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ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Empirical evaluation of spatial and non-spatial European-scale multimedia fate models:
Results and implications for chemical risk assessment

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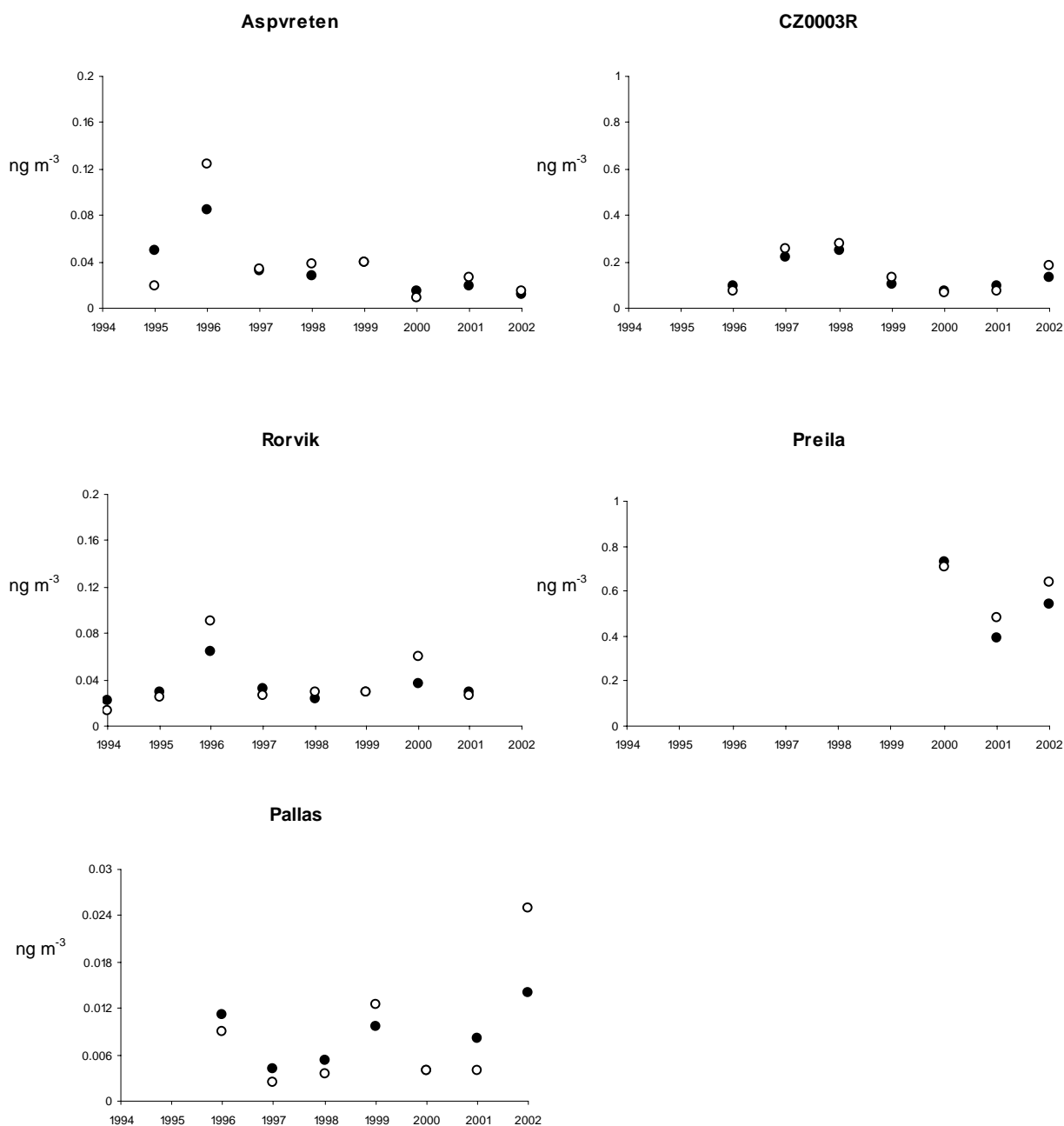


Figure S1. Temporal trends of annual geometric mean (closed circle) and median (open circle) BaP concentrations (ng m^{-3}) from EMEP monitoring sites (1994 – 2002)

Table S1. Range of median observed concentrations calculated for individual EVn-BETR and IMPACT 2002 model zones containing monitoring data

(a) Air compartment (ng m^{-3})

	EVn-BETR	IMPACT2002
Chemical	Range	Range
BaP	0.01 - 0.64	0.03 - 0.14
BbF	0.02 - 0.21	0.05 - 0.21
BkF	0.02 - 0.14	0.05 - 0.14
IP	0.01 - 0.18	0.04 - 0.18
HCB	0.02 - 0.06	0.02 - 0.06

(b) Freshwater compartment (ng L^{-1})

	EVn-BETR	IMPACT2002
Chemical	Range	Range
BaP	1.7 - 15	0.2 - 15
BbF	2.2 - 23	0.6 - 23
BkF	1.0 - 10	0.2 - 10
IP	0.3 - 15	0.3 - 15

(c) Sediment compartment (ng g^{-1})

	EVn-BETR	IMPACT2002
Chemical	Range	Range
BaP	44 - 430	9.3 - 660
BbF	70 - 600	10 - 700
BkF	40 - 290	6.2 - 360
IP	4.1 - 350	13 - 505
HCB	0.4 - 45	0.3 - 150

(d) Soil compartment (ng g^{-1})

	EVn-BETR	IMPACT2002
Chemical	Range	Range
BaP	0.3 - 140	12 - 150
BbF	0.6 - 150	16 - 155
BkF	0.2 - 80	10 - 80
IP	11 - 13	11 - 13
HCB	0.2 - 1.1	0.2 - 1.5

Table S2. Comparison of median and range of predicted concentrations across the entire model domain and for model zones containing monitoring data for EVn-BETR and IMPACT2002 and predicted concentrations generated by SimpleBox 3.0.

(a) Air compartment (ng m⁻³)

SimpleBox 3.0			EVn-BETR				IMPACT2002			
Chemical	Value	Range	Entire Model Domain		With Monitoring Data		Entire Model Domain		With Monitoring Data	
			Median	Range	Median	Range	Median	Range	Median	Range
BaP	0.16	-	0.047	0.003 - 0.42	0.12	0.01 - 0.35	0.043	0.0004 - 0.38	0.11	0.04 - 0.26
BbF	0.50	-	0.065	0.003 - 0.45	0.14	0.01 - 0.23	0.049	0.0006 - 0.43	0.22	0.13 - 0.31
BkF	0.09	-	0.033	0.002 - 0.21	0.05	0.02 - 0.14	0.033	0.0003 - 0.18	0.10	0.07 - 0.13
IP	0.14	-	0.044	0.003 - 0.38	0.07	0.01 - 0.18	0.029	0.0004 - 0.33	0.08	0.03 - 0.22
HCB	0.11	-	0.028	0.007 - 0.07	0.01	0.007 - 0.03	0.043	0.0005 - 0.43	0.10	0.08 - 0.12

(b) Freshwater compartment (ng L⁻¹)

SimpleBox 3.0			EVn-BETR				IMPACT2002			
Chemical	Value	Range	Entire Model Domain		With Monitoring Data		Entire Model Domain		With Monitoring Data	
			Median	Range	Median	Range	Median	Range	Median	Range
BaP	1.79	-	0.037	0.001 - 0.5	0.077	0.03 - 0.18	0.78	0.01 - 4.5	1.8	0.5 - 3.0
BbF	0.27	-	0.014	0.001 - 0.2	0.034	0.01 - 0.08	0.83	0.01 - 4.2	1.9	0.6 - 4.2
BkF	1.22	-	0.023	0.001 - 1.9	0.051	0.02 - 0.11	0.56	0.01 - 2.9	1.1	0.4 - 2.0
IP	1.06	-	0.028	0.001 - 0.4	0.059	0.01 - 0.12	0.51	0.01 - 5.1	1.3	0.3 - 2.1

Table S2 (continued). Comparison of median and range of predicted concentrations across the entire model domain and for model zoned containing monitoring data for EVn-BETR and IMPACT2002 and predicted concentrations generated by SimpleBox 3.0.

(c) Sediment compartment (ng g⁻¹)

SimpleBox 3.0			EVn-BETR				IMPACT2002			
Chemical	Value	Range	Entire Model Domain		With Monitoring Data		Entire Model Domain		With Monitoring Data	
			Median	Range	Median	Range	Median	Range	Median	Range
BaP	13.8	-	4.3	0.11 - 62	8.5	2.7 - 24	1.8	0.02 - 11	4.2	0.7 - 10
BbF	1.2	-	1.4	0.05 - 20	3.3	0.9 - 8.4	1.2	0.01 - 6.4	2.8	0.5 - 6.4
BkF	9.1	-	3.0	0.08 - 36	5.4	1.8 - 15	1.3	0.02 - 6.6	2.8	0.5 - 6.4
IP	17.4	-	4.7	0.14 - 65	7.8	2.3 - 21	1.8	0.02 - 13	4.4	1.4 - 7.6
HCB	0.02	-	0.2	0.05 - 1.3	0.3	0.1 - 0.5	0.001	4e-05 - 0.003	0.002	0.001 - 0.003

(d) Soil compartment (ng g⁻¹)

SimpleBox 3.0			EVn-BETR				IMPACT2002			
Chemical	Value	Range	Entire Model Domain		With Monitoring Data		Entire Model Domain		With Monitoring Data	
			Median	Range	Median	Range	Median	Range	Median	Range
BaP	0.16	-	0.10	0.001 - 0.55	0.11	0.04 - 0.33	0.07	0.002 - 0.28	0.20	0.04 - 0.27
BbF	0.02	-	0.02	0.001 - 0.16	0.02	0.01 - 0.08	0.05	0.001 - 0.22	0.18	0.16 - 0.20
BkF	0.11	-	0.06	0.001 - 0.35	0.07	0.03 - 0.21	0.04	0.001 - 0.19	0.13	0.12 - 0.13
IP	0.18	-	0.08	0.001 - 0.47	0.19	0.13 - 0.28	0.06	0.002 - 0.29	0.23	0.17 - 0.29
HCB	0.0002	-	0.002	0.0003 - 0.006	0.002	0.001 - 0.003	2e-05	1e-05 - 2e-04	3e-05	2e-05 - 8e-05

Table S3. Input parameters varied and default confidence Factors (CFs) used for Sensitivity and Propagation of Uncertainty Analysis

1. Chemical Properties	
Property Temperature (C)	1
Molar Mass (g/mol)	1
Melting point (C)	1
Aqueous solubility (g/m ³)	1.5
Vapor pressure (Pa)	1.5
Kow (<i>not</i> Log Kow)	3
Kaw (<i>not</i> Log Kow)	3
Kow (<i>not</i> Log Kow)	3
Koa (<i>not</i> Log Kow)	3
Air Reaction half-life (h)	3
Vegetation Reaction half-life (h)	3
Fresh Water Reaction half-life (h)	3
Coastal Water Reaction half-life (h)	3
Soil Reaction half-life (h)	3
Sediment Reaction half-life (h)	3
Enthalpy of vaporization (from water to air) (J/mol)	1.2
Enthalpy of solution (from octanol to water) (J/mol)	1.2
2. Emission Parameters in All Regions	
Emissions to Bulk Upper Air (kg/y)	3
Emissions to Bulk Lower Air (kg/y)	3
Emissions to Bulk Vegetation (kg/y)	3
Emissions to Bulk Fresh Water (kg/y)	3
Emissions to Bulk Coastal Water (kg/y)	3
Emissions to Bulk Soil (kg/y)	3
Emissions to Bulk Sediment (kg/y)	3
Background Upper Air Conc (ng/m ³)	3
Background Lower Air Conc (ng/m ³)	3
Background Fresh Water Conc (ng/L)	3
Background Coastal Water Conc (ng/L)	3

3. Environmental Characteristics in All Regions	
Total Surface Area (km ²)	1
% Surface covered by fresh water	1.1
% Surface covered by coastal water	1.5
% Soil covered by vegetation	1.1
Leaf Area Index (m ² /m ²)	1.5
vegetation mass per square meter (kg/m ²)	1.5
Average lower air compartment height (km)	1.5
Average upper air compartment height (km)	1.5
Average fresh water depth (m)	1.5
Average coastal water depth (m)	1.5
Average soil depth (cm)	1.5
Average fresh water sediment depth (cm)	3
Volume Fraction Particles in upper air	3
Volume Fraction Particles in lower air	3
Volume Fraction Particles in fresh water	3
Volume Fraction Fish in fresh water	3
Volume Fraction Particles in coastal water	3
Volume Fraction Fish in coastal water	3
Volume Fraction Air in soil	1.1
Volume Fraction Water in soil	1.1
Volume Fraction Soil solids	1.1
Volume Fraction Sediment pore water	1.1
Volume Fraction Sediment solids	1.1
Volume Fraction Water in vegetation	1.1
Volume Frac (Pseudo)Octanol in vegetation flesh	3
Winter mean temperature (oC)	1.1
Summer mean temperature (oC)	1.1
Fraction OC Particles in fresh water	1.5
Fraction OC Particles in coastal water	1.5
Fraction OC Soil solids	1.5
Fraction OC Sediment solids	1.5
Average Vegetation Cycle	1.1
density of air particles (1,2) (2,2)	1.5
density of water (4,1)	1.05
density of water particles (4,2)	1.5
density of water biota (4,3)	1.05
density of soil solids (6,3)	1.5
density of sediment solids (7,2)	1.5
density of coastal biota (5,3)	1.05
density of vegetation flesh (3,2)	1.5
1 air side air-fresh water MTC	3
2 water side air-fresh water MTC	3
3 rain rate	3
4 aerosol depositon	3
5 soil air phase diffusion MTC	3
6 soil water phase diffusion MTC	3
7 soil air boundary layer MTC	3
8 sediment-water diffusion MTC	3
9 sediment deposition	3

10 sediment resuspension	3
11 soil water runoff	3
12 soil solids runoff	3
13 sediment burial	3
14 diffusion to stratosphere	3
15 leaching from soil	3
16 leaf side air-veg. MTC	3
17 air side air-veg. MTC	3
18 veg. water uptake velocity	3
19 upper-lower air mixing MTC	10
20 air side air-coastal water MTC	3
21 water side air-coastal water MTC	3
rain scavenging ratio	10
Snow scavenging ratio	10
Fraction of rain intercepted by foliage	1.1
4. Inter-regional Flow Rates (Matrix G values)	
Upper air flow rate (m ³ /h)	3
Lower air flow rate (m ³ /h)	3
Fresh water flow rate (m ³ /h)	3
Runoff water flow rate (m ³ /h)	3
Coastal water flow rate (m ³ /h)	3