

S1. Derivation of the concentration fields

Although the wind direction was randomised in the meteorological data used in short-range dispersion modelling, the resulting concentration fields were not symmetrical due to the influence of short-term events such as very stable periods. In order to obtain generic concentration fields that can be used in the sub-grid model, this asymmetry was removed by fitting polynomial regression curves, of the form $ax^3 + bx^2 + cx + d$, to the modelled concentrations (natural log of concentrations vs. natural log of distance (m) from source centre), as shown in Figure A2.1. For each source height, the mean value of the predictions from all regression curves was used to calculate the concentration fields used in the sub-grid model (Table A2.1).

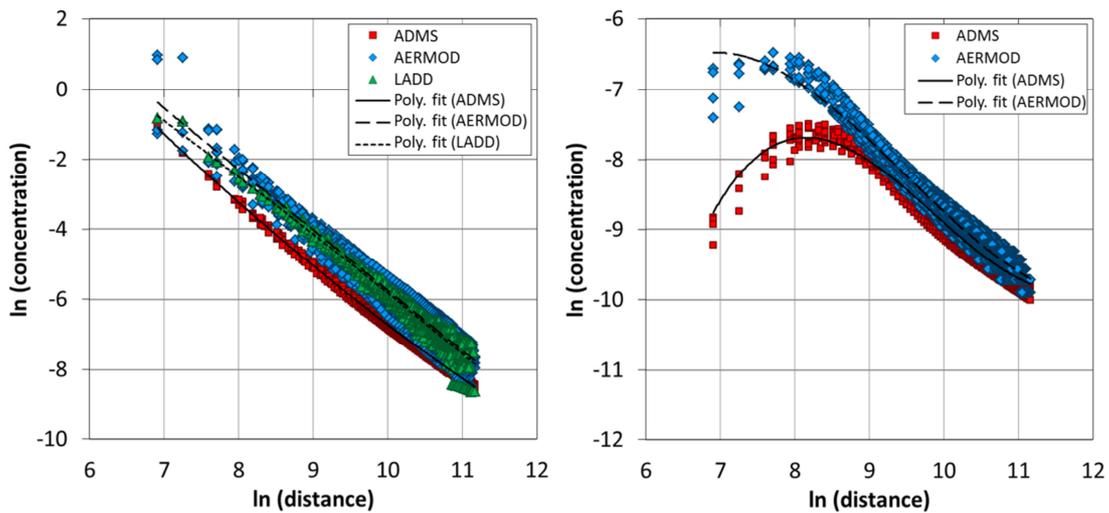


Figure S1.1: Natural log of modelled concentration plotted against the natural log of distance from source centre for a ground level source (left) and a 400 m high stack source (right).

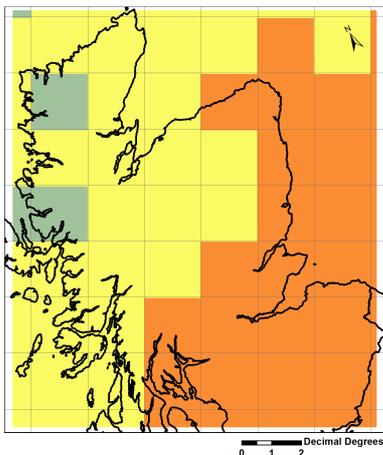
Table S1.1: Regression coefficients of the polynomial fits (of the form: $ax^3 + bx^2 + cx + d$) to the natural log of modelled concentration vs. the natural log of distance (m) from the source centre for all source heights and models.

Emission height: 0 m					
Model	a	b	c	d	Value for emission square
ADMS	--	-0.0356	-0.964	7.46	1.69
AERMOD	--	0.0747	-3.08	16.6	0.864
LADD	--	-0.0189	-1.32	9.28	1.32
Mean model	--	--	-1.67	10.7	1.34
Emission height: 25 m					
Model	a	b	c	d	Value for emission square
ADMS	-0.0192	0.573	-7.03	25.5	-0.895
AERMOD	-0.0261	0.602	-5.56	15.9	-1.88
Mean model	-0.0295	0.754	-7.58	23.8	-1.27
Emission height: 50 m					
Model	a	b	c	d	Value for emission square
ADMS	0.0109	-0.294	1.28	-1.40	-2.35
AERMOD	-0.0241	0.692	-7.56	24.1	-3.02
Mean model	-0.0105	0.318	-4.31	15.1	-2.63
Emission height: 100 m					
Model	a	b	c	d	Value for emission square
ADMS	0.00850	-0.259	1.49	-4.84	-4.45
AERMOD	-0.0213	0.572	-6.00	16.8	-4.02
Mean model	-0.00610	0.149	-2.22	5.96	-4.22
Emission height: 200 m					
Model	a	b	c	d	Value for emission square
ADMS	0.0283	-0.813	6.85	-23.5	-6.88
AERMOD	-0.0290	0.885	-9.80	30.3	-5.39
Mean model	-0.00150	0.0705	-1.82	4.58	-5.88
Emission height: 400 m					
Model	a	b	c	d	Value for emission square
ADMS	0.108	-3.20	30.6	-103	-12.7
AERMOD	0.0532	-1.52	13.4	-44.0	-7.21
Mean model	0.0666	-1.93	17.7	-59.3	-7.90
Emission height: 800 m					
Model	a	b	c	d	Value for emission square
ADMS	0.189	-6.00	62.7	-225	-51.0
AERMOD	0.109	-3.30	32.3	-111	-9.90
Mean model	0.0900	-2.81	28.2	-101	-10.6

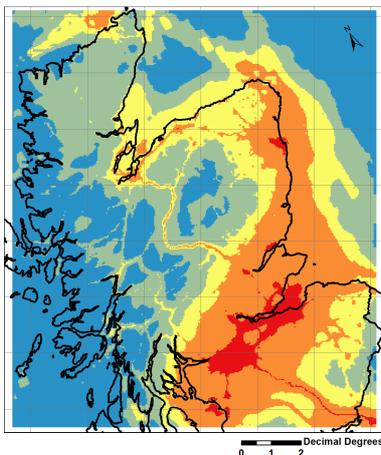
S2. Converting “sub-grid distributions” to “sub-grid concentrations”

Example: Annual mean NO₂ concentrations for the central Scotland domain

Starting datasets:



EMEP annual mean NO₂
concentration (50 × 50 km²)



Sub-grid annual mean NO₂
distribution (1 × 1 km²)

Process flowchart

