

1 **Supplementary material**

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3 Table S1: Parameters used for the size resolved anthropogenic primary particle  
 4 emissions. Since the particle number size distribution properties and chemical  
 5 properties were found in different studies, the exact size resolved chemical  
 6 composition used in this study will not be identical with the references.

	<b>Mode 1</b>	<b>Mode 2</b>	<b>Mode 3</b>	<b>Mode 4</b>	<b>Mode 5</b>
<b>Dp road (nm)</b>	3.0 <sup>a</sup>	20.0 <sup>a</sup>	77.0 <sup>a</sup>	-	-
<b><math>\sigma</math> road</b>	1.25 <sup>a</sup>	1.9 <sup>a</sup>	1.75 <sup>a</sup>	-	-
<b><math>N_{mode\ i}/N_{tot}</math> road</b>	0.02 <sup>a</sup>	0.90 <sup>a</sup>	0.08 <sup>a</sup>	-	-
<b>EC fraction road</b>	0 <sup>b</sup>	0.2 <sup>b</sup>	0.64 <sup>b</sup>	-	-
<b>POA fraction road</b>	1 <sup>b</sup>	0.8 <sup>b</sup>	0.27 <sup>b</sup>	-	-
<b>Mineral fraction road</b>	0	0	0.09	-	-
<b>Dp ship (nm)</b>	14.0 <sup>c</sup>	90.0 <sup>c</sup>	-	-	-
<b><math>\sigma</math> ship</b>	1.45 <sup>c</sup>	1.52 <sup>c</sup>	-	-	-
<b><math>N_{mode\ i}/N_{tot}</math> ship</b>	0.438 <sup>c</sup>	0.562 <sup>c</sup>	-	-	-
<b>EC fraction ship</b>	0 <sup>d</sup>	0.52 <sup>d</sup>	-	-	-
<b>POA fraction ship</b>	1 <sup>d</sup>	0.08 <sup>d</sup>	-	-	-
<b>Mineral fraction ship</b>	0	0.4	-	-	-
<b>Dp wood (nm)</b>	7.7 <sup>e</sup>	23.8 <sup>e</sup>	64.2 <sup>e</sup>	150.0 <sup>e</sup>	530.0 <sup>e</sup>
<b><math>\sigma</math> wood</b>	1.26 <sup>e</sup>	1.49 <sup>e</sup>	1.50 <sup>e</sup>	1.60 <sup>e</sup>	1.30 <sup>e</sup>
<b><math>N_{mode\ i}/N_{tot}</math> wood</b>	0.032 <sup>e</sup>	0.241 <sup>e</sup>	0.497 <sup>e</sup>	0.227 <sup>e</sup>	0.003 <sup>e</sup>
<b>EC fraction wood</b>	0	0	0.025 <sup>f</sup>	0.025 <sup>f</sup>	0.025 <sup>f</sup>
<b>POA fraction wood</b>	1	1	0.96 <sup>f</sup>	0.96 <sup>f</sup>	0.96 <sup>f</sup>
<b>Mineral fraction wood</b>	0	0	0.015	0.015	0.015

7 <sup>a</sup>Value from Kristensson et al. (2004) for LDV at 70 km/h, <sup>b</sup>Values estimated from data in Pohjola et al.  
 8 (2007), <sup>c</sup>Values from Petzold et al. (2008), <sup>d</sup>Values estimated from data in Moldanová et al. (2009),  
 9 <sup>e</sup>Values from Kristensson (2005), <sup>f</sup>Values from Schauer et al. (2001).

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1 Table S2. Parameters used to calculate temperature dependent aerosol yields for  
 2 oxidation products of different organic compounds.

<b>Org. comp.</b>	<b>Ox. Agent</b>	$\alpha_1$	$\alpha_2$	$K_{om,1}$ ( $m^3/\mu g$ )	$K_{om,2}$ ( $m^3/\mu g$ )	$\Delta H_1$ ( $kJ/mol$ )	$\Delta H_2$ ( $kJ/mol$ )	$T_{ref,1}$ ( <b>K</b> )	$T_{ref,2}$ ( <b>K</b> )
$\alpha$ -pinene	OH	0.5 <sup>a</sup>	-	0.02 <sup>a</sup>	-	40 <sup>a</sup>	-	320 <sup>a</sup>	-
	O <sub>3</sub>	0.08 <sup>a</sup>	0.42 <sup>a</sup>	0.5 <sup>a</sup>	0.005 <sup>a</sup>	100 <sup>a</sup>	38 <sup>a</sup>	310 <sup>a</sup>	310 <sup>a</sup>
	NO <sub>3</sub>	0.1 <sup>a</sup>	-	0.02 <sup>a</sup>	-	40 <sup>a</sup>	-	310 <sup>a</sup>	-
$\beta$ -pinene	OH	1.0 <sup>a</sup>	-	0.02 <sup>a</sup>	-	60 <sup>a</sup>	-	310 <sup>a</sup>	-
	O <sub>3</sub>	0.03 <sup>a</sup>	0.38 <sup>a</sup>	0.5 <sup>a</sup>	0.005 <sup>a</sup>	100 <sup>a</sup>	40 <sup>a</sup>	310 <sup>a</sup>	300 <sup>a</sup>
	NO <sub>3</sub>	1.0 <sup>b</sup>	-	0.0163 <sup>b</sup>	-	60 <sup>b</sup>	-	~310 <sup>b</sup>	-
$\Delta^3$ - carene	OH	0.054 <sup>b</sup>	0.517 <sup>b</sup>	0.043 <sup>b</sup>	0.0042 <sup>b</sup>	100 <sup>c</sup>	40 <sup>c</sup>	~310 <sup>b</sup>	~310 <sup>b</sup>
	O <sub>3</sub>	0.128 <sup>b</sup>	0.068 <sup>b</sup>	0.337 <sup>b</sup>	0.0036 <sup>b</sup>	100 <sup>c</sup>	40 <sup>c</sup>	~310 <sup>b</sup>	~310 <sup>b</sup>
	NO <sub>3</sub>	0.743 <sup>b</sup>	0.257 <sup>b</sup>	0.0088 <sup>b</sup>	0.0091 <sup>b</sup>	80 <sup>c</sup>	40 <sup>c</sup>	~310 <sup>b</sup>	~310 <sup>b</sup>
D- limonene	OH	0.239 <sup>b</sup>	0.363 <sup>b</sup>	0.055 <sup>b</sup>	0.0053 <sup>b</sup>	100 <sup>c</sup>	40 <sup>c</sup>	~310 <sup>b</sup>	~310 <sup>b</sup>
	O <sub>3</sub>	0.03 <sup>c</sup>	0.38 <sup>c</sup>	0.055 <sup>c</sup>	0.0053 <sup>c</sup>	40 <sup>c</sup>	100 <sup>c</sup>	~310 <sup>b</sup>	~310 <sup>b</sup>
	NO <sub>3</sub>	1.0 <sup>c</sup>	-	0.055 <sup>c</sup>	-	80 <sup>c</sup>	80 <sup>c</sup>	~310 <sup>b</sup>	~310 <sup>b</sup>
Isoprene	OH	0.232 <sup>d</sup>	0.0288 <sup>d</sup>	0.00862 <sup>d</sup>	1.62 <sup>d</sup>	-	-	-	-
	O <sub>3</sub>	0.232 <sup>d</sup>	0.0288 <sup>d</sup>	0.00862 <sup>d</sup>	1.62 <sup>d</sup>	-	-	-	-
	NO <sub>3</sub>	0.232 <sup>d</sup>	0.0288 <sup>d</sup>	0.00862 <sup>d</sup>	1.62 <sup>d</sup>	-	-	-	-
Benzene	OH+NO	0.072 <sup>e</sup>	0.888 <sup>e</sup>	3.315 <sup>e</sup>	0.0090 <sup>e</sup>	40 <sup>c</sup>	40 <sup>c</sup>	300 <sup>c</sup>	300 <sup>c</sup>
	OH+HO <sub>2</sub>	0.37 <sup>e</sup>	-	-	-	-	-	-	-
Toluene	OH+ NO	0.095 <sup>a</sup>	0.20 <sup>a</sup>	0.5 <sup>a</sup>	0.005 <sup>a</sup>	40 <sup>a</sup>	40 <sup>a</sup>	300 <sup>a</sup>	300 <sup>a</sup>
	OH+HO <sub>2</sub>	0.36 <sup>e</sup>	-	-	-	-	-	-	-
Xylene	OH+NO	0.044 <sup>a</sup>	0.15 <sup>a</sup>	0.5 <sup>a</sup>	0.005 <sup>a</sup>	60 <sup>a</sup>	60 <sup>a</sup>	300 <sup>a</sup>	300 <sup>a</sup>
	OH+HO <sub>2</sub>	0.30 <sup>e</sup>	-	-	-	-	-	-	-

3 <sup>a</sup>Values from Svendby et al., 2008, <sup>b</sup>Values from Griffin et al., 1999, <sup>c</sup>Estimated values for this work,

4 <sup>d</sup>Values from Henze and Seinfeld, 2006, <sup>e</sup>Values from Ng et al., 2007

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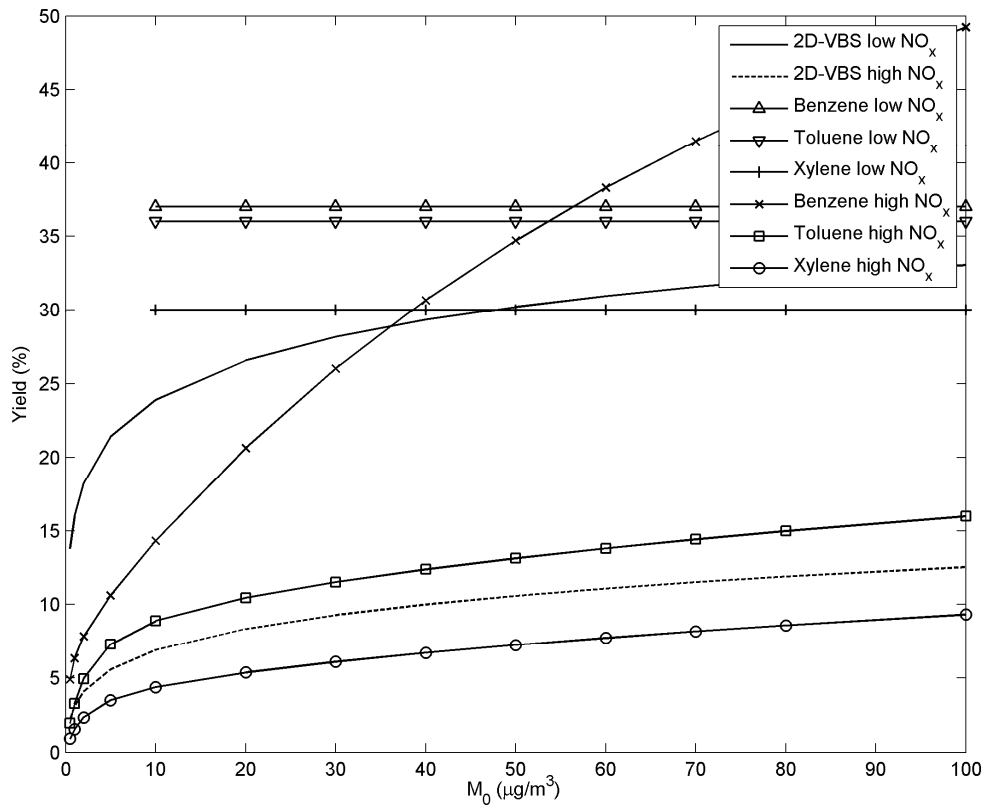
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1 Table S3. Emission fractions of existing non-volatile POA emissions if treating the  
 2 POA as semi-volatile and including IVOC emissions.

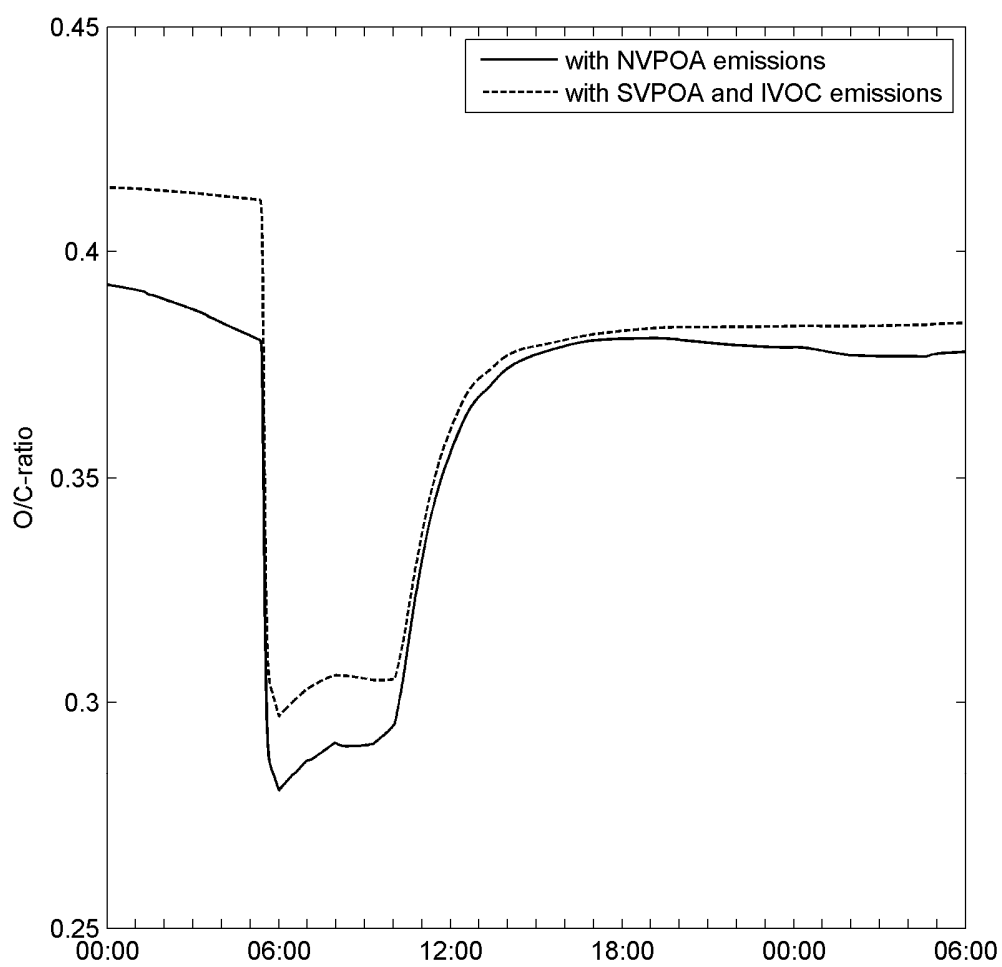
C* at 298 K ( $\mu\text{g}/\text{m}^3$ )	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$	$10^3$	$10^4$	$10^5$	$10^6$
Emission fractions <sup>a</sup> SVPOA	0.03	0.06	0.09	0.14	0.18	0.30	0.20	0.50	0.80
Emission fractions <sup>a</sup> IVOCs	0	0	0	0	0	0	0.20	0.50	0.80

3 <sup>a</sup>Mass ratio to existing EMEP POA emissions, values adopted from Robinson et al. (2007), Shrivastava  
 4 et al. (2008) and Tsimpidi et al. (2010).

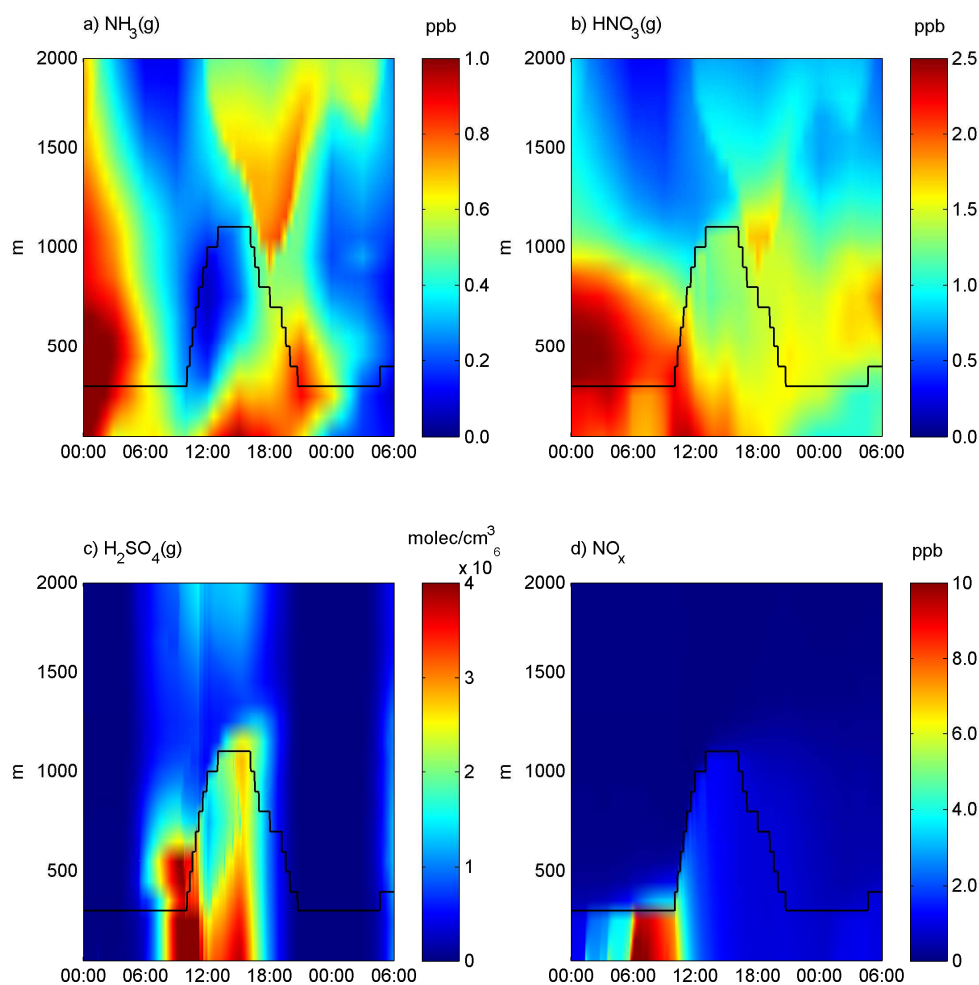
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 2 Figure S1. SOA Yield for benzene, toluene and xylene (BTX), at 300 K, at high  $\text{NO}_x$   
 3 and low  $\text{NO}_x$  conditions (Ng et al., 2007) and BTX SOA yield at 300 K from 2D-VBS  
 4 model used in ADCHEM.  
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2 Figure S2. Modeled O/C-ratio in the center of the urban plume with non-volatile POA  
3 (NVPOA) emissions (base case) or with semi-volatile (SVPOA) and intermediate  
4 VOC (IVOC) emissions from anthropogenic sources.



1  
 2 Figure S3. Modeled ammonia (a), nitric acid (b), sulfuric acid (c) and  $\text{NO}_x$  (d), from 6  
 3 hours before Malmö (00:00) until 24 hours downwind Malmö, in vertical direction (0-  
 4 2000 m a.g.l.), in the center of the urban plume. The mixing height along the  
 5 trajectory is also displayed.

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## 7 References

- 8 Griffin R. J., Cocker III D. R., Flagan R. C., Seinfeld J. H. Organic aerosol formation  
 9 from the oxidation of biogenic hydrocarbons. *J. Geophys. Res.*, 107, D3, 3555-3567,  
 10 1999.
- 11 Henze D. K. and Seinfeld J. H. Global secondary organic aerosol from isoprene  
 12 oxidation. *Geophysical Research Letters*, 33 L09812, 2006.

- 1 Kristensson A. Johansson C., Westerholm R., Swietlicki E., Gidhagen L., Widequist  
2 U. and Vesely V. Real-world traffic emission factors of gases and particles measured  
3 in a road tunnel in Stockholm, Sweden. *Atmospheric Environment* 38, 657-673, 2004.
- 4 Kristensson A. Aerosol Particle Sources Affecting the Swedish Air Quality at Urban  
5 and Rural Level. Doctoral Dissertation at Department of Physics, Lund University.  
6 ISBN: 91-628-6573-0, 2005.
- 7 Moldanová J., Fridell E., Popovicheva O., Demirdjian B., Tishkova V., Faccinetto A.  
8 and Focsa C. Characterisation of particulate matter and gaseous emissions from a  
9 large ship diesel engine. *Atmospheric Environment*, 43, 2632-2641, 2009.
- 10 Ng N.L., Kroll J. H., Chan A. W. H., Chhabra P. S., Flagan R. C. and Seinfeld J. H.  
11 Secondary organic aerosol formation from m-xylene, toluene, and benzene.  
12 *Atmospheric Chemistry and Physics*, 7, 3909-3922, 2007.
- 13 Petzold A., Hasselbach J., Lauer P., Baumann R., Franke K., Gurk C., Schlager H.  
14 and Weingartner E. Experimental studies on particle emissions from cruising ship,  
15 their characteristic properties, transformation and atmospheric lifetime in the marine  
16 boundary layer. *Atmospheric Chemistry and Physics*, 8, 2387-2403, 2008.
- 17 Pohjola M. A., Pirjola L., Karppinen A., Härkönen J., Korhonen H., Hussein T.,  
18 Ketzler M. and Kukkonen J. Evaluation and modelling of the size fractionated aerosol  
19 particle number concentration measurements nearby a major road in Helsinki-Part I:  
20 Modelling results within the LIPIKA project. *Atmospheric Chemistry and Physics*, 7,  
21 4065-4080, 2007.
- 22 Robinson A. L., Donahue N. M., Shrivastava M. K., Weitkamp E. A., Sage A. M.,  
23 Grieshop A. P., Lane T. E., Pierce J. R., Pandis S. N. Rethinking organic aerosols:  
24 Semivolatile emissions and photochemical aging. *Science*, 315, 1259-1262, 2007.
- 25 Schauer J. J., Kleeman M. J., Cass G. R. and Simoneit B. R. T. Measurement of  
26 Emissions from Air Pollution Sources. 3. C-C Organic Compounds from Fireplace  
27 Combustion of Wood. *Environmental Science and Technology*, 35, 1716-1728, 2001.
- 28 Shrivastava M. K., Lane T. E., Donahue N. M., Pandis S. N. and Robinson A. L.  
29 Effects of gas particle partitioning and aging of primary emissions on urban and

1 regional organic aerosol concentrations. *Journal of Geophysical Research*, 113,  
2 D18301, doi:10.1029/2007JD009735, 2008.

3 Svendby T. M., Lazaridis M. and Tørseth K. Temperature dependent secondary  
4 organic aerosol formation from terpenes and aromatics. *Journal of Atmospheric*  
5 *Chemistry*, 59, 25-46, 2008.

6 Tsimpidi A. P., Karydis V. A., Zavala M., Lei W., Molina L., Ulbrich I. M., Jimenez  
7 J. L. and Pandis S. N. Evaluation of the volatility basis-set approach for the simulation  
8 of organic aerosol formation in the Mexico City metropolitan area. *Atmos. Chem.*  
9 *Phys.*, 10, 525–546, 2010.