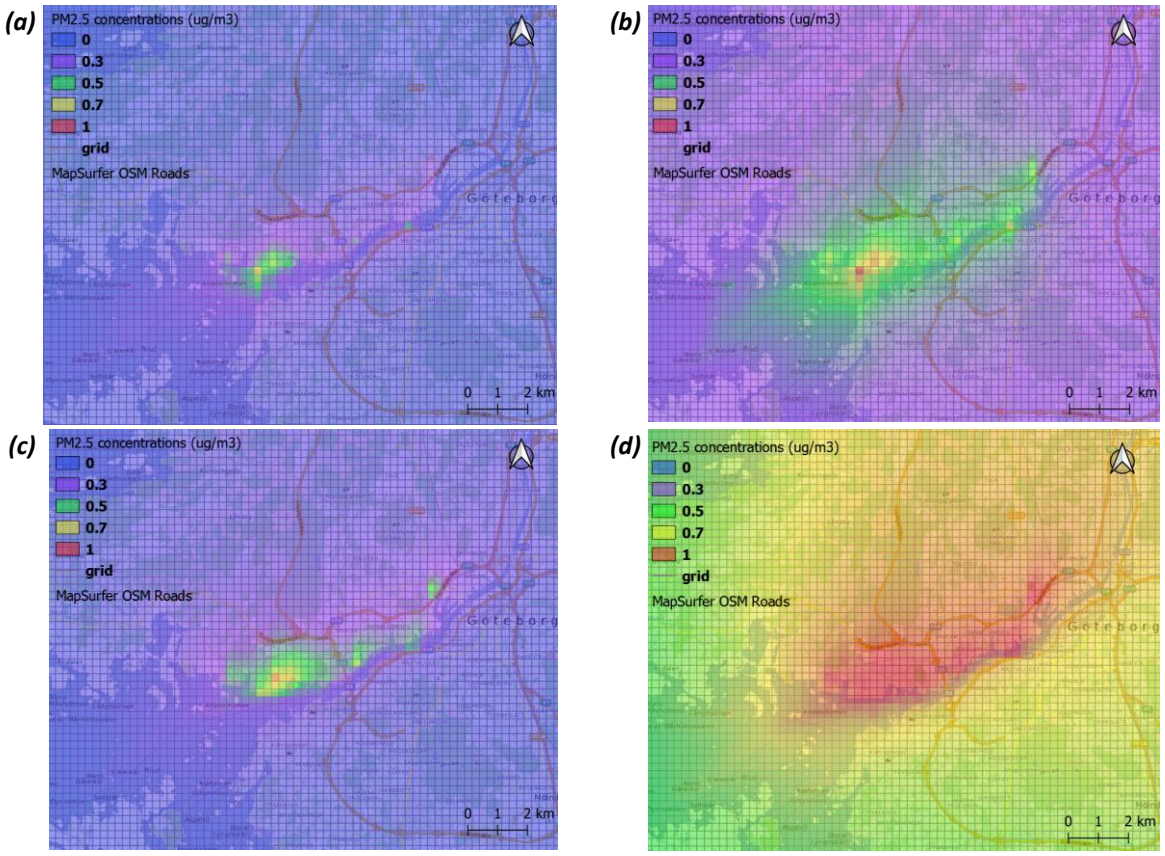


Figure S6: Contributions of shipping to air concentration of $PM_{2.5}$ (µg m^{-3}) as mean of winter months (DJF) and summer months (JJA) in year 2012: (a) Local shipping contribution in winter; (b) Local and regional shipping contributions in winter; (c) Local shipping contribution in summer; (d) Local and regional shipping contributions in summer. Base map credits: © OpenStreetMap contributors (openstreetmap.org). Distributed under a Creative Commons BY-SA License.

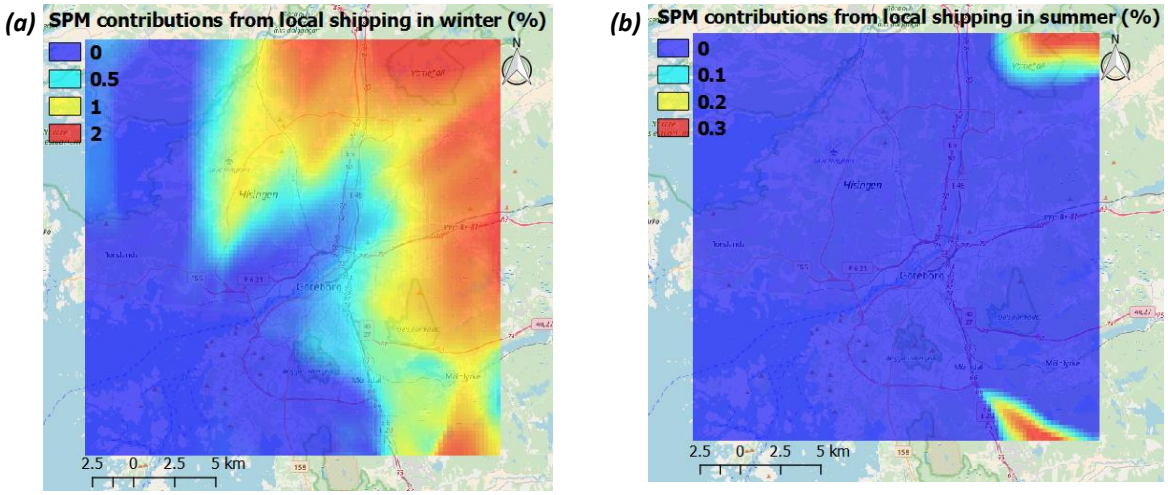


Figure S7: The contributions (%) of secondary particulate matter (SPM) from local shipping emissions corresponding to $PM_{2.5}$ concentrations in (a) winter and (b) summer. Base map credits: © OpenStreetMap contributors (openstreetmap.org). Distributed under a Creative Commons BY-SA License.

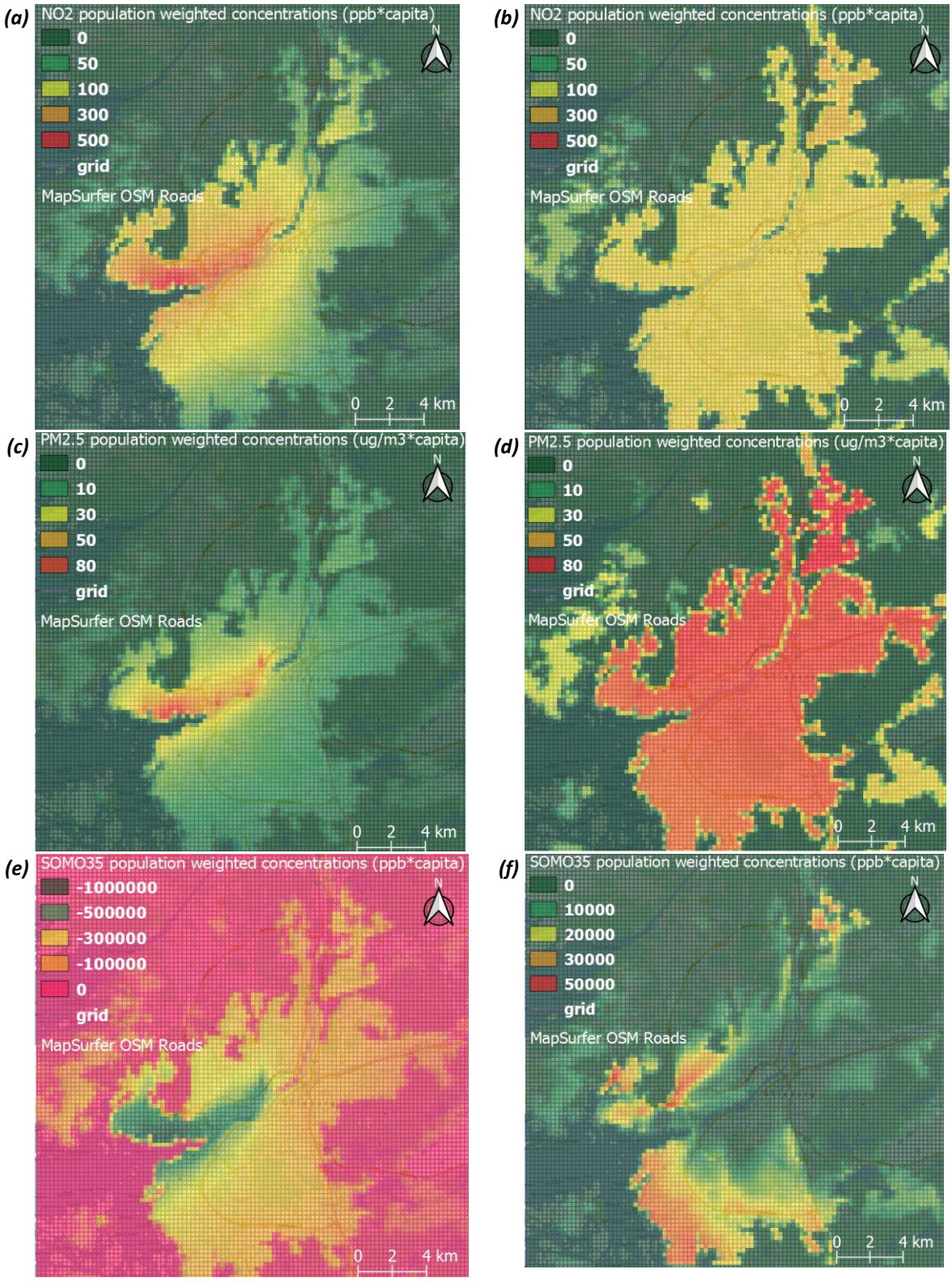


Figure S8: The annual average population weighted concentrations for NO_2 (ppb × capita), $PM_{2.5}$ (μg m^{-3} × capita) and SOMO35 (ppb × h × capita): (a) NO_2 from local shipping; (b) NO_2 from regional shipping; (c) $PM_{2.5}$ from local shipping; (d) $PM_{2.5}$ from regional shipping; (e) SOMO35 from local shipping; (f) SOMO35 from regional shipping. Base map credits: © OpenStreetMap contributors (openstreetmap.org). Distributed under a Creative Commons BY-SA License.