

Supplementary Information:

Potential reductions in ambient NO₂ concentrations from meeting diesel vehicle emissions standards

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S1. Model Simulations

S1.1. European simulations

The setup for the European simulation has been described in Mar et al. (2016) with a small number of changes, described here. The horizontal resolution was 22.5 km x 22.5 km; the model domain had 230 and 186 grid points in the west-east and south-north directions, respectively. Given the short duration of the simulation, no four-dimensional data assimilation was applied. Emissions for the base simulation were taken from the TNO-MACCI3 inventory for 2011 and prepared as described in Mar et al. (2016), except that all emissions were emitted at the surface rather than into higher vertical levels, as the model results for this setup showed little sensitivity to the distribution of emissions above the surface layer (see Mar et al, 2016). For the US EPA scenario, NO_x emissions were calculated as described in Section 2.4, namely, the reduction factor for going from HBEFA to US EPA emission factors for LDVs was applied to diesel exhaust emissions for road transport based on the ratio of LDVs to LDVs+HDVs for each country (Kuenen, 2015). Application of these diesel LDV emission reductions led to a reduction of domain-total NO_x emissions of 12% for the US EPA scenario compared to the base scenario. WRF-Chem simulations were performed using both the MOZART-4 and RADM2 gas-phase chemical mechanisms. In the text results from the simulations done with the RADM2-mechanism are discussed to parallel the Berlin simulations. Results from both mechanisms are presented in Table 3.

S1.2. Berlin simulations

The setup focusing on the greater Berlin area is described in Kuik et al., (2016), and uses the same settings as the European simulations, limited to the RADM2 chemical mechanism. The setup has three nested domains with 15 km x 15 km, 3 km x 3 km and 1 km x 1 km horizontal resolution. The coarsest domain covers large parts of Europe, but only the results from the 1 km x 1 km domain covering the greater Berlin area are discussed here. Results at this resolution should be considered representative of the urban background environment for urban areas. A consistency check showed that the results from the 15 km x 15 km domain are consistent with the results obtained with the European simulation setup. As the setup is focused on the urban area of Berlin, it includes three urban land use classes as well as updated input parameters to the urban scheme (Kuik et al., 2016). In order to match the resolution of the emission input data with the model resolution, the emissions for Berlin were downscaled to a horizontal resolution of ca. 1 km as described in Kuik et al., (2016). In addition, the emissions were distributed vertically into seven model layers. The setup mainly covers Germany and thus the fraction of diesel LDV in Germany (43%) has been used in the US EPA scenario simulation.

Table S1. Summary of WRF-Chem model simulations for the European simulation and the Berlin simulation.

	European simulations	Berlin simulations
Main reference	Mar et al., 2016	Kuik et al., 2016
Chemical mechanism	MOZART and RADM2	RADM2
Horizontal resolution	22.5 km x 22.5 km	15 km x 15 km 3 km x 3 km 1 km x 1 km
Emissions	TNO-MACC III (7 km x 7 km hor. res.) No vertical distribution	TNO-MACC III (7 km x 7 km hor. res.) Distributed vertically into 7 model layers Downscaled to 1 km x 1 km over 1 km x 1 km domain
EPA scenario emissions	Using country-specific LDV/HDV ratios (TNO – add reference)	Using LDV/HDV ratio for Germany (TNO – add reference)
Urban processes		Single-layer urban canopy model with modified input parameters (Kuik et al., 2016) 3 urban land use categories
Further changes with respect to main reference	No FDDA applied	Using physics options of Mar et al., 2016

Table S2. Comparison of modeled (Berlin simulation, 1km x 1km resolution) and measured surface NO₂ concentrations. The statistics include the mean bias and normalized mean bias over the whole month of July 2011, as well as the correlation coefficient (R) of daily mean NO₂ concentrations. FAC2 denotes the fraction of modeled concentrations within a factor of 2 of the observations.

Station	Code	Mean bias (ug/m3)	Normalized mean bias (%)	R	FAC2 (%)
Urban background					
Amrumer Str.	DEBE010	-6.1	-31	0.63	77
Belziger Straße	DEBE018	-4.1	-23	0.74	90
Brückenstraße	DEBE068	-5.5	-28	0.44	80
Johanna und Willi Brauer Platz	DEBE066	-3.4	-25	0.06	80
Nansenstraße	DEBE034	-6.5	-30	0.56	84
Suburban/rural background					
Buch	DEBE051	-0.05	-1	0.56	77
Grunewald	DEBE032	0.4	6	0.50	90
Müggelseedamm	DEBE056	-0.2	-3	0.13	87
Frohnau	DEBE062	-0.4	-5	0.44	71

S2. Observation-based calculations

Table S3. Estimated reduction in ambient concentrations of daily mean NO₂ at the roadside and for the urban background of Berlin from the observation-based calculations. Estimates for both the national and city level fraction of LDV diesel are included. Values are (top) monthly average daily mean values and (bottom) annual average daily mean values, both with standard deviation. All units are in µg m⁻³.

	National fleet (43% LDV)		City fleet (80% LDV)	
	Roadside	Urban background	Roadside	Urban background
Monthly Average (July)				
Euro 5	10 ± 2.5	1.3 ± 0.43	19 ± 4.6	2.3 ± 0.80
Euro 6 (conformity factor, Sept 2017)	11 ± 2.5	1.3 ± 0.44	20 ± 4.6	2.4 ± 0.81
Euro 6	12 ± 2.9	1.5 ± 0.50	23 ± 5.3	2.7 ± 0.94
US EPA	14 ± 3.3	1.6 ± 0.53	26 ± 6.2	2.9 ± 0.99
Monthly Average (January)				
Euro 5	8.3 ± 2.3	0.94 ± 0.49	15 ± 4.3	1.7 ± 0.92
US EPA	11 ± 3.1	1.1 ± 0.60	21 ± 5.8	2.1 ± 1.1
Annual Average				
Euro 5	9.0 ± 2.8	1.2 ± 0.65	17 ± 5.2	2.2 ± 1.2
Euro 6 (conformity factor, Sept 2017)	9.1 ± 2.8	1.2 ± 0.66	17 ± 5.2	2.2 ± 1.2
Euro 6	11 ± 3.2	1.4 ± 0.76	20 ± 6.0	2.6 ± 1.4
US EPA	12 ± 3.8	1.5 ± 0.80	23 ± 7.0	2.7 ± 1.5

Table S4. The relationship between NO₂ and NO_x concentrations. The slope of the linear fit (NO₂:NO_x) and r² values are provided.

	Site type	Slope	r ²
Annual		0.35	0.88
July	traffic	0.48	0.94
January		0.31	0.90
Annual	urban	0.55	0.85
July	background	0.82	0.98
January		0.56	0.89

Figure S1. Hourly NO_x versus NO₂ concentrations in $\mu\text{g m}^{-3}$ by site type for July 2014. Station names are listed in the legend. Linear fits to the lines shown are included in Table S4.

