

Supporting Information

Dechlorane Plus in the Environment: A Review

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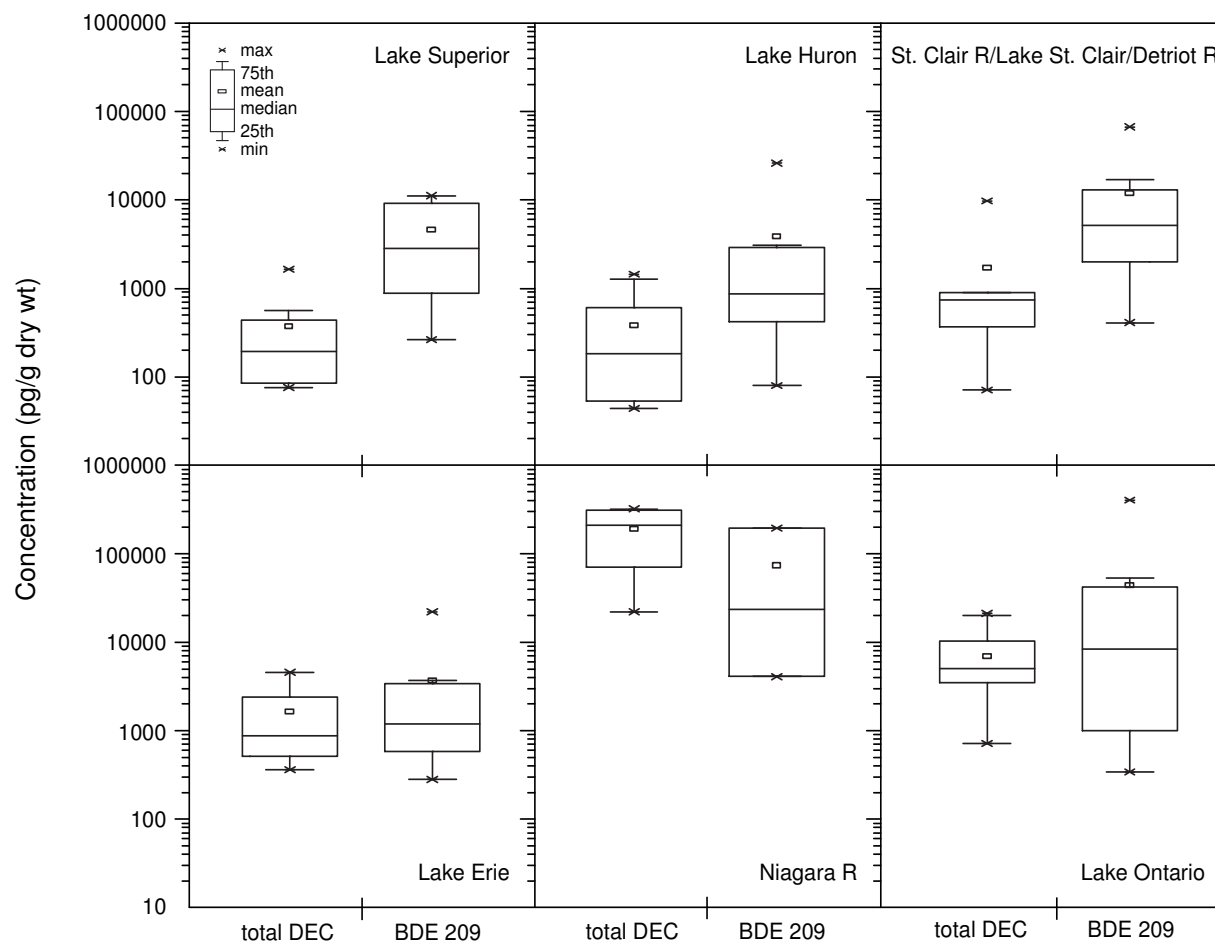
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Figure SI-1. Boxplots comparing total DEC and BDE 209 concentrations in tributary sediments of the Great Lakes; from Shen et al., 2011.



SI-A. Physical-chemical properties and model estimates

Physical-chemical property and half-life estimates for DP and DP analogs are summarized in Tables SI-1 to SI-4. At this time it is not possible to quantify possible differences in DP isomer properties. Values selected from this compilation were used to run The OECD Tool to calculate characteristic travel distances (*CTD*; km), transfer efficiency (TE; %), and overall persistence (P_{OV} ; d). Figures SI-2 and SI-3 compare these model calculations for DP and DP analogs with model calculations for benchmark chemicals including listed POPs (see Table SI-4) (Cowan-Ellsberry et al., 2009; Wegmann et al., 2009) assuming 100% emissions to air and 100% emissions to water, respectively. DP and DP analogs fall in the same range as some listed POPs. Notably the TE is greater and more comparable to the benchmark POPs when emissions are to air. Importantly, concentrations in remote regions, such as the Arctic, are also a function of the quantity of chemical emissions.

A method to estimate *in vivo* metabolic biotransformation rates in fish (Arnot et al., 2008) was applied to laboratory dietary test data for the *anti*- and *syn*-Dechlorane Plus isomers (Tomy et al., 2008). The estimated metabolic biotransformation rate constants (normalized to a 10 g fish at 15 °C and notated $k_{M,N}$, were 0.015 d⁻¹ and 0.0083 d⁻¹, respectively. The confidence (uncertainty) factors associated with these estimates were 3.2 and 3.3, respectively, indicating that 95% of the expected values are approximately within an order of magnitude of the estimates. Qualitatively, these rates of biotransformation are considered to be slow (Arnot et al., 2009).

Table SI-5 summarizes screening-level model calculations for the bioaccumulation factor (BAF; L-water/kg-wet weight) of DP and DP analogs in lower, middle, and upper trophic level fish species (Arnot & Gobas, 2003; U.S. EPA, 2009).

Table SI-1: Chemical identification, SMILES notation for physical-chemical property estimation, molar mass (g/mol), and melting point (°C) (U.S. EPA, 2009).

Chemical	CAS RN	SMILES	Molar mass (g/mol)	Melting point (°C)
DP	13560-89-9	<chem>ClC2=C(Cl)C3(Cl)C1CCC4C(CCC1C2(Cl)C3(Cl)Cl)C5(Cl)C(Cl)=C(Cl)C4(Cl)C5(Cl)Cl</chem>	653.7	206.45
Dec 602	31107-44-5	<chem>O(C(C(C(=C(C12Cl)Cl)Cl)(C2(Cl)Cl)Cl)C1C3C(C(=C(C45Cl)Cl)Cl)(C4(Cl)Cl)Cl)C35</chem>	613.6	190.16
Dec 603	N/A	<chem>ClC5=C(Cl)C6(Cl)C4C1CC(C2C1C3(Cl)C(Cl)=C(Cl)C2(Cl)C3(Cl)Cl)C4C5(Cl)C6(Cl)Cl</chem>	637.7	198.39
Dec 604	N/A	<chem>ClC3(Cl)C2(Cl)CC(ClCC(Br)c(Br)c(Br)c1Br)C3(Cl)C(Cl)=C2Cl</chem>	692.5	202.55
CP	N/A	<chem>ClC4=C(Cl)C5(Cl)C1C(CC2C1C3(Cl)C(Cl)=C(Cl)C2(Cl)C3(Cl)Cl)C4(Cl)C5(Cl)Cl</chem>	611.7	188.69

Table SI-2: Solid state water solubility (mg/L) and vapor pressures (Pa) for DP and DP analogs (U.S. EPA, 2009; University of Georgia, 2010).

Chemical	Water solubility (S _w ; mg/L)				Vapor pressure (P _s ; Pa)		
	WSKOWWIN	WATERNT	SPARC	Measured or average ¹	MPBPVP	SPARC	Average
DP	1.69 E-08	6.54 E-07	1.75 E-08	4.40 E-08	9.41 E-08	7.40 E-11	4.71 E-08
Dec 602	1.75 E-05	4.81 E-06	3.20 E-06	8.49 E-06	1.09 E-06	1.60 E-08	5.53 E-07
Dec 603	2.45 E-08	6.38 E-07	2.30 E-07	2.97 E-07	3.17 E-07	1.60 E-09	1.59 E-07
Dec 604	3.75 E-08	4.70 E-06	1.90 E-06	2.21 E-06	1.69 E-07	6.20 E-11	8.47 E-08
CP	5.79 E-07	6.12 E-07	1.70 E-06	9.64 E-07	1.36 E-06	1.70 E-08	6.88 -07

1. The value for DP is measured; the others are averaged.

Table SI-3: Air-water ($\log K_{AW}$), octanol-water ($\log K_{OW}$), and octanol-air ($\log K_{OA}$) partition coefficients at 25 °C.

Chemical	HenryWin	Log K_{AW}		KOWWIN	Log K_{OW}		Log K_{OA} ¹
		SPARC	Average		SPARC	Average ²	
DP	-3.52	-2.95	-3.24	11.27	11.55	9.0 (1.5)	12.26
Dec 602	-6.96	-3.45	-5.21	8.05	9.75	7.1 (1.4)	12.27
Dec 603	-4.00	-2.75	-3.37	11.20	11.07	8.5 (1.6)	11.83
Dec 604	-4.34	-5.05	-4.70	10.56	9.38	8.5 (0.9)	13.22
CP	-3.89	-2.63	-3.26	9.80	10.36	8.0 (1.4)	11.25

1. Calculated as $\log K_{OW} - \log K_{AW}$
2. Average (and standard deviation) of KOWWIN (U.S. EPA, 2009), SPARC (University of Georgia, 2010) and eight other K_{OW} model predictions (Tetko, 2005).

Table SI-4: DP, DP analogs, and benchmark chemicals and their properties (Cowan-Ellsberry et al., 2009; Wegmann et al., 2009) used in The OECD Tool calculations for LRTP and P_{OV} .

Chemical Name	Molar Mass (g/mol)	Log K_{AW}	Log K_{OW}	Half-life in air (hours)¹	Half-life in water (hours)	Half-life in soil (hours)
α -HCH	290.8	-3.59	3.88	1200	10560	15840
HCB	284.8	-1.51	5.61	15600	24000	36000
PCB-101	326.4	-2.08	6.38	480	28800	43200
PCB-180	395.3	-2.51	7.15	1920	52800	79200
PCB-28	257.6	-1.93	5.66	144	7200	10800
Atrazine	215.7	-6.84	2.73	9.6	1200	1800
Biphenyl	154.2	-1.96	4.06	72	360	540
<i>p</i> -cresol	108.1	-4.26	1.97	7.2	120	180
HBCD	641.7	-4.28	5.77	31.2	2040	2040
CP	611.7	-3.26	7.99	22.68	4320	8640
Dec 602	613.6	-5.21	7.06	18.26	4320	8640
Dec 603	637.7	-3.37	8.46	18.40	4320	8640
Dec 604	692.5	-4.70	8.52	49.23	4320	8640
DP	653.7	-3.24	9.03	13.68	4320	8640

1. Half-lives in air are largely based on gaseous phase reactions and do not take into account possibly longer half-lives following sorption to particles

2. **Figure SI-2:** Characteristic travel distance (CTD ; km), transfer efficiency (TE , %), and overall persistence (P_{OV} ; d) of DP, DP analogs, and benchmark chemicals calculated with The OECD Tool assuming that 100% of the chemical emissions are to air.

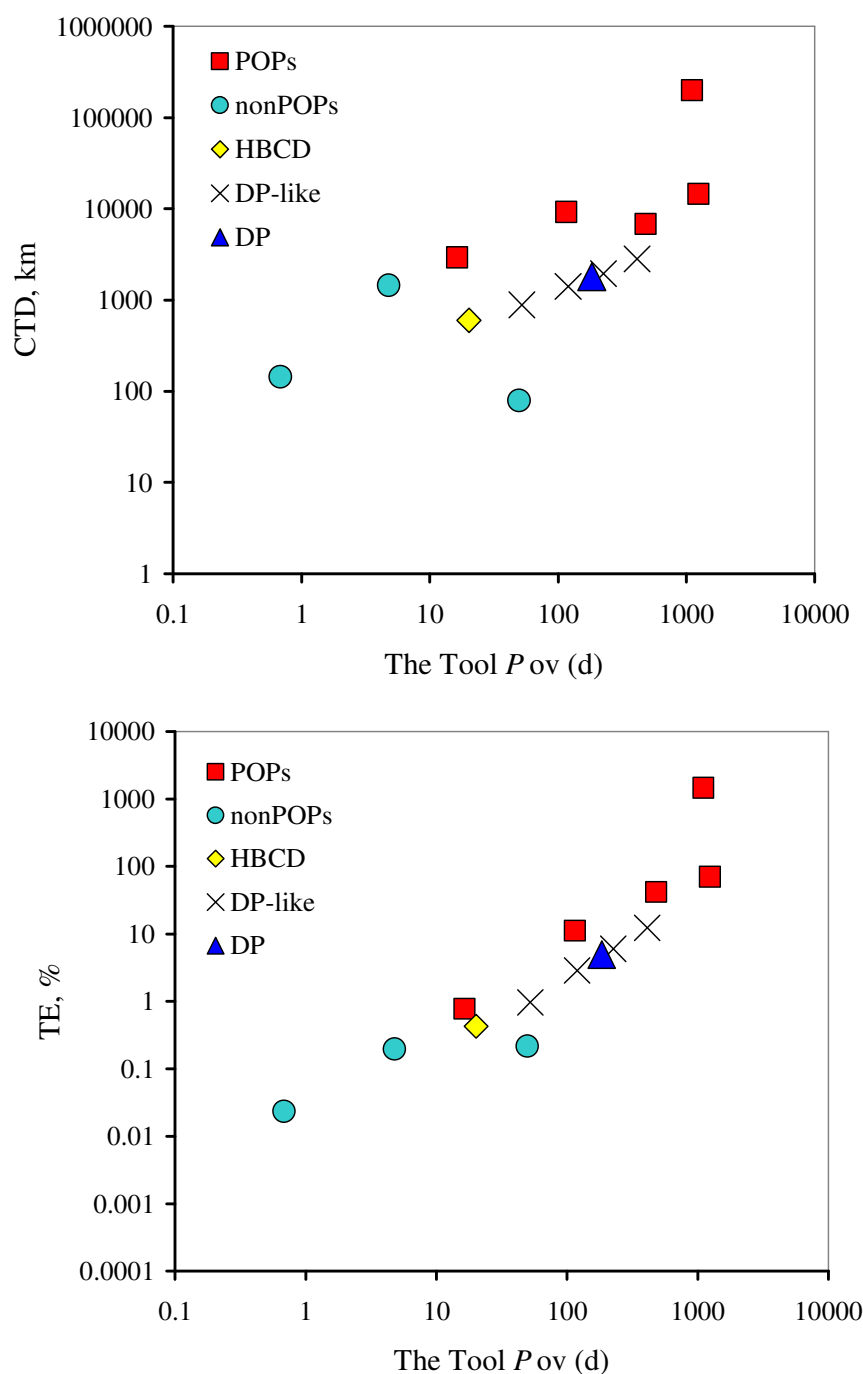


Figure SI-3: Characteristic travel distance (*CTD*; km), transfer efficiency (TE, %), and overall persistence (P_{OV} ; d) of DP, DP analogs, and benchmark chemicals calculated with The OECD Tool assuming that 100% of the chemical emissions are to water. Two non-POPs have TE < 0.000001%.

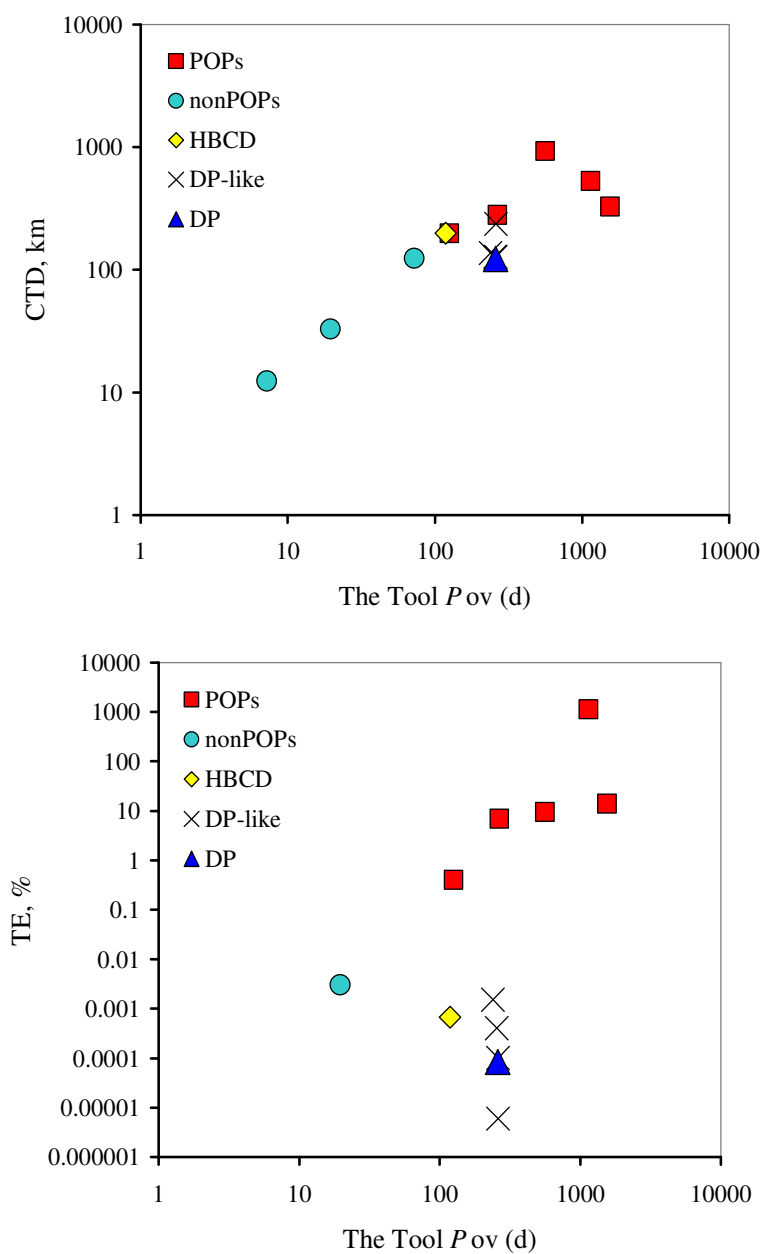


Table SI-5: Screening-level bioaccumulation factors (BAFs, L-water/kg-wet weight) based on total water concentrations in lower, middle, and upper trophic level fish species (Arnot and Gobas, 2003; U.S. EPA, 2009). Log 5000 = 3.69.

Chemical	Input parameters			log BAF (L/kg)		
	log K _{OW}	$k_{M,N}$ (d ⁻¹)	HL_N^3 (d)	Lower	Middle	Upper
<i>anti</i> -DP	9.03	1.48 E-02 ¹	47	4.77	4.85	4.97
<i>syn</i> -DP	9.03	8.21 E-03 ¹	84	5.03	5.19	5.41
Dec 602	7.06	2.27 E-04 ²	3100	6.45	6.73	7.07
Dec 603	8.46	2.39 E-05 ²	29000	6.28	6.56	6.91
Dec 604	8.52	1.72 E-03 ²	400	5.97	6.22	6.55
CP	7.99	9.65 E-05 ²	7,200	6.47	6.74	7.09

1. In vivo estimate from laboratory data (Tomy et al., 2008)
2. Screening-level QSAR estimate (U.S. EPA, 2009)
3. HL_N – primary biotransformation half-life normalized to a 10-g fish.

SI-C. Air-surface exchange

The fugacity fraction (ff) is used to assess the equilibrium status of a chemical between two interacting phases, and for soil and air, it takes the form (Hippelein & McLachlan, 2000; Meijer et al. 2003)

$$ff = C_s \rho_s / (C_s \rho_s + 0.41 \phi'_{SOM} K_{OA} C_A) \quad (1)$$

where C_A is the air concentration (in pg/m³), C_s is the soil concentration (in pg/g dw), ρ_s is the density of the dry soil (in g/m³), ϕ'_{SOM} is the mass fraction of SOM [soil organic matter, ϕ'_{SOM} is often estimated as 1.8 ϕ'_{SOC} , where ϕ'_{SOC} is the mass fraction of SOC (soil organic carbon)], and K_{OA} is the octanol/air partition coefficient.

Values of ff equal to 0.5 indicate soil–air equilibrium and no net gas exchange. Values > 0.5 indicate net volatilization from soil, and values < 0.5 indicate net gaseous deposition to soil. If soil-air equilibrium is assumed to be achieved, then the ratio of C_A/C_s given by

$$C_A / C_s = \rho_s / (0.41 \phi'_{SOM} K_{OA}) \quad (2)$$

Wang and co-workers (2010) measured both air and soil samples concurrently collected near a DP manufacturing facility. DP concentrations in both gas and particle phases from three air samples were measured for three consecutive days (October 10-12, 2009); see Figure SI-5. It is interesting to note that, while the level of particle-DP in air during the three sampling days varied widely (7330-26300 pg/m³) due to local wind directions and speed, the levels of gas-phase DP were quite stable (390-430 pg/m³). Furthermore, the values of f_{anti} for the gas phase DP were 0.74 ± 0.04 , which was close to that in soil (0.78 ± 0.11), but less than those for particle phase DP (0.63 ± 0.01), which is close to that of DP produced by the manufacturer. This may indicate

the differences in sources of DP in the two phases. Therefore, we hypothesize that the particle DP in air measured near this DP manufacturer in October 10-12, 2009, originated from the DP production facility, while the gas-phase DP was volatilization from soil.

In order to explore this idea further, the ratio of C_A/C_S was calculated by using Equation (2). We used the $\log K_{OA}$ value for DP of 12.26 (See Table SI-3). In the gridded soil density map, as generated by Jia et al. (2009), the soil densities varied from 0.53 to 1.79 g/cm³. Thus, in our calculation, the mean soil density ρ_S was 1.2 g/cm³ and ϕ'_{SOM} was 0.1. If we adapt the value for all parameters above, we can get the following equation at equilibrium:

$$C_A(\text{in pg / m}^3) / C_S(\text{in pg / g dw}) \approx 3.2 \times 10^{-5} \quad (3)$$

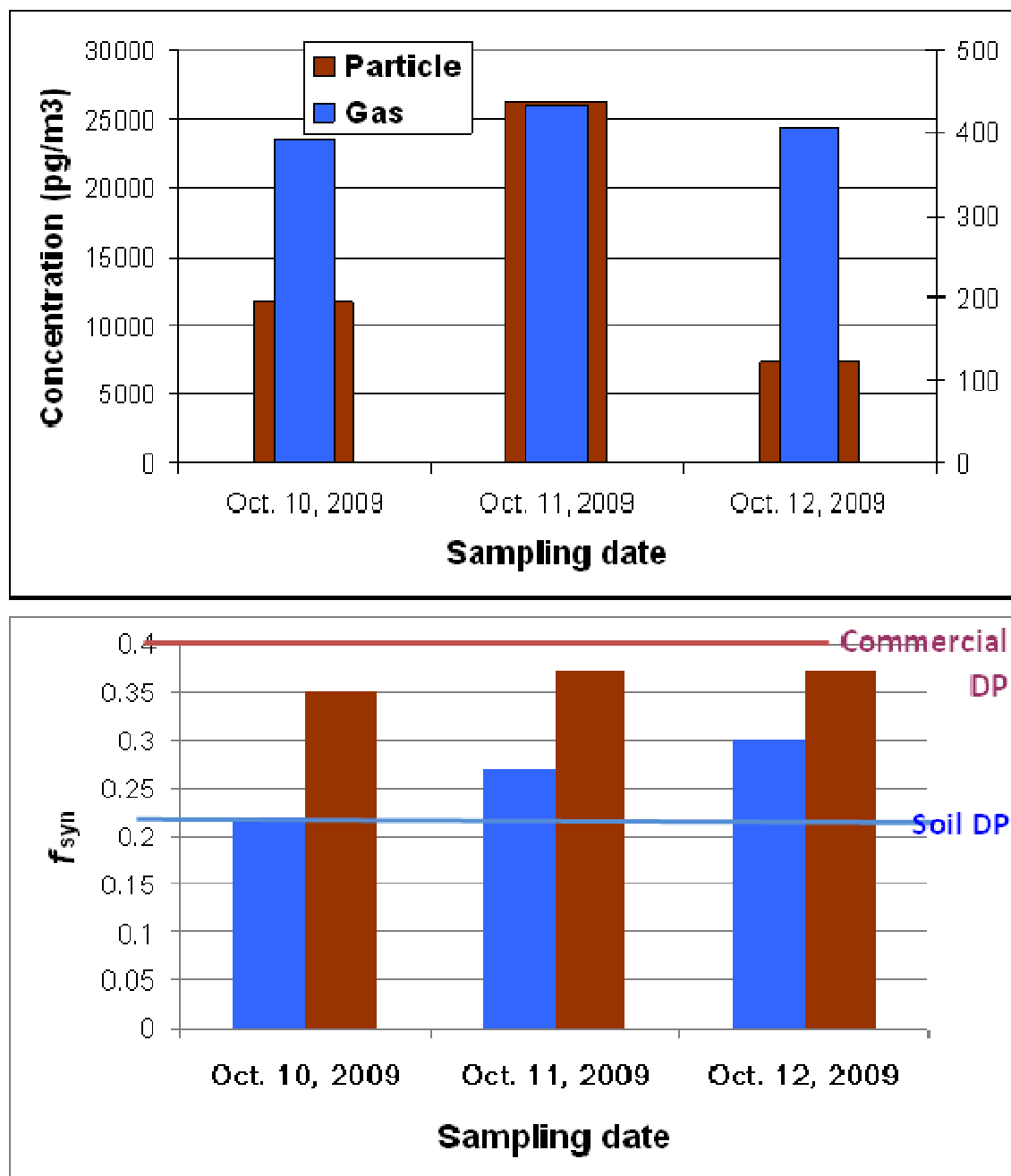
The concentration of DP in the soil sample collected nearest the air sampler was 13,400 ng/g dw (dry weight). By using the above equation, air concentrations of DP in the gas-phase at the equilibrium state were calculated as 430 pg/m³, which is very close to the measured values (390-430 pg/m³) in the same area for the three days.

The fugacity fraction (ff) is used to assess equilibrium status of a chemical between two interacting phases, in this case air and water,

$$ff = C_A / (C_A + K_{AW}C_W) \quad (4)$$

Values of ff equal to 0.5 indicate air–water equilibrium and no net gas exchange. Values < 0.5 indicate net volatilization from water, and values > 0.5 indicate net gaseous deposition to water.

Figure SI-5. Data for the three air samples collected near the DP manufacturing facility for three consecutive days (October 10-12, 2009); from Wang et al., 2010. Concentrations of DP in both gas and particle phases (top panel; particle phase, left axis; gas phase, right axis) and the fractional abundances of the *syn* isomer (bottom panel) are given.



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