Supplementary Material for

"PAH Concentrations Simulated with AURAMS-PAH over Canada and the USA"

E. Galarneau*, P.A. Makar, Q. Zheng, J. Narayan, J. Zhang, M.D. Moran, M.A. Bari, S. Pathela, A. Chen, and R. Chlumsky

* Corresponding Author: Elisabeth Galarneau, Air Quality Research Division, Environment Canada, 4905 Dufferin Street, Toronto, ON, M3H 5T4, Canada, elisabeth.galarneau@ec.gc.ca, Telephone: 1-416-739-4431

Table of Contents

1. AURAMS-PAH Model Parameters

Table S1.1: Physicochemical Parameters used in the AURAMS-PAH Model

Parameter	Units	RP[a]	PHEN[a]	ANTH[a]	FLRT[a]	PYR[a]	BaA[a]	C+T[a]	BaP[a]
Gas-phase diffusivity (298K) [b]	$cm^2\ s^{-1}$	-	5.97×10^{-2}	5.97×10^{-2}	5.74×10^{-2}	5.74×10^{-2}	5.28×10^{-2}	5.28×10^{-2}	5.12×10^{-2}
Gas-phase OH reaction rate constant, k_{OH} [c]	$cm^3\ molec^{-1}\ s^{-1}$	-	13×10^{-12}	40×10^{-12}	29×10^{-12}	50×10^{-12}	50×10^{-12}	50×10^{-12}	50×10^{-12}
Saturated vapour pressure, p_L^0 [d]	Pa	m	-3706.04	-3710.87	-4081.11	-4153.89	-4563.27	-4577.21	-5046.88
Octanol-air partition coefficient, K_{OA} [e]	dimensionless	m	3293	3316	3904	3985	4746	4754	5382
		b	-3.37	-3.41	-4.34	-4.56	-5.64	-5.65	-6.50
Soot-water partition coefficient, K_{SW} [f]	$L\ kg^{-1}$	-	4.34×10^{5}	1.55×10^{6}	2.24×10^{6}	1.70×10^{6}	3.74×10^{7}	2.82×10^{7}	9.59×10^{7}
Air-water partition coefficient, K_{AW} [g]	dimensionless	m	-5689.20	-5629.06	-4654.80	-5159.97	-7986.53	-12136.16	-4437.1
		b	12.750	12.750	8.420	10.103	19.124	32.235	3.9881
Solid-phase density [h]	$kg\ m^{-3}$	-	1174	1280	1252	1271	1254	1273	1351

[a] Explanation of abbreviations: RP = regression parameter for semi-logarithmic temperature-dependent form (m = slope, b = intercept), PHEN = phenanthrene, ANTH = anthracene, FLRT = fluoranthene, PYR = pyrene, BaA = benz[a]anthracene, C+T = chrysene+triphenylene, BaP = benzo[a]pyrene; [b] for diffusivity at another temperature, multiply the result in the table by $(T/298)^{1.75}$; [c] U.S. EPA (2005), $d[PAH]/[PAH] = -k_{OH}[OH]dt$; [d] Offenberg and Baker (1999), $\log p_L^0$ (Pa) = m/T(K) + b; [e] Odabasi et al. (2006), $\log K_{OA}$ = m/T(K) + b; [f] Jonker and Koelmans (2002), see text; [g] Bamford et al. (1999), $\ln K_{AW}$ = m/T(K) + b; [h] Mackay et al. (2006)

2. Network and Station Information for Measurement Data Sources

NAPS

The National Air Pollution Surveillance (NAPS) network is a multi-agency collaboration administered by Environment Canada. In 2002, there were 17 NAPS stations that collected PAH data. Samples were collected for 24 hours beginning and ending at midnight. High-volume samplers using Teflon-coated glass fibre filters and polyurethane foam plugs were used to collect particulate and gaseous PAHs. Both were analysed together to arrive at a measured total PAH concentration.

NAPS stations are listed in Table S2.1 from west to east. Note that there were no NAPS stations measuring PAHs in 2002 in the provinces of British Columbia, Saskatchewan or Prince Edward Island. The model domain for this evaluation did not extend northward into the Yukon Territory, Northwest Territories or Nunavut.

Table S2.1: NAPS Stations with Data Used in AURAMS-PAH Evaluation

Station Name	Code	Province/State
Edmonton East	EDM	AB
65 Ellen Street (Winnipeg)	WPG	MB
College & South (Windsor)	WIN	ON
Experimental Farm (Simcoe)	SIM	ON
Beasley Park[1] (Hamilton)	HMB	ON
Egbert	EGB	ON
Confederation Park[1] (Hamilton)	HMC	ON
Judson & Etona[2] (Toronto)	JET	ON
Junction Triangle[2] (Toronto)	JCT	ON
Gage Institute[2] (Toronto)	GAG	ON
Point Petre	PPT	ON
1125 Ontario[3] (Montréal)	MTL	QC
Rivière-des-Prairies[3] (Montréal)	RDP	QC
Parc Berthier (Jonquière)	JON	QC
Forest Hills (Saint John)	SAJ	NB
Kejimkujik National Park	KEJ	NS
354 Water Street (St. John's)	STJ	NF

[1] Beasley Park and Confederation Park stations lie in the same AURAMS-PAH 42-km grid square.
[2] Gage Institute, Judson & Etona, and Junction Triangle lie in the same AURAMS-PAH 42-km grid square.
[3] 1125 Ontario and Rivière-des-Prairies lie in the same AURAMS-PAH 42-km grid square.

IADN

The Integrated Atmospheric Deposition Network (IADN) was mandated by the 1987 Canada-US Water Quality Agreement. PAHs were collected by high-volume sampler for periods of 24 hours beginning at 08:00 Eastern time. At Canadian sites, glass fibre filters and polyurethane foam collected the particulate and gaseous fractions, whereas the US stations collected these with quartz fibre filters and XAD resin. Station information for

the eight IADN sites collecting PAH data in 2002 are presented in Table S2.2 from west to east.

Table S2.2: IADN Stations with Data Used in AURAMS-PAH Evaluation

Station Name	Code	Province/State
Brule River[1]	BRR	WI
Eagle Harbor	EGH	MI
Illinois Institute of Technology (Chicago)	IIT	IL
Sleeping Bear Dunes	SBD	MI
Burnt Island	BNT	ON
Egbert[2]	EGB	ON
Sturgeon Point	STP	NY
Point Petre[2,3]	PPT	ON

[1] Brule River is no longer operating.
[2] Egbert and Point Petre hosted both NAPS and IADN stations.
[3] Point Petre hosts IADN samplers from Canada and the US.

CARB

In 2002, the California Air Resources Board (CARB) reported data for a single PAH, benzo[a]pyrene, on $PM_{2.5}$ sampled on quartz fiber filters using high volume samplers at seventeen sites. CARB stations are listed from north to south in Table S2.3.

Table S2.3: CARB Stations with Data Used in AURAMS-PAH Evaluation

Station Name	Code	Province/State
Chico	CHI	CA
Roseville	ROS	CA
Stockton	STO	CA
San Francisco	SFR	CA
Fremont	FRE	CA
San Jose – Jackson Street	SJJ	CA
San Jose – 4th Street	SJF	CA
Fresno	FRS	CA
Bakersfield	BAK	CA
Simi Valley	SMV	CA
Burbank	BUR	CA
Fontana	FON	CA
Los Angeles	LAX	CA
Riverside – Rubidoux	RIV	CA
North Long Beach	NLB	CA
El Cajon	ELC	CA
Chula Vista	CHU	CA

Rio Tinto Alcan

Rio Tinto Alcan operates an aluminum smelter in Kitimat, British Columbia. In 2002, they monitored PAHs using high-volume filter-PUF samplers at three sites in the area and these are listed in Table S2.4.

Table S2.4: Rio Tinto Alcan Kitimat Stations with Data Used in AURAMS-PAH Evaluation

Station Name	Code	Province/State
Haul Road[1]	HAU	BC
Kitamaat Village[1]	KIT	BC
Whitesail	WHI	BC

[1] Haul Road and Kitamaat Village lie in the same AURAMS-PAH 42km grid square.

3.. Maps of Modelled Annual Average PAH Concentrations

Figure 3.1: Map of modelled (JP) annual average total (gas + particle) phenanthrene concentrations (ng m^{-3}).

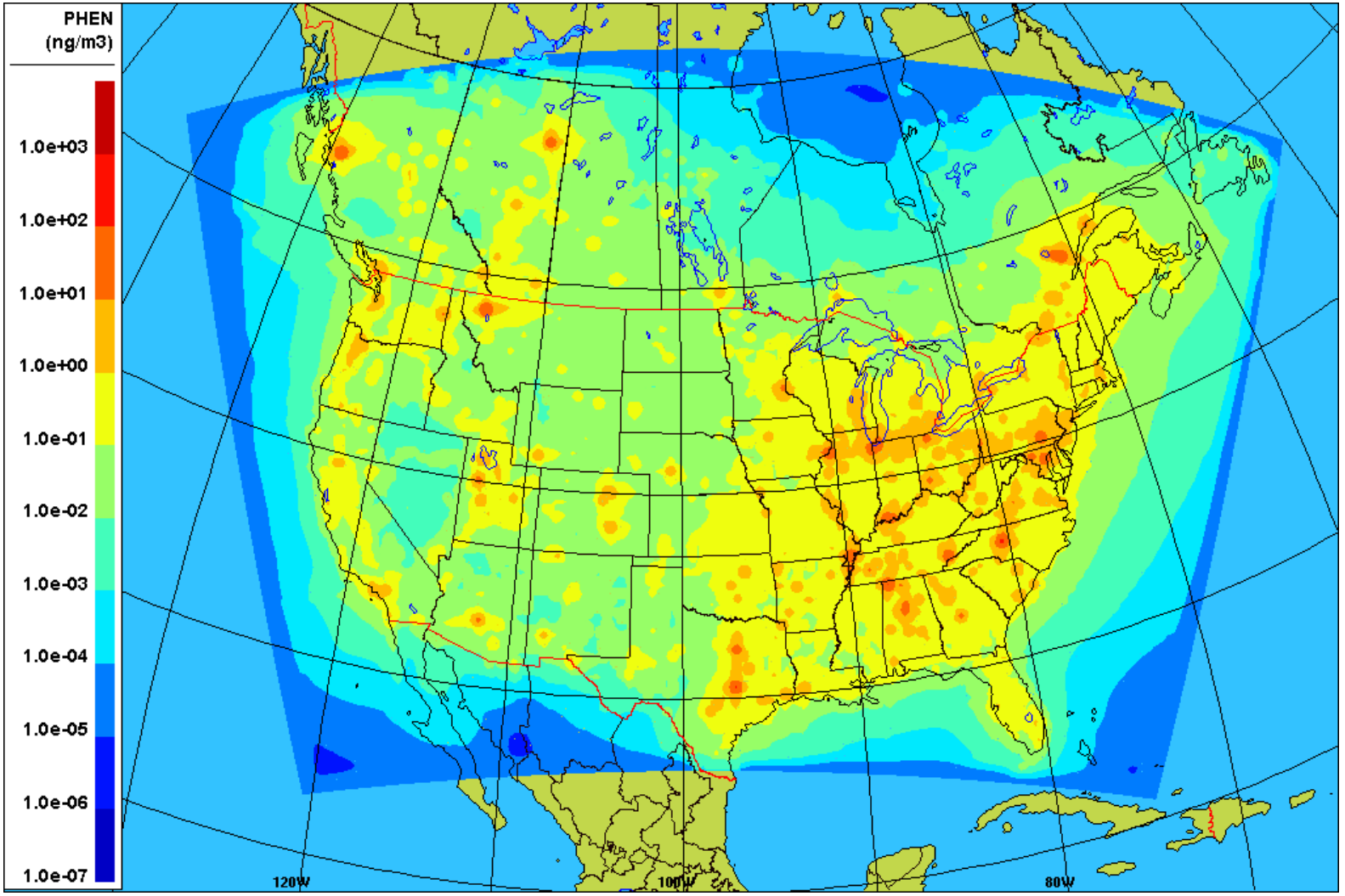


Figure 3.2: Map of modelled (DE) annual average total (gas + particle) phenanthrene concentrations (ng m^{-3}).

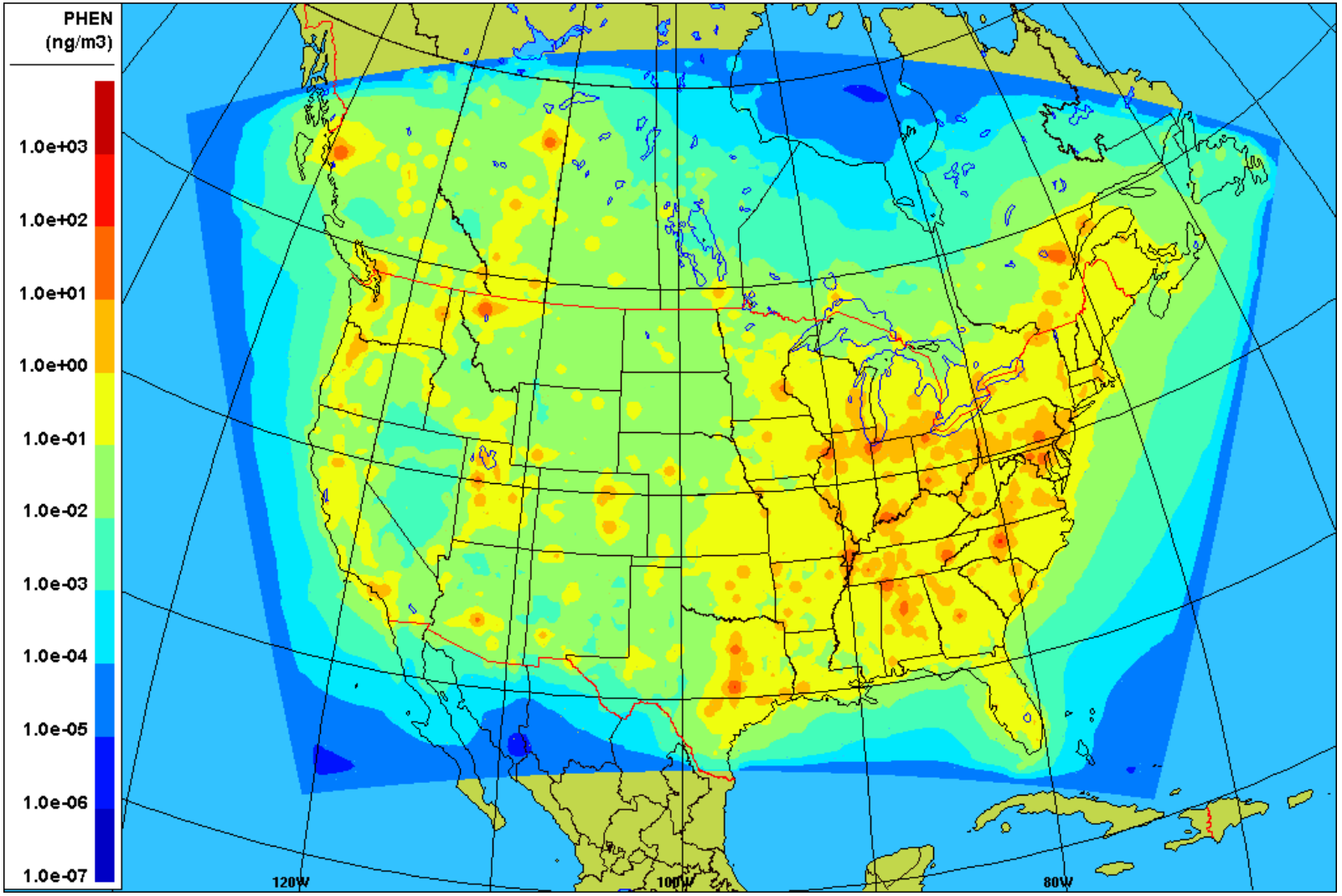


Figure 3.3: Map of modelled (JP) annual average total (gas + particle) anthracene concentrations (ng m^{-3}).

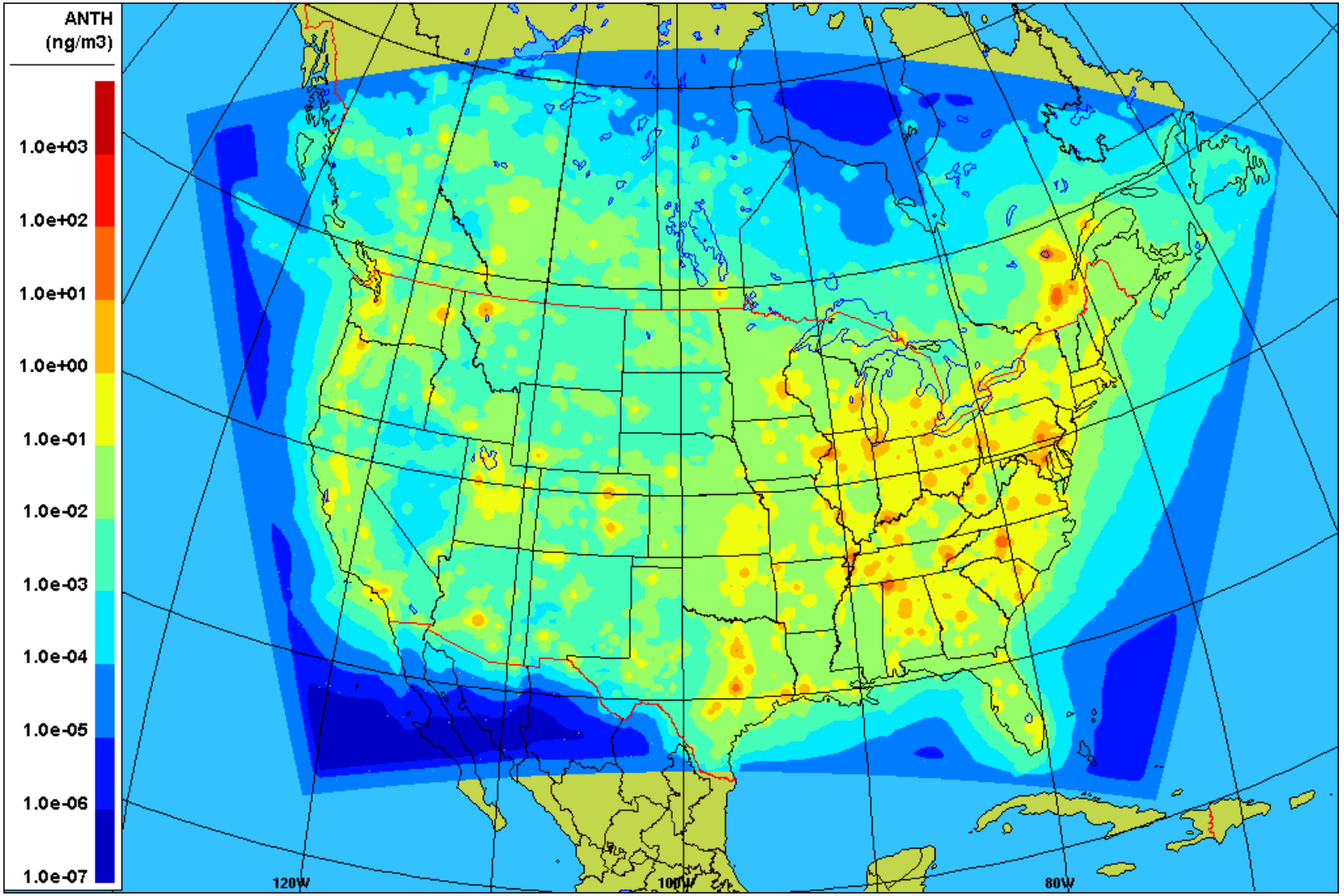


Figure 3.4: Map of modelled (DE) annual average total (gas + particle) anthracene concentrations (ng m^{-3}).

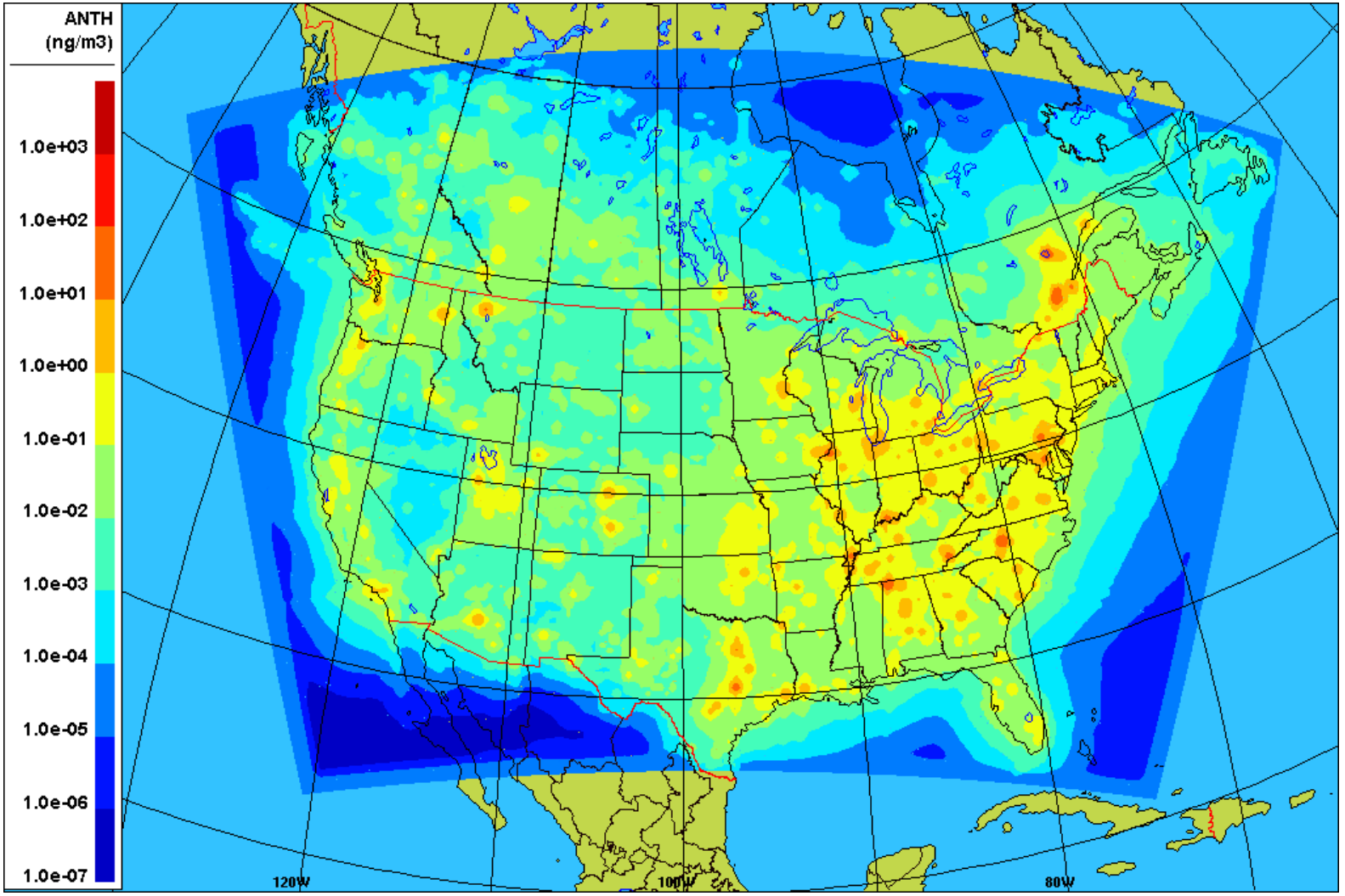


Figure 3.5: Map of modelled (DE) annual average total (gas + particle) fluoranthene concentrations (ng m^{-3}).

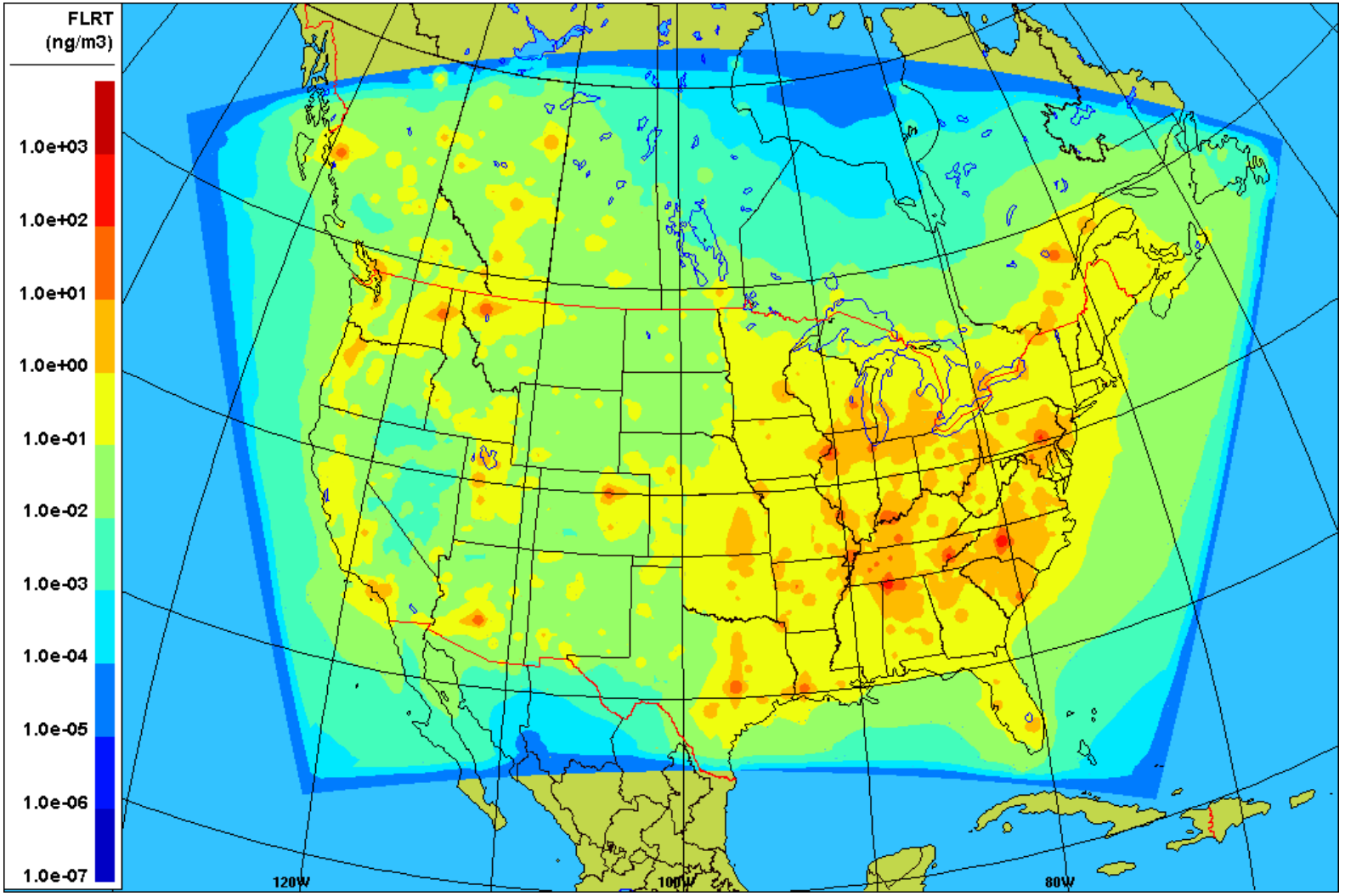


Figure 3.6: Map of modelled (JP) annual average total (gas + particle) pyrene concentrations (ng m^{-3}).

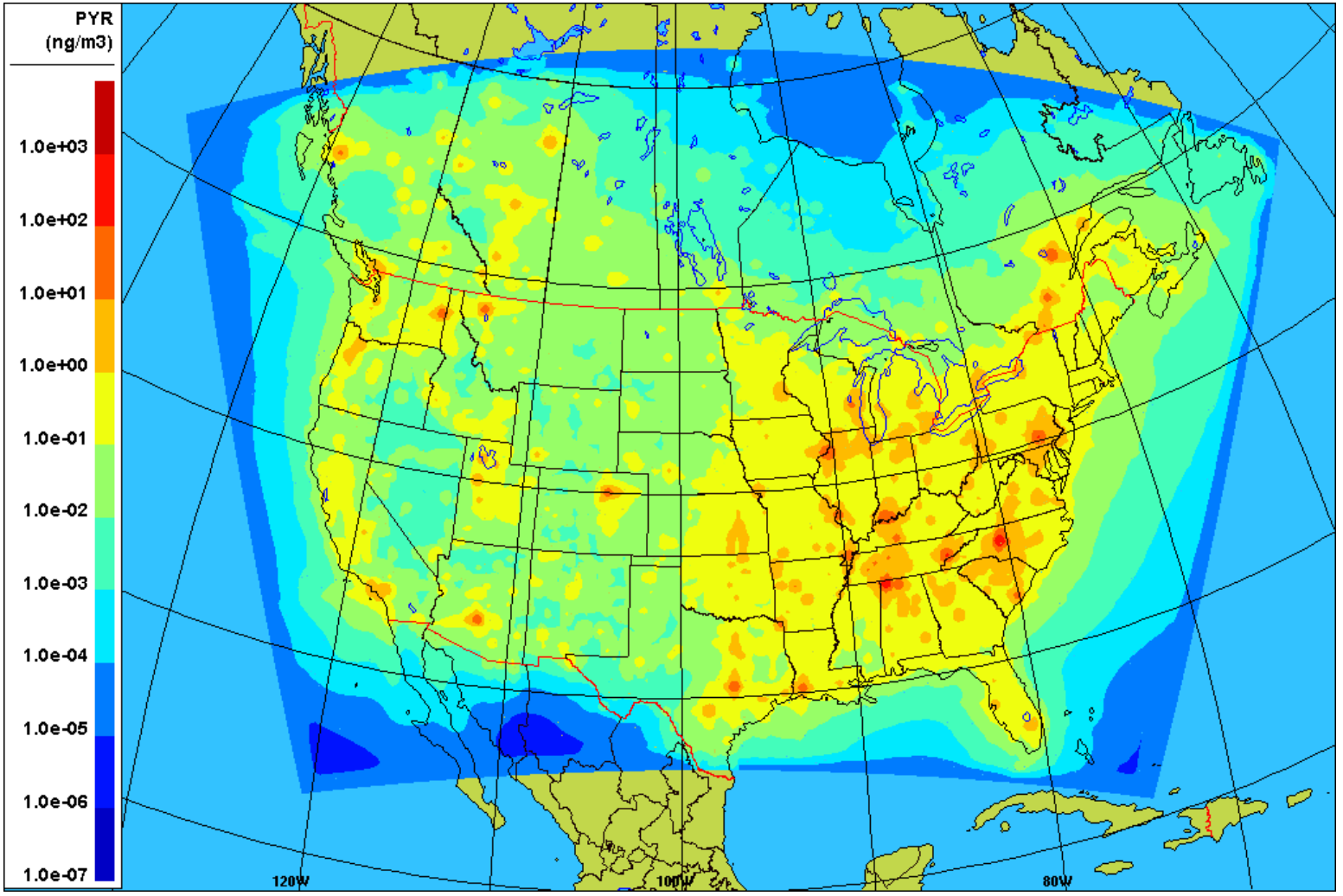


Figure 3.7: Map of modelled (DE) annual average total (gas + particle) pyrene concentrations (ng m^{-3}).

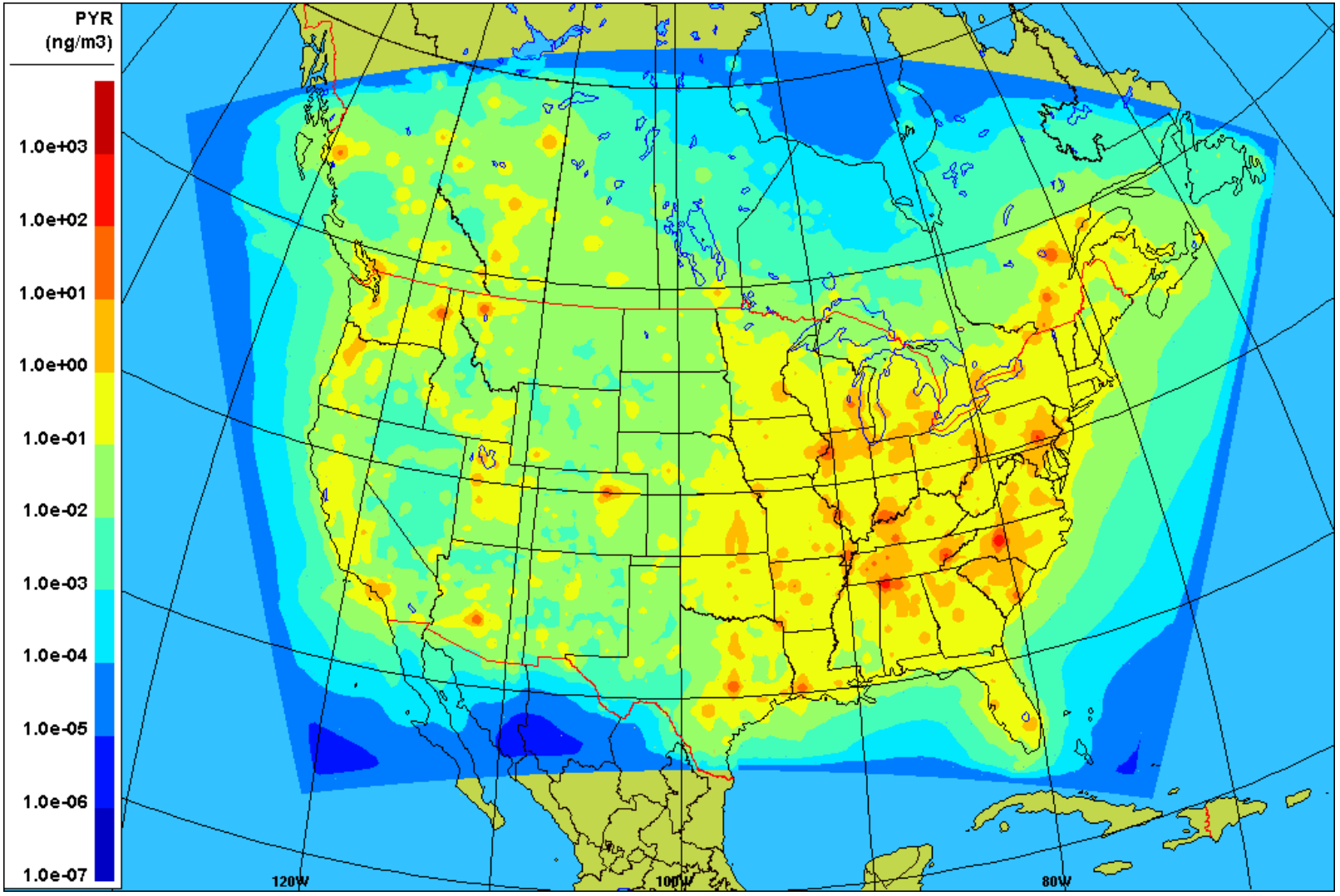


Figure 3.8: Map of modelled (JP) annual average total (gas + particle) benz[a]anthracene concentrations (ng m^{-3}).

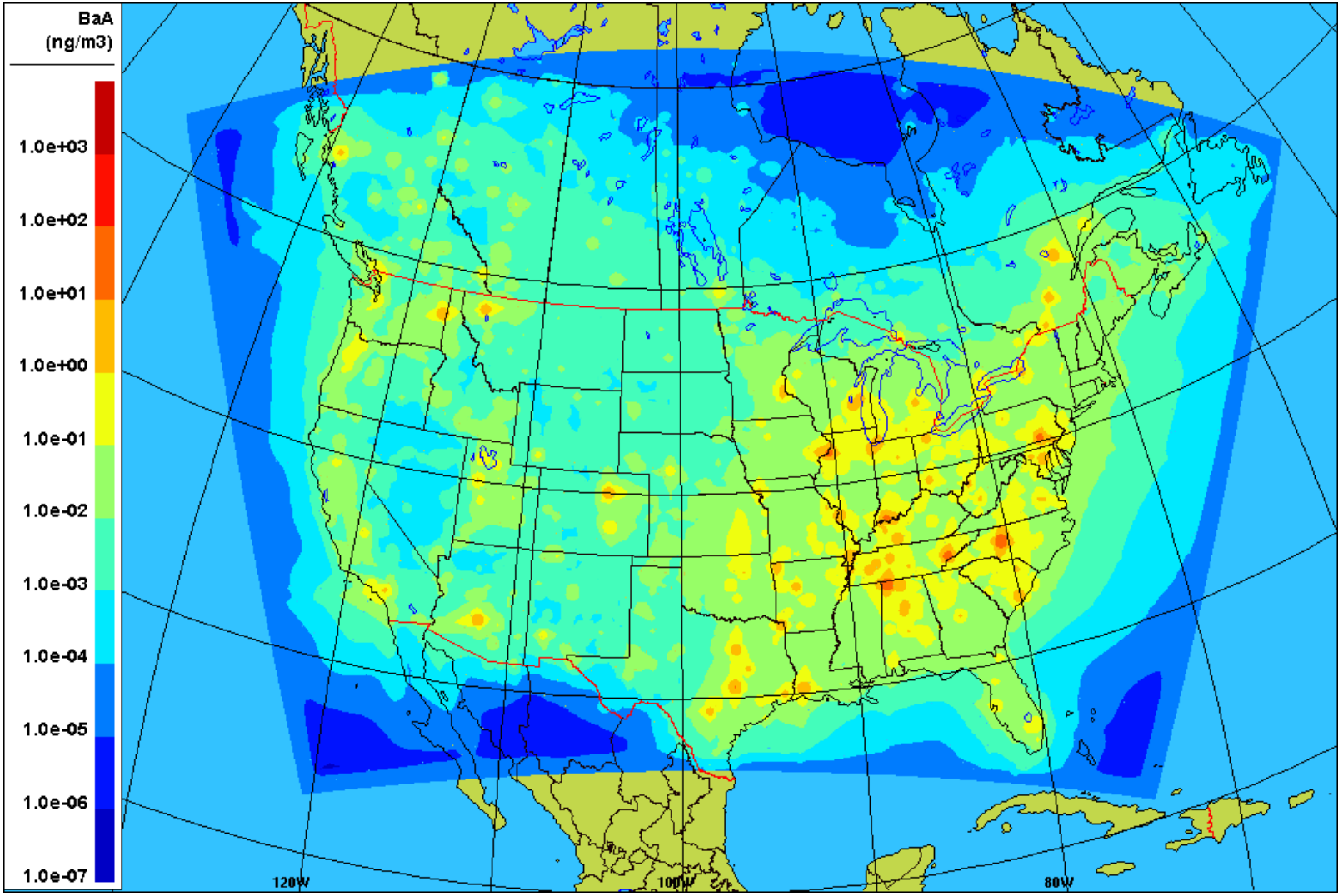


Figure 3.9: Map of modelled (DE) annual average total (gas + particle) benz[a]anthracene concentrations (ng m^{-3}).

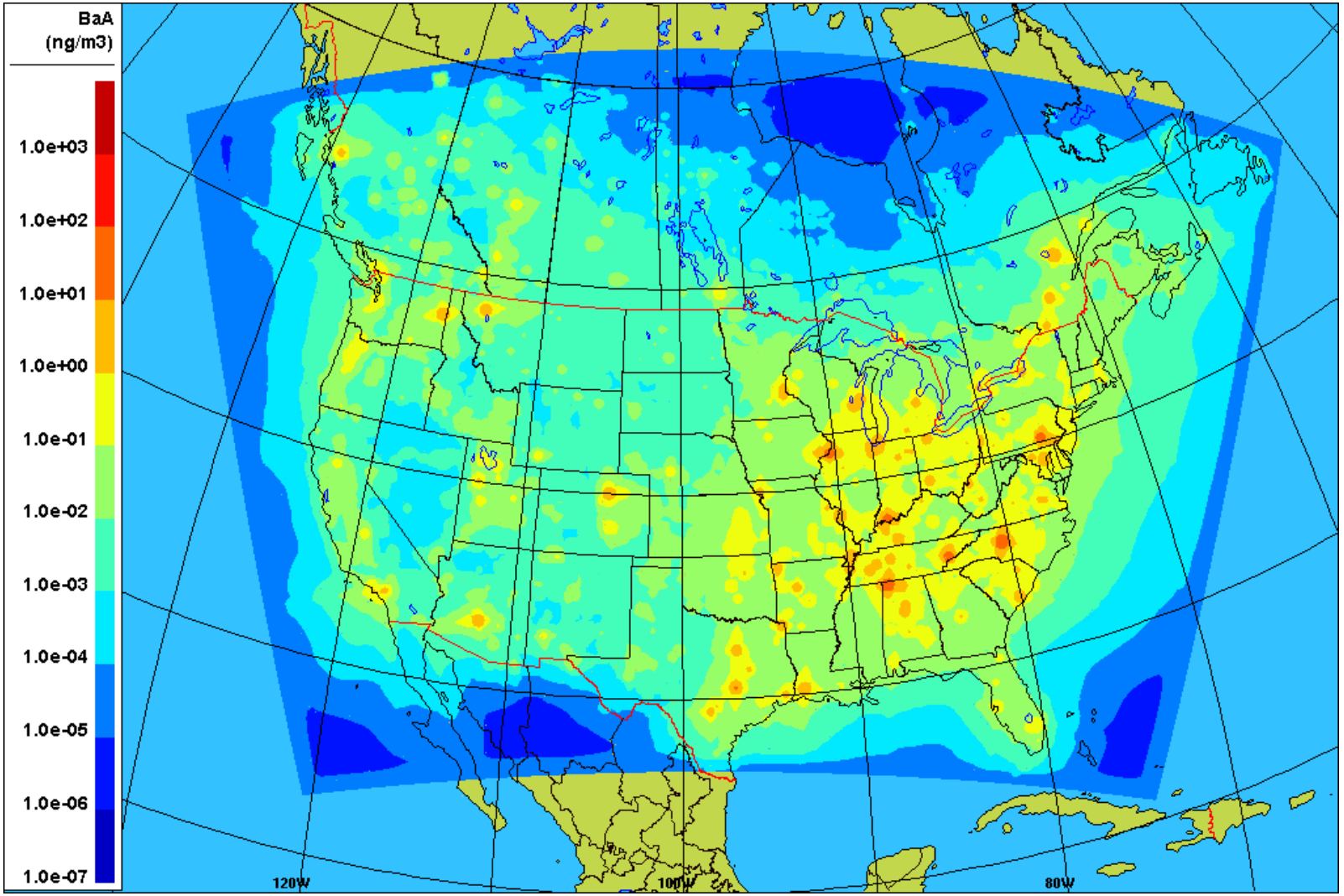


Figure 3.10: Map of modelled (JP) annual average total (gas + particle) chrysene + triphenylene concentrations (ng m^{-3}).

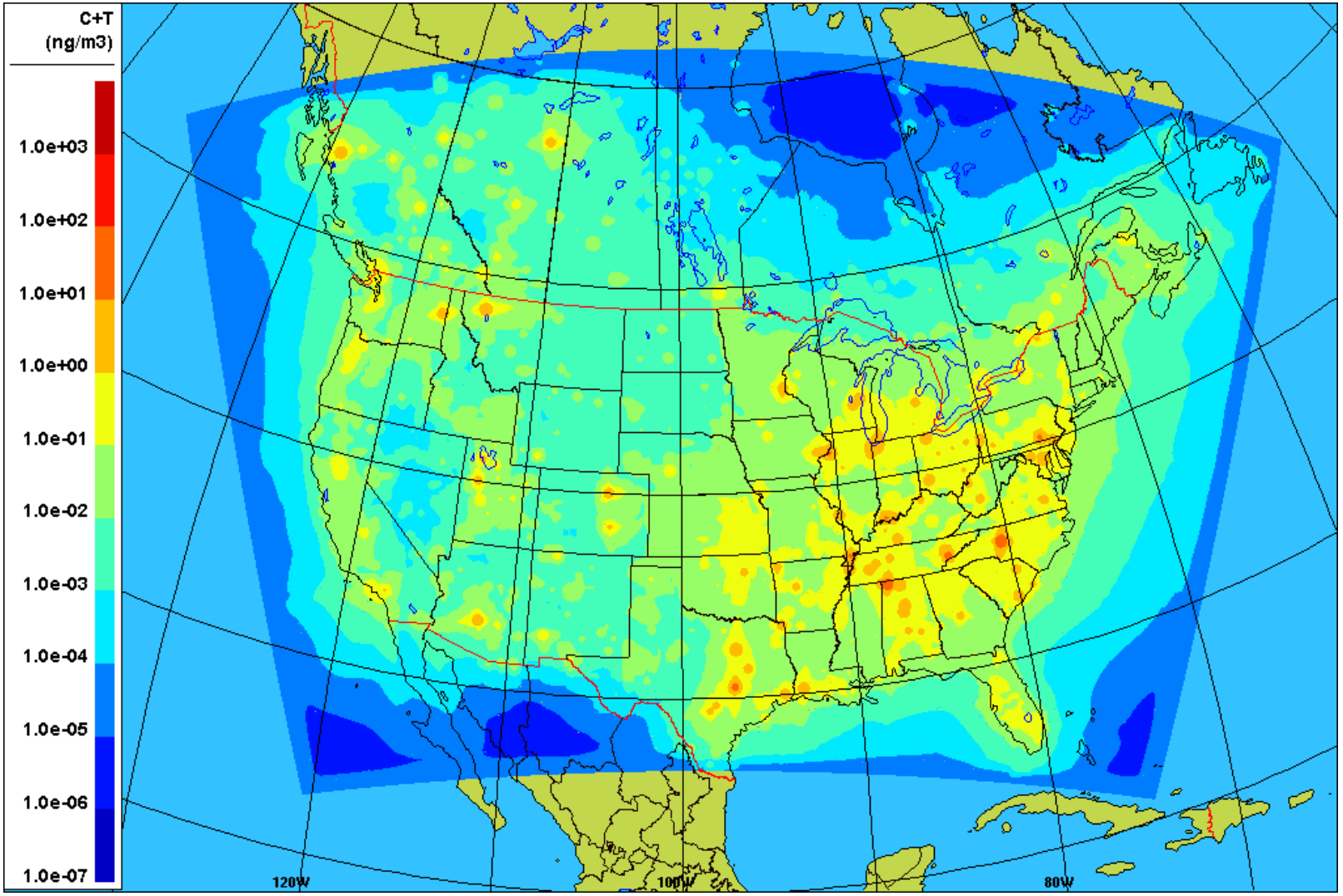


Figure 3.11: Map of modelled (DE) annual average total (gas + particle) chrysene + triphenylene concentrations (ng m^{-3}).

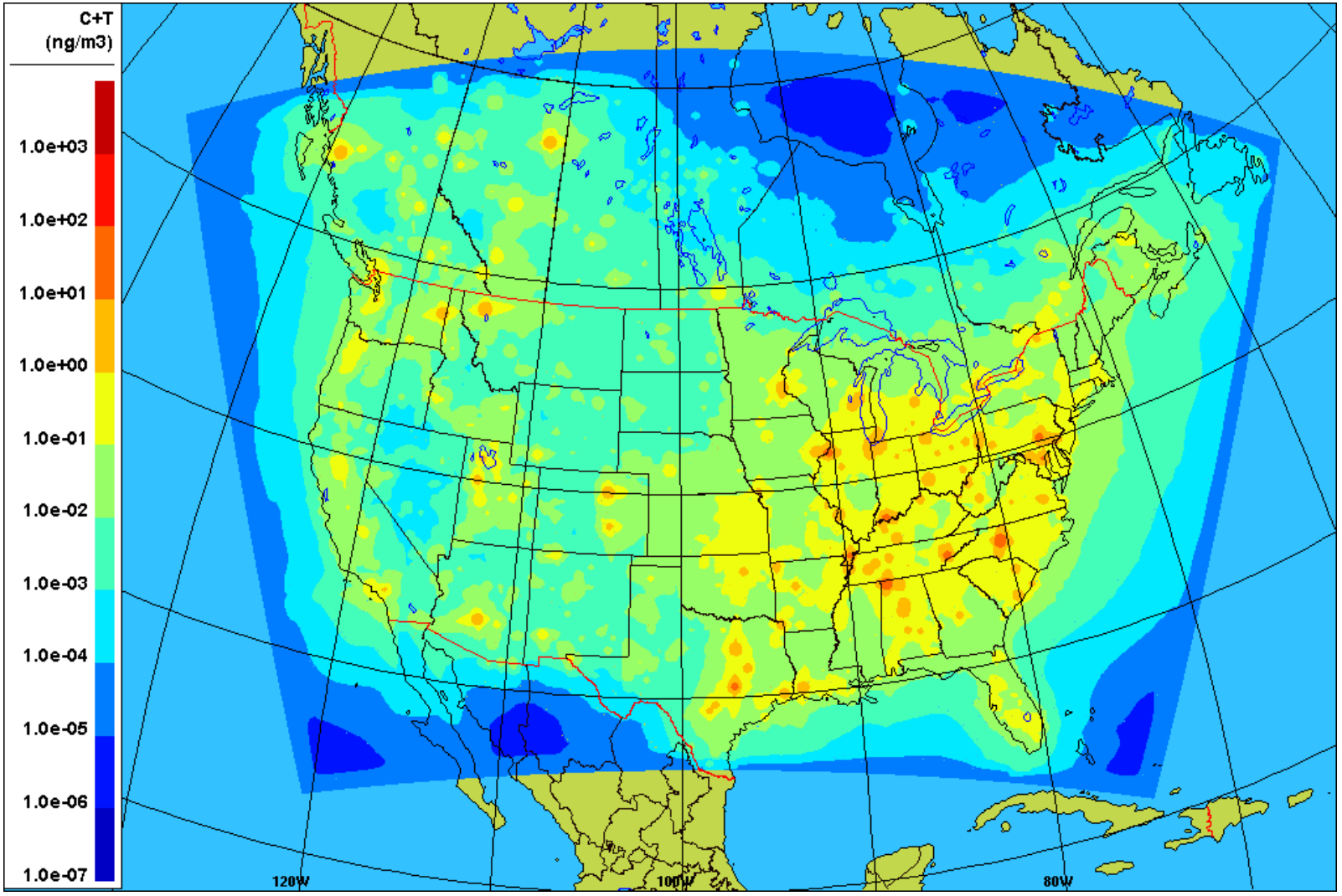


Figure 3.12: Map of modelled (JP) annual average total (gas + particle) benzo[a]pyrene concentrations (ng m^{-3}).

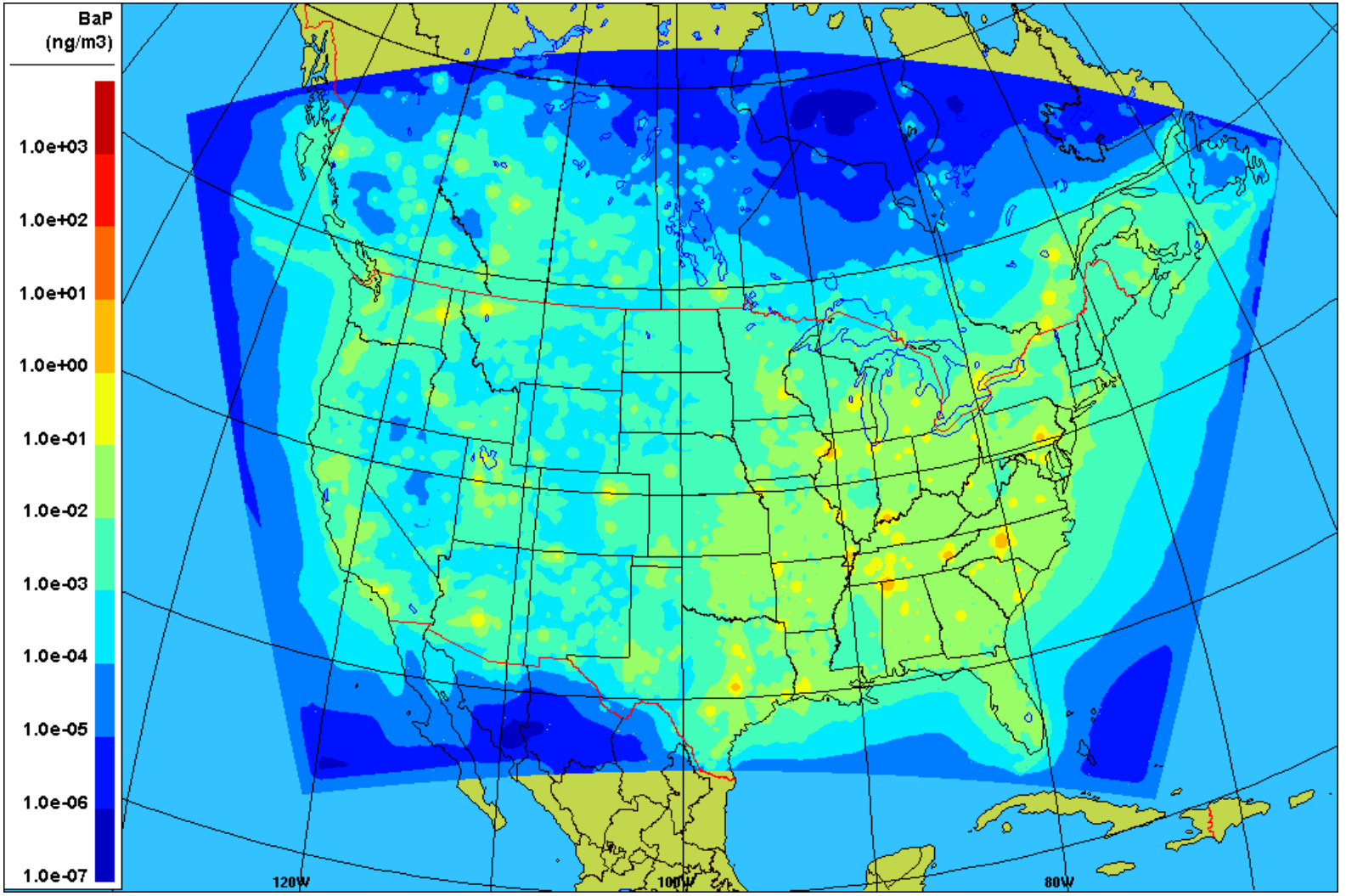
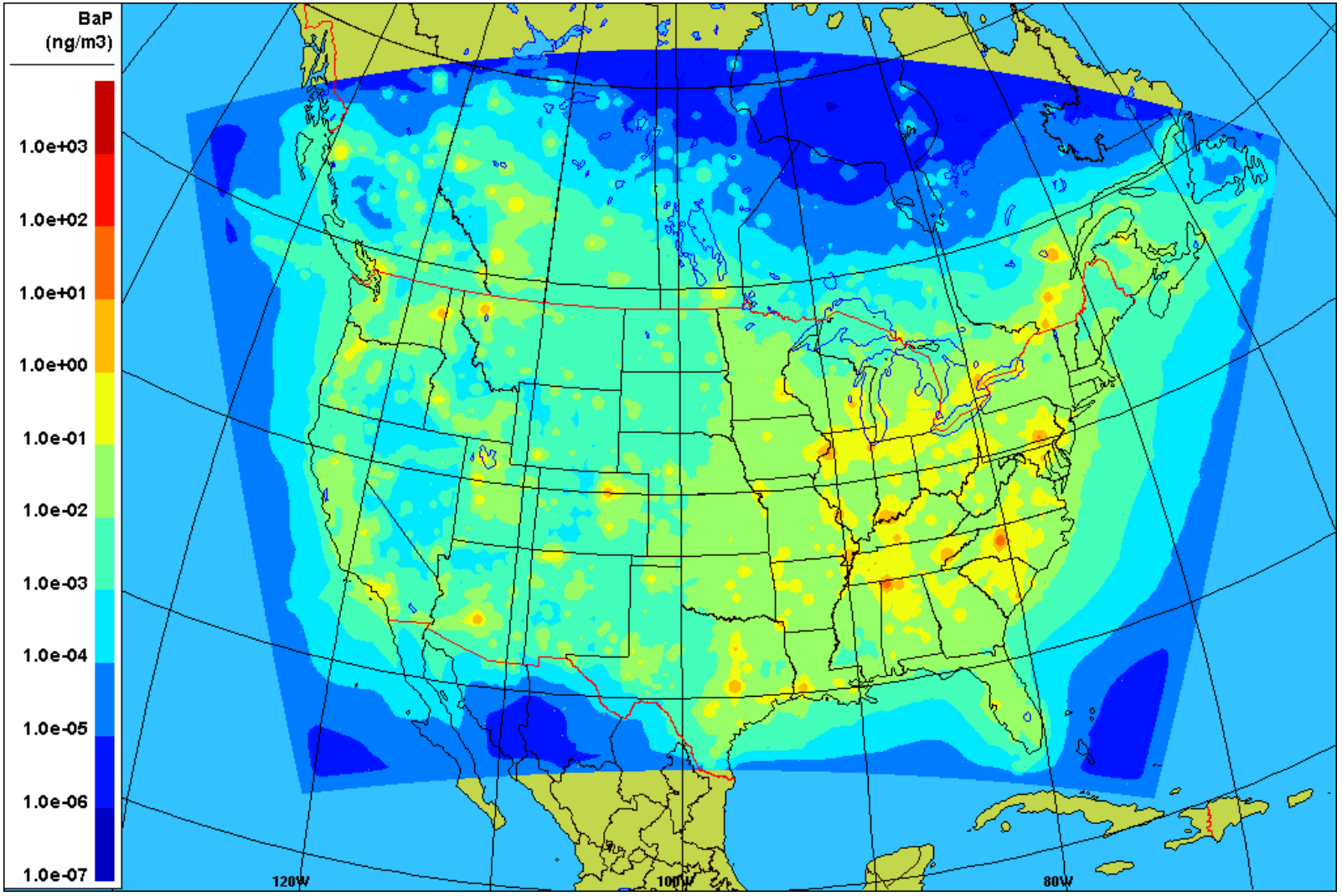


Figure 3.13: Map of modelled (DE) annual average total (gas + particle) benzo[a]pyrene concentrations (ng m^{-3}).



4. Additional Model Performance Metrics for 2002 AURAMS-PAH Simulation

Table S4.1: Model Performance Metrics for Total PAH Concentration – Junge-Pankow Partitioning

Performance Metric	PHEN	ANTH	FLRT	PYR	BaA	C+T	BaP
Mean Bias (ng m-3)	-23.30	-1.89	-2.40	-0.01	-0.10	-1.79	0.27
Mean Error (ng m-3)	34.54	3.04	10.03	6.97	1.73	3.79	1.51
Mean Normalized Bias (unitless)	-0.27	3.40	1.15	1.91	7.08	23.65	11.16
Mean Normalized Error (unitless)	1.00	4.12	1.73	2.37	7.38	24.19	11.54
Normalized Mean Bias (unitless)	-0.65	-0.67	-0.26	0.00	-0.07	-0.54	0.30
Normalized Mean Error (unitless)	0.96	1.09	1.09	1.22	1.30	1.15	1.67
Mean Fractional Bias (unitless)	-0.98	-0.10	-0.02	0.20	0.66	0.11	0.58
Mean Fractional Error (unitless)	1.20	1.20	0.93	0.97	1.16	1.03	1.22
Root Mean Square Error (RMSE, ng m-3)	-97.95	-9.90	-17.78	-8.81	-3.49	-17.94	-1.04
Slope (unitless)	0.06	-0.01	0.12	0.22	0.16	0.01	0.15
Intercept (ng m-3)	10.54	0.93	5.71	4.47	1.01	1.49	1.04
Coefficient of Determination (r2, unitless)	0.05	0.00	0.07	0.15	0.17	0.00	0.06
Percentage Within a Factor of 2 (%)	21.90	25.96	34.22	34.14	23.28	30.65	22.86
Percentage Within a Factor of 3 (%)	34.18	39.94	57.03	49.68	35.57	49.51	33.78
Percentage Within a Factor of 10 (%)	71.90	64.34	85.80	85.35	75.74	80.86	66.05
Number of Modelled-Measured Data Pairs	790	701	789	785	610	721	595

Table S4.2: Model Performance Metrics for Total PAH Concentration – Dachs-Eisenreich Partitioning

Performance Metric	PHEN	ANTH	FLRT	PYR	BaA	C+T	BaP
Mean Bias (ng m-3)	-23.30	-1.89	-2.29	0.28	0.00	-1.83	0.52
Mean Error (ng m-3)	34.54	3.04	10.03	7.05	1.78	3.77	1.73
Mean Normalized Bias (unitless)	-0.27	3.36	1.15	1.96	7.65	25.78	14.44
Mean Normalized Error (unitless)	1.00	4.07	1.73	2.42	7.94	26.33	14.78
Normalized Mean Bias (unitless)	-0.65	-0.68	-0.25	0.05	0.00	-0.55	0.57
Normalized Mean Error (unitless)	0.96	1.08	1.09	1.23	1.35	1.14	1.92
Mean Fractional Bias (unitless)	-0.99	-0.10	-0.02	0.21	0.69	0.13	0.67
Mean Fractional Error (unitless)	1.20	1.20	0.93	0.98	1.19	1.04	1.27
Root Mean Square Error (RMSE, ng m-3)	-97.95	-9.90	-17.50	-7.63	-3.21	-18.32	-0.52
Slope (unitless)	0.06	0.00	0.12	0.26	0.19	0.01	0.16
Intercept (ng m-3)	10.54	0.92	5.76	4.54	1.08	1.46	1.28
Coefficient of Determination (r2, unitless)	0.05	0.00	0.07	0.17	0.18	0.00	0.05
Percentage Within a Factor of 2 (%)	22.03	25.96	34.09	34.39	22.13	30.10	19.33
Percentage Within a Factor of 3 (%)	34.05	40.09	57.67	49.68	33.93	48.54	31.43
Percentage Within a Factor of 10 (%)	71.90	64.62	85.80	85.48	74.10	81.00	61.68
Number of Modelled-Measured Data Pairs	790	701	789	785	610	721	595