Supplement of Atmos. Chem. Phys., 16, 15327–15345, 2016
http://www.atmos-chem-phys.net/16/15327/2016/
doi:10.5194/acp-16-15327-2016-supplement

Atmospheric Chemistry and Physics Open Access EGU

Supplement of

Evaluation of gas-particle partitioning in a regional air quality model for organic pollutants

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Contents

1 Table S1. Summary of atmospheric processes and other features incorporated in recent regional scale modelling studies of POPs.

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Reference	Galarneau[1]	Silibello[2]	Aulinger[3]	San Jose[4]	Inomata[5]	Matthias[6] Bieser[9]	Meng[7]	Cooter[8]
Model Name	AURAMS	FARM	CMAQ	CMAQ	RAQM	CMAQ	CMAQ	CMAQ
Domain	USA & Canada	Italy	Europe	Spain	N.E. Asia	Europe	USA	NE USA
Compound(s)	PAHs (BaP)	BaP	BaP	BaP	PAHs (BaP)	BaP	PCBs PCDD/Fs	Atrazine
Gas-phase reaction	Yes (Off-line)	Yes (SAPRC99)	Yes (CB4)	No (inert)	Yes	Yes (CB4)	Yes (CB4)	Yes (CB4)
Adsorption model (J-P)	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Aerosol water dissolution	No	Yes	Yes	No	No	Yes	No	Yes
Absorption to OM	Yes	Yes	Yes	No	No	Yes	Yes	Yes
Adsorption to EC/BC	Yes	No	No	No	No	No	No	No
Heterogeneous chemistry (e.g. O_3 reaction)	No	No	No	Yes	No	Yes	No	No

[1]Galarneau et al., 2014; [2]Silibello et al., 2012; [3]Aulinger et al., 2007; [4]San José et al., 2013; [5]Inomata et al., 2012; [6]Matthias et al., 2009; [7]Meng et al., 2007; [8]Cooter and Hutzell, 2002; [9]Bieser et al., 2012

Table S2. Detailed information about the BaP concentration and deposition measurement stations operated by EMEP during 2006.

Code	Country	Station	Latitude (°N)	Longitude (°E)	Altitude (m)	Concentration sampling	Deposition sampling
CZ0003R	Czech Republic	Kosetice	49.58	15.08	534	1 day per week, air+aerosol	1 day per week, wet deposition
ES0008R	Spain	Niembro	43.44	-4.85	134	1 day per week, air+aerosol	NA
FI0036R	Finland	Pallas	68	24.24	340	1 week per month, air+aerosol	1 week per month, precip+dry deposition
LV0010R	Latvia	Rucava	56.16	21.17	18	Monthly, aerosol	NA
LV0016R	Latvia	Zoseni	57.14	25.91	188	Monthly, aerosol	NA
SE0012R	Sweden	Aspvreten	58.8	17.38	20	1 week per month, air+aerosol	Monthly (4wk), precip+dry deposition
SE0014R	Sweden	Råö	57.39	11.91	5	2 week per month, air+aerosol	Monthly (4wk), precip+dry deposition
GB0014R	U.K.	High Muffles	54.33	-0.81	267	3 months per yr, ads_tube	NA
DE0009R	Germany	Zingst	54.43	12.73	1	NA	Monthly (4wk), wet deposition
DE0001R	Germany	Westerland	54.93	8.31	12	NA	Monthly (4wk), wet deposition

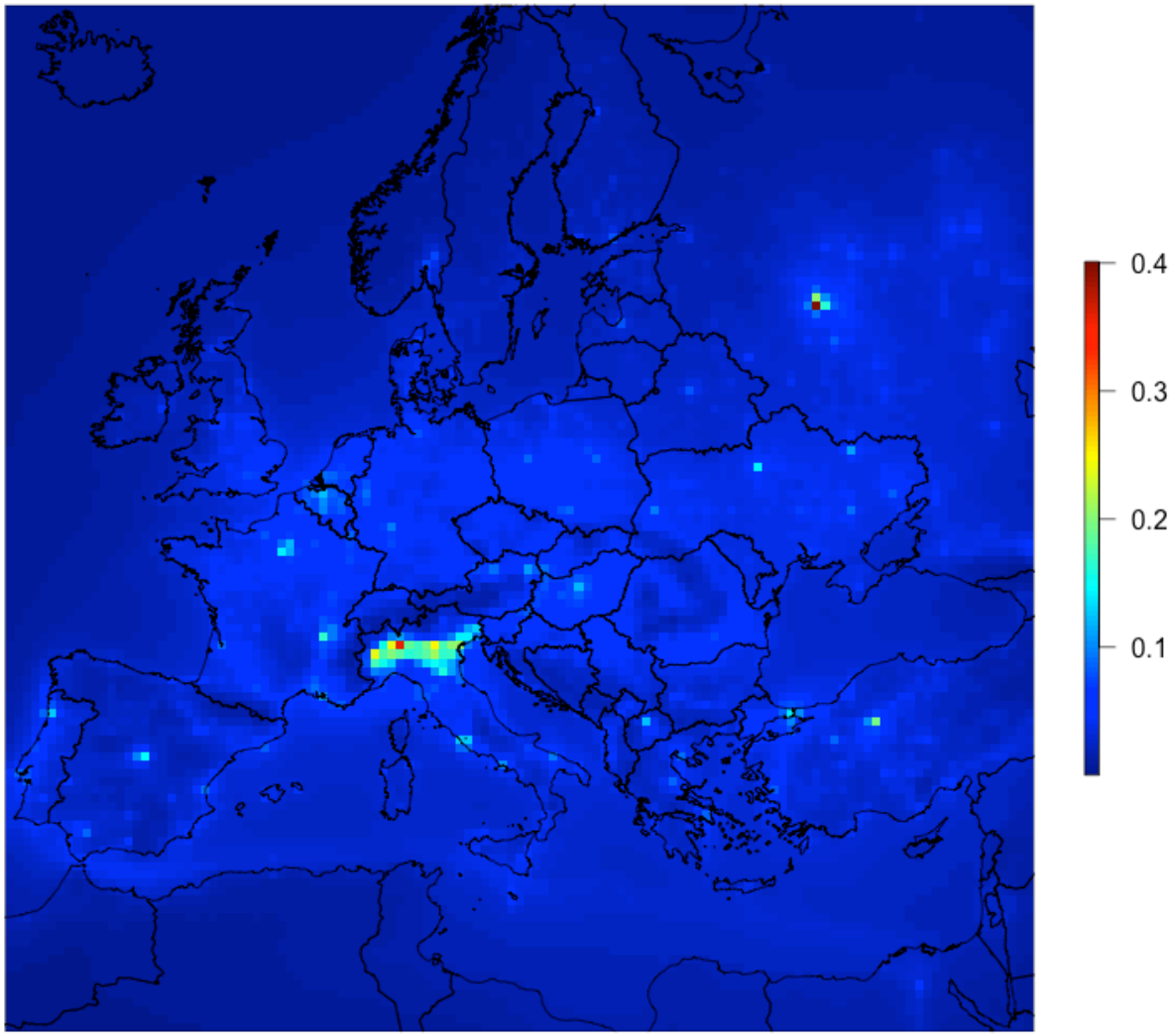

Figure S3. Annual average total elemental carbon (EC) concentrations (μg m^{-3}) calculated at the level of the surface layer by WRF-CMAQ-BaP during 2006.

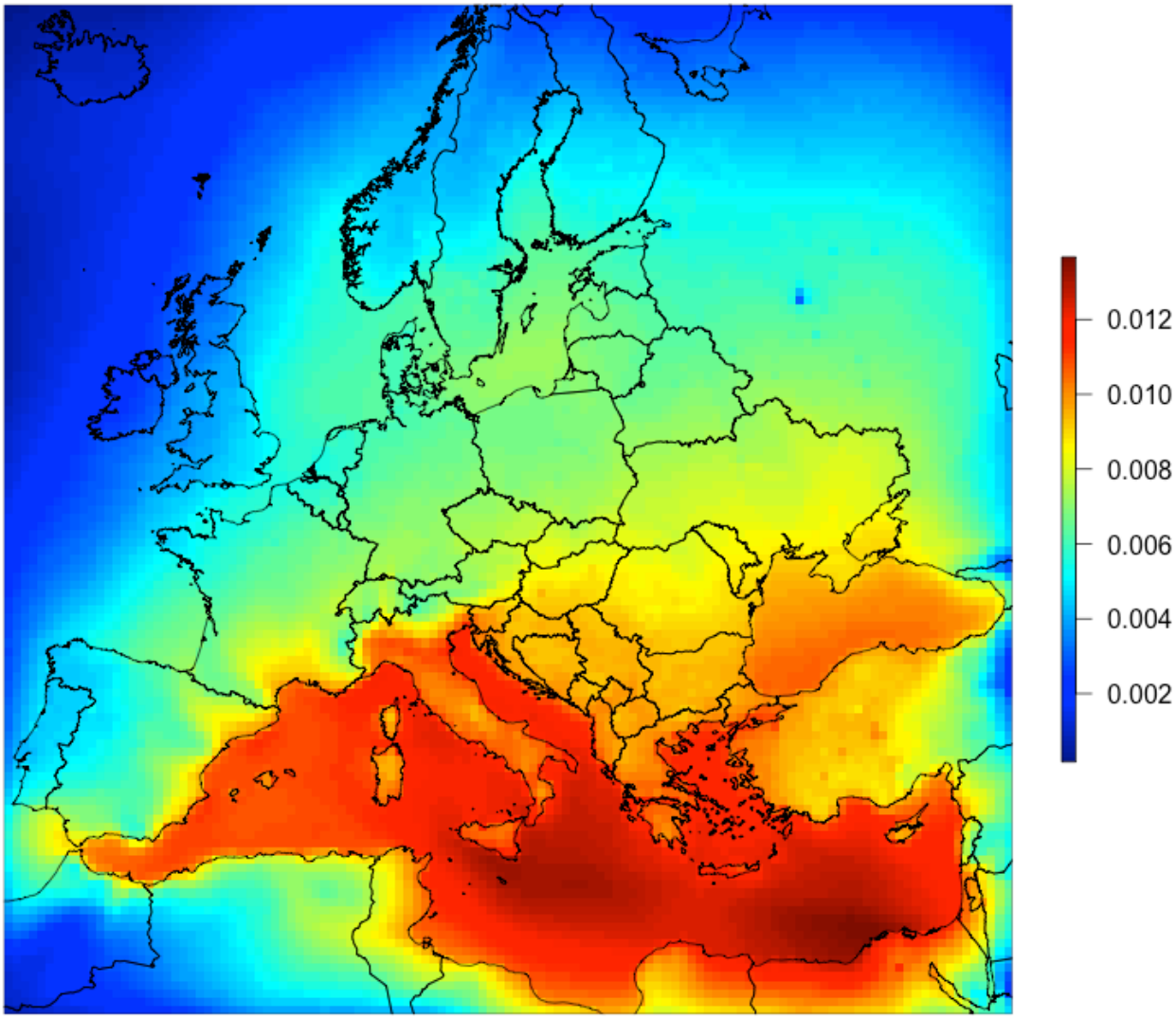

Figure S4. Annual average ozone concentrations (ppmV) calculated at the level of the surface layer by WRF-CMAQ-BaP during 2006.

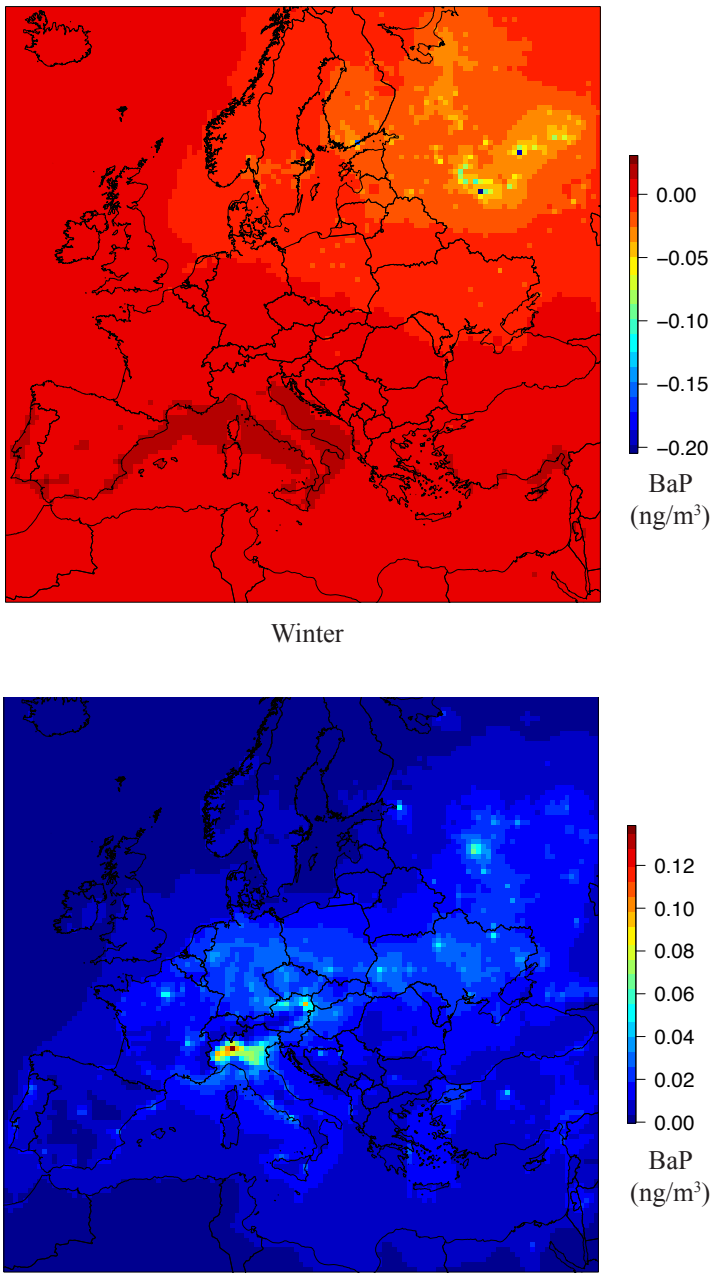

Figure S5. Seasonal differences in average surface-level BaP concentrations simulated by the dual GPP model (scenario 4) between the typical K_{oa} estimates based on K_{ow} (Beyer, 2000), minus the semi-logarithmic temperature-dependent form proposed by Odabasi (2006).

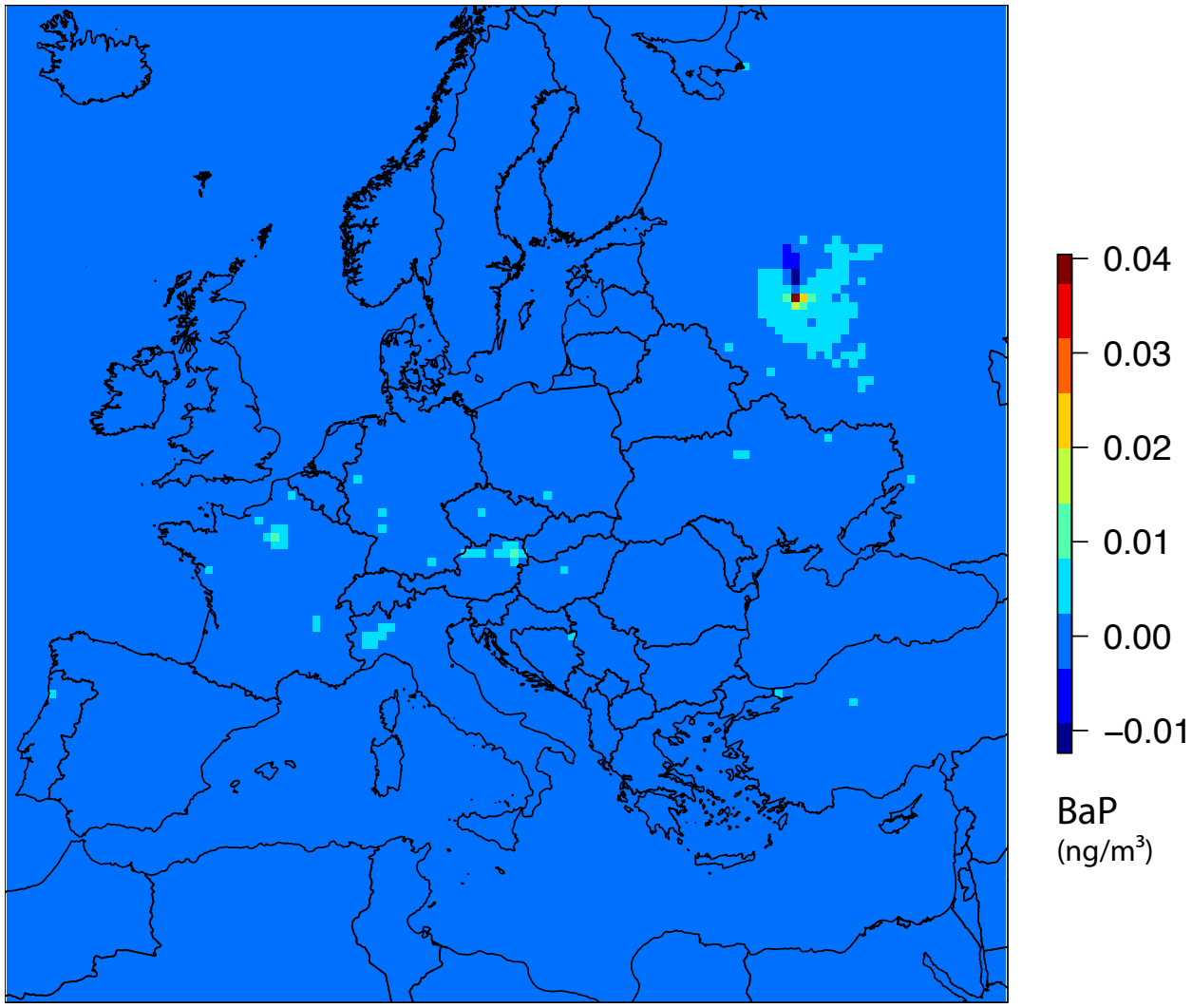

Figure S6. Wintertime differences (Method B – Method A) in average surface-level BaP concentrations simulated by the dual GPP model (scenario 4) using two different methods for estimating the soot-air partitioning coefficient K_{SA} (Method A: Dachs et al., 2000; Method B: van Noort, 2008).

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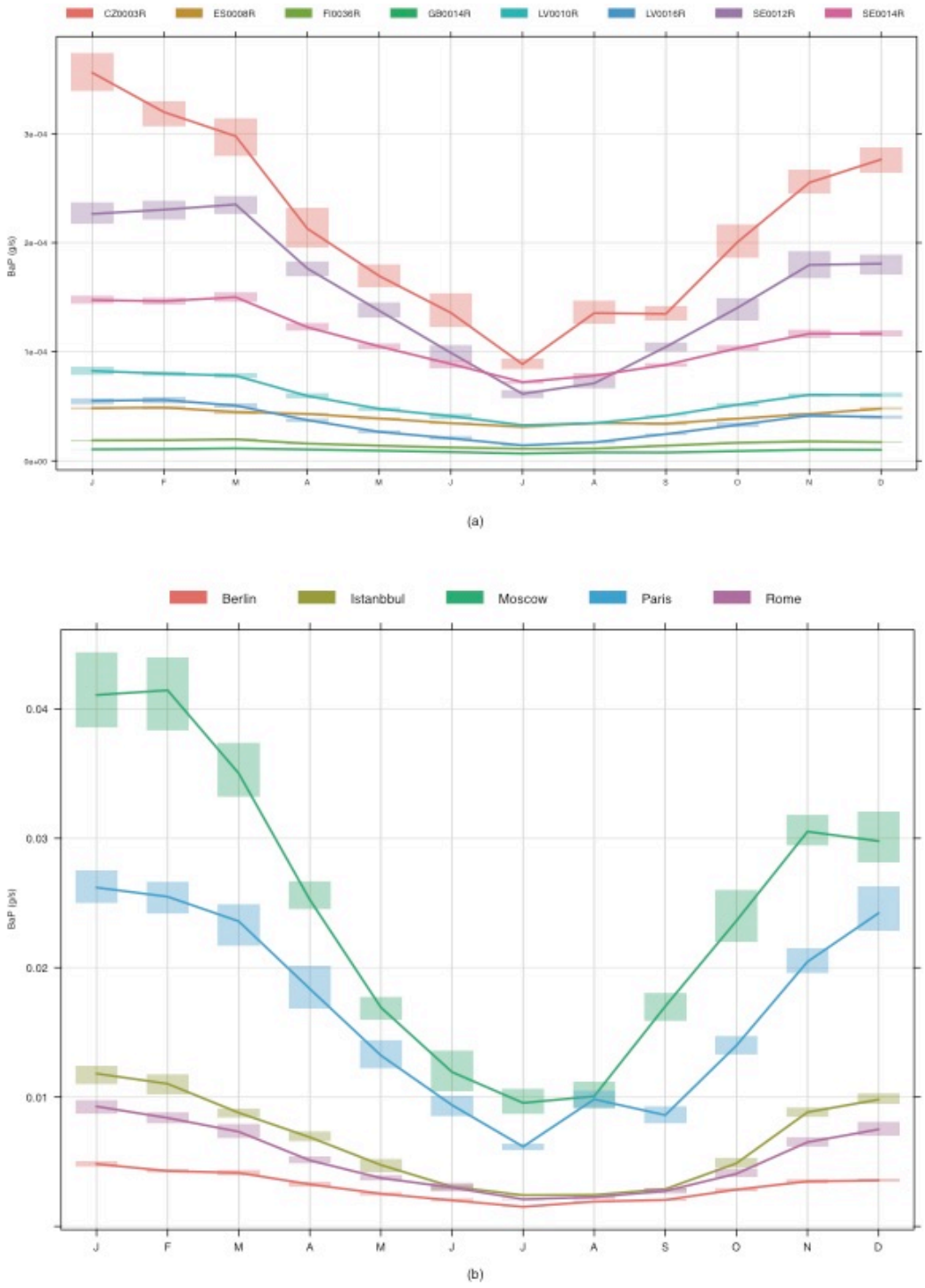


Figure S7. Annual average BaP emission fluxes (g/s) in the model cells (a) enclosing EMEP monitoring site locations, and (b) selected metropolitan areas of Europe during 2006.

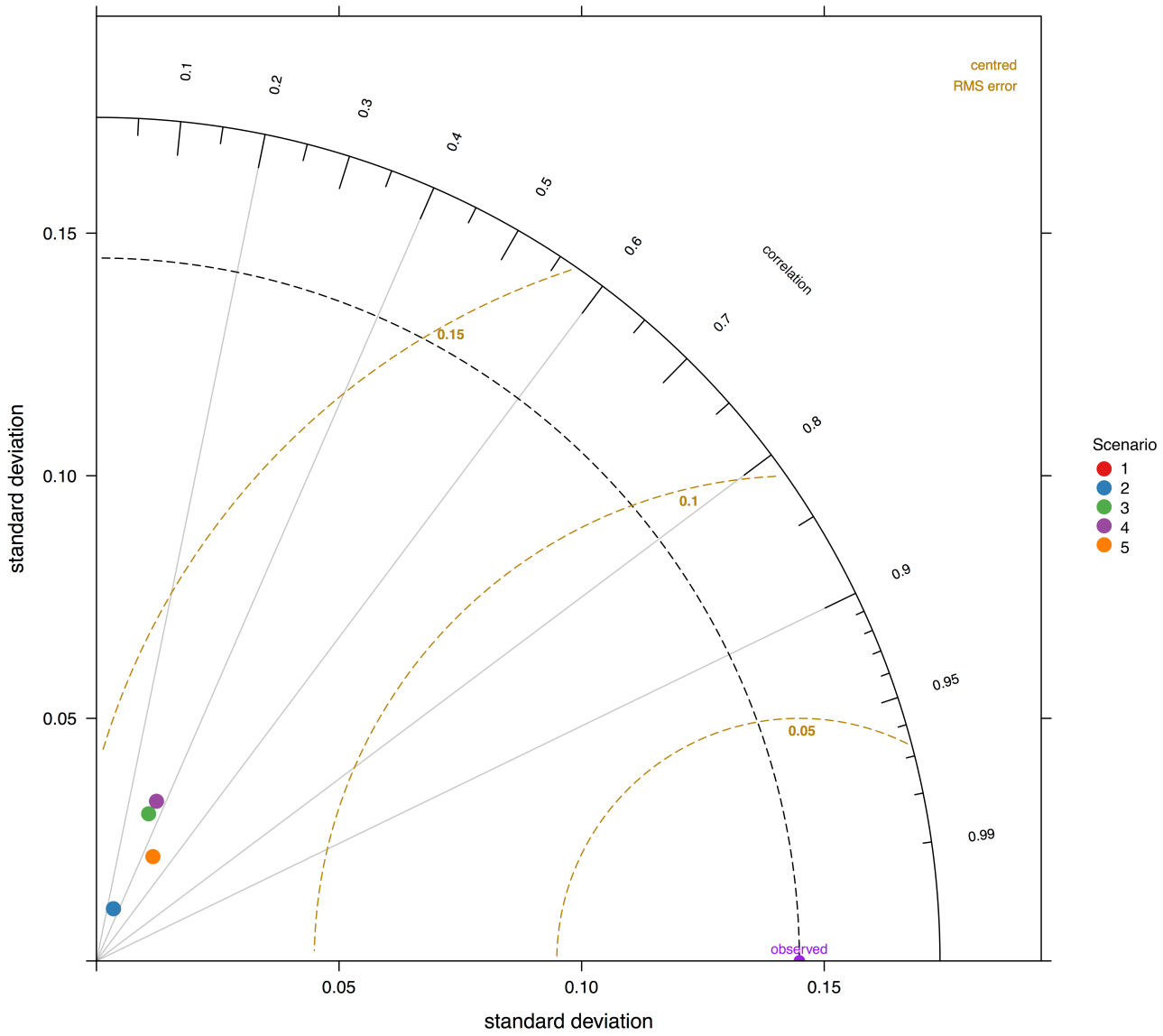


Figure S8. Taylor diagram showing how three complementary model performance statistics (correlation coefficient, standard deviation, and the centred root-mean-square error) vary simultaneously for each one of the 2006 WRF-CMAQ-BaP simulation scenarios against EMEP measurements.

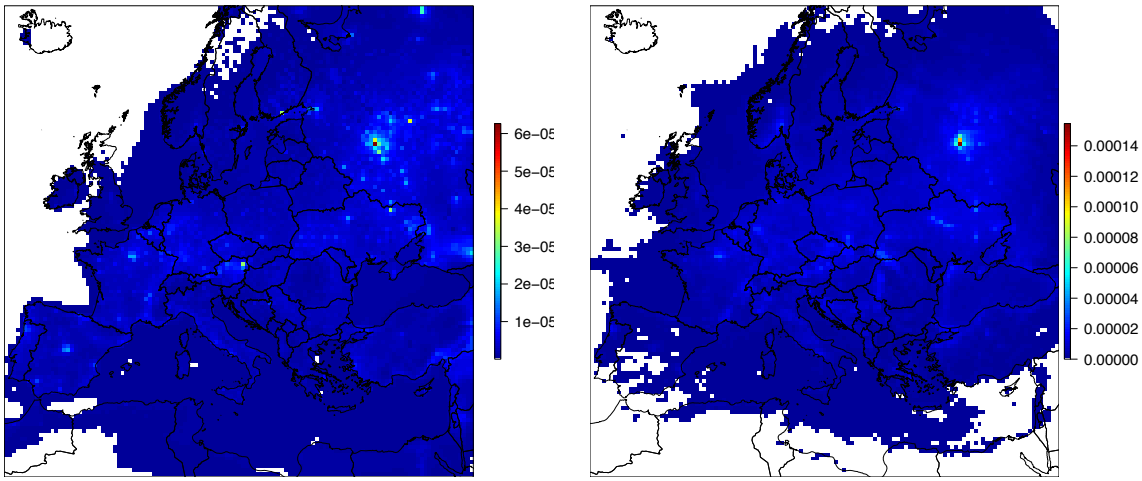
Table S9. Comparison between modelled and measured BaP concentrations for the entire 2006 EMEP dataset along with performance metrics and ranking for each individual site.

CZ0003R (n=49)										
Rank	Scenario	FAC2	MB	MGE	NMB	NMGE	RMSE	r	COE	IOA
1	5	0.36735	-0.08637	0.09609	-0.70689	0.78640	0.19376	0.54963	0.32679	0.66339
2	3	0.36735	-0.07212	0.10288	-0.59027	0.84202	0.19932	0.23115	0.27917	0.63958
3	4	0.32653	-0.05801	0.10339	-0.47476	0.84617	0.19225	0.28326	0.27562	0.63781
4	1	0.44898	-0.09848	0.10690	-0.80599	0.87492	0.21169	0.32111	0.25101	0.62550
5	2	0.44898	-0.09848	0.10690	-0.80601	0.87493	0.21169	0.32112	0.25100	0.62550
ES0008R (n=49)										
Rank	Scenario	FAC2	MB	MGE	NMB	NMGE	RMSE	r	COE	IOA
1	4	0.26531	-0.02635	0.02964	-0.69933	0.78686	0.04848	-0.02821	-0.27066	0.36467
2	3	0.08163	-0.03105	0.03232	-0.82423	0.85797	0.05036	-0.00232	-0.38549	0.30726
3	5	0.06122	-0.03357	0.03369	-0.89104	0.89434	0.05158	-0.04224	-0.44422	0.27789
4	1	0.00000	-0.03446	0.03446	-0.91481	0.91481	0.05190	0.03887	-0.47727	0.26136
5	2	0.00000	-0.03449	0.03449	-0.91550	0.91550	0.05192	0.02794	-0.47839	0.26081
FI0036R (n=12)										
Rank	Scenario	FAC2	MB	MGE	NMB	NMGE	RMSE	r	COE	IOA
1	4	0.50000	-0.01179	0.01358	-0.72184	0.83163	0.03614	0.89444	0.36985	0.68492
2	3	0.41667	-0.01268	0.01373	-0.77616	0.84042	0.03627	0.90937	0.36319	0.68159
3	5	0.33333	-0.01427	0.01473	-0.87360	0.90210	0.03984	0.38981	0.31645	0.65823
4	1	0.16667	-0.01560	0.01560	-0.95507	0.95507	0.04070	0.45114	0.27631	0.63815
5	2	0.08333	-0.01563	0.01563	-0.95708	0.95708	0.04072	0.42418	0.27479	0.63739
LV0010R (n=11)										
Rank	Scenario	FAC2	MB	MGE	NMB	NMGE	RMSE	r	COE	IOA
1	4	0.00000	-0.27764	0.27764	-0.92828	0.92828	0.36661	0.80956	-0.32366	0.33817
2	3	0.00000	-0.28174	0.28174	-0.94198	0.94198	0.36970	0.84842	-0.34319	0.32841
3	5	0.00000	-0.28967	0.28967	-0.96852	0.96852	0.37933	0.51157	-0.38103	0.30948
4	1	0.00000	-0.29504	0.29504	-0.98646	0.98646	0.38476	0.85236	-0.40662	0.29669
5	2	0.00000	-0.29527	0.29527	-0.98722	0.98722	0.38496	0.85706	-0.40770	0.29615

Continued on next page

Table S8 Continued

LV0016R (n=12)										
Rank	Scenario	FAC2	MB	MGE	NMB	NMGE	RMSE	r	COE	IOA
1	4	0.08333	-0.07158	0.07227	-0.72059	0.72752	0.09057	0.88148	-0.33827	0.33086
2	3	0.08333	-0.07546	0.07570	-0.75964	0.76204	0.09297	0.88465	-0.40177	0.29911
3	5	0.08333	-0.08749	0.08749	-0.88077	0.88077	0.10770	0.84240	-0.62019	0.18991
4	1	0.08333	-0.09485	0.09485	-0.95487	0.95487	0.11846	0.87319	-0.75649	0.12176
5	2	0.08333	-0.09488	0.09488	-0.95517	0.95517	0.11850	0.87173	-0.75705	0.12148
SE0012R (n=12)										
Rank	Scenario	FAC2	MB	MGE	NMB	NMGE	RMSE	r	COE	IOA
1	4	0.50000	-0.05197	0.05303	-0.71114	0.72557	0.08451	0.79238	0.22525	0.61262
2	3	0.50000	-0.05462	0.05490	-0.74732	0.75119	0.08590	0.78000	0.19790	0.59895
3	5	0.25000	-0.05926	0.05940	-0.81079	0.81274	0.09213	0.72644	0.13217	0.56609
4	1	0.00000	-0.06656	0.06656	-0.91074	0.91074	0.09943	0.69886	0.02753	0.51377
5	2	0.00000	-0.06675	0.06675	-0.91333	0.91333	0.09972	0.68275	0.02477	0.51238
SE0014R (n=24)										
Rank	Scenario	FAC2	MB	MGE	NMB	NMGE	RMSE	r	COE	IOA
1	4	0.33333	-0.03390	0.04240	-0.59250	0.74120	0.07728	0.75338	0.25318	0.62659
2	3	0.37500	-0.03674	0.04275	-0.64223	0.74734	0.07807	0.78464	0.24699	0.62349
3	5	0.33333	-0.04268	0.04564	-0.74610	0.79780	0.08329	0.72657	0.19615	0.59807
4	1	0.29167	-0.05009	0.05066	-0.87565	0.88547	0.09049	0.67532	0.10782	0.55391
5	2	0.29167	-0.05042	0.05089	-0.88133	0.88948	0.09073	0.68208	0.10378	0.55189
GB0014R (n=4)										
Rank	Scenario	FAC2	MB	MGE	NMB	NMGE	RMSE	r	COE	IOA
1	4	0.25000	-0.02517	0.02613	-0.71395	0.74117	0.03611	0.99549	-0.10005	0.44997
2	3	0.25000	-0.02812	0.02812	-0.79784	0.79784	0.03768	0.98569	-0.18416	0.40792
3	5	0.00000	-0.03169	0.03169	-0.89900	0.89900	0.04143	0.95280	-0.33431	0.33285
4	1	0.00000	-0.03296	0.03296	-0.93504	0.93504	0.04339	0.29286	-0.38780	0.30610
5	2	0.00000	-0.03297	0.03297	-0.93543	0.93543	0.04341	0.27833	-0.38837	0.30581



(a) (b)

Figure S10. Modelled annual average (a) wet and (b) dry deposition (kg/hectare) of BaP during 2006.