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Simulation of Observed PCBs and Pesticides in the Water Column during the North Atlantic Bloom Experiment

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Supporting Information for

Simulation of observed PCBs and pesticides in the water column during the North Atlantic Bloom Experiment.

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SI Tables

Table SI- 1 . Amount of Blanks for PCBs in Air, Water, and Zooplankton Samples. Recoveries for ^{13}C-PCB Surrogates.

Average Blanks (pg)	PCB8	PCB18	PCB28	PCB52	PCB44	PCB66	PCB 101	PCB 118	PCB 153	PCB 138
Air Blanks	76.3	54.1	119.8	138.4	84.4	154.0	185.0	95.3	128.7	97.4
S.D.	14.0	23.9	40.7	98.4	52.5	72.6	32.2	46.9	60.4	55.3
Water Blanks	150.2	93.9	197.1	95.1	51.6	113.3	106.8	35.4	76.9	79.2
S.D.	41.0	33.9	37.0	26.1	19.1	42.3	11.2	10.9	44.8	26.1
Zooplankton Blanks	81.8	59.2	97.3	62.8	31.2	21.8	64.9	34.8	64.8	43.6
S.D.	13.1	12.4	17.7	18.4	22.0	17.7	34.2	15.8	17.7	21.4

Average Recoveries	^{13}C-PCB 8	^{13}C-PCB 28	^{13}C-PCB 52	^{13}C-PCB 118	^{13}C-PCB 138	^{13}C-PCB 180	^{13}C-PCB 209
Air	90%	95%	91%	97%	97%	107%	80%
S.D.	17.0%	19.0%	16.1%	16.2%	16.3%	21.1%	17.1%
Water	79%	82%	81%	83%	84%	86%	85%
S.D.	8%	10%	10%	10%	11%	12%	9%
Zooplankton	70%	87%	79%	84%	84%	89%	66%
S.D.	20%	20%	18%	20%	21%	25%	23%

Table SI- 2 . PCB Concentrations (pg m^{-3}) in the Gas Phase on the Year-day of 2008.

Year-day	PCB 8	PCB 18	PCB 28	PCB 52	PCB 44	PCB 66	PCB 101	PCB 118	PCB 153	PCB 138	Σ_{ICES} PCB
121.5	72.4	25.7	28.5	11.9	7.2	6.1	9.3	3.4	5.4	3.4	61.9
122.0	82.3	25.4	27.1	12.5	7.4	7.9	12.2	4.6	9.2	5.3	70.9
122.5	61.6	17.2	18.1	10.5	5.6	6.8	11.3	4.3	7.7	4.6	56.4
123.0	70.1	20.0	21.0	8.8	5.9	6.3	9.3	3.4	5.9	4.3	52.7
123.5	18.4	7.1	9.0						4.4		14.3
124.0	22.9	7.8	7.4	3.1	1.8	1.8			2.3	1.4	14.2
125.5	18.4	7.6	9.9	7.4	4.1	4.1	6.4	2.1	4.0	2.5	32.4
126.0	6.7	2.6									
126.5	18.3	6.6	6.0								6.0
127.0	26.7	7.6	6.0								6.0
127.5	18.3	5.7	4.9								4.9
128.0	16.9	5.0	4.6								4.6
128.5	11.2	3.8									
129.0	13.0	4.6									
129.5	12.3	4.7									
130.0	14.0	5.0									
130.5	22.5	6.5	5.4								5.4
131.0											
132.0	11.0	4.1	4.6								4.6
135.0	49.5	17.8	23.0	4.4	3.2	2.7					27.4
136.0	25.7	7.7	8.8								8.8
137.0	12.8	5.1	6.3								6.3
138.0	9.1	4.0	4.4								4.4
139.0	8.1	4.7	2.4								2.4
140.0	8.9	3.2	2.6								2.6
141.0	10.6	3.6									
142.0	13.6	4.2									
142.5	10.4	3.1									

Table SI- 3. PCB Concentrations (pg L^{-1}) in the Dissolved Phase on the Year-day of 2008.

Year-day	PCB8	PCB 18	PCB 28	PCB 52	PCB 44	PCB 66	PCB 101	PCB 118	PCB 153	PCB 138	Σ_{ICES} PCB
123.0	0.85	0.44	1.24	1.13	0.51	1.80	1.32	0.18	1.30	0.13	5.29
123.5	0.16	0.32	0.98	0.75	0.38	1.19	0.79	0.21	1.37		4.11
124.0	0.97	0.20	0.23	0.18	0.28	0.25		0.07	0.24		0.72
125.5	0.73	0.20	0.63	0.60	0.21	1.03	0.71	0.24	1.12		3.30
126.0											
126.5											
127.0			0.15	0.32	0.20	1.08	0.62	0.55	0.98		2.62
127.5			0.03	0.89	0.65	2.65	0.40	1.73	2.58		5.64
128.0	0.73	1.27	1.52	0.58	0.61	0.92	0.50	0.68	0.12		3.40
128.5	1.34	0.34									
129.0	0.80	0.25									
129.5	0.98	0.03									
130.0	1.74	0.36						0.37			0.37
130.5	5.36	1.12						0.16			0.16
131.0	1.66	0.68			0.17			0.23	0.35		0.58
132.0	3.17	0.69	0.34								0.34
135.0	11.24	2.44	2.71	0.57	0.26	0.19		0.24	0.04		3.56
136.0	7.10	1.23	1.04					0.09			1.13
137.0	5.73	1.00	0.63	0.31		0.01		0.30	0.21		1.45
138.0	4.23	1.45	0.39								0.39
139.0	3.36	0.72						0.05			0.05
140.0	4.96	0.25	0.22					0.18			0.39
141.0	4.68	0.54	0.23					0.12			0.35
142.0	0.84										
142.5	13.55	1.66						0.12	0.53		0.65

Table SI- 4. Fugacity Ratios for Various PCB Congeners as a Function of Julian Day 2008.

Julian Day	PCB8	PCB 18	PCB 28	PCB 52	PCB 44	PCB 66	PCB 101	PCB 118	PCB 153	PCB 138
123.0	21.69	7.56	3.10	1.58	3.98	0.55	2.40	12.60	1.90	9.03
123.5	29.76	3.66	1.66						1.33	
124.0	5.91	6.09	5.74	3.38	2.11	1.09			3.69	
125.5	5.96	5.69	2.57	2.26	6.01	0.56	2.72	5.08	1.31	
126.0										
126.5										
127.0			7.47							
127.5			30.2							
128.0	5.93	0.64	0.53							
128.5	2.16	1.82								
129.0	4.08	2.84								
129.5	3.31	25.49								
130.0										
130.5	1.10	0.97								
131.0										
132.0	0.89	0.97	2.41							
135.0	1.11	1.16	1.49	1.51	4.12	2.08				
136.0	0.92	1.00	1.49							
137.0	0.56	0.82	1.76							
138.0	0.54	0.44	2.00							
139.0	0.60	1.03								
140.0	0.46	2.05	2.10							
141.0	0.58	1.06								
142.0	4.13									
142.5	0.21	0.32								

Table SI- 5. Air-Water Exchange Velocities (m/d) Calculated Using Three Different Wind Speed Dependency Relationships; Liss and Merlivat 1986 (LM86), Nightingale et al 2000 (N00), and Wanninkhof and McGillis 1999 (WM99).

Velocity (m/d)	PCB 28			PCB 153		
Year-Day	LM86	N00	WM99	LM86	N00	WM99
123.0	0.79	0.90	1.25	0.54	0.60	0.76
123.5	0.90	1.04	1.52	0.61	0.68	0.89
124.0	1.79	2.34	4.01	1.16	1.39	1.94
125.5	1.58	1.99	3.37	1.05	1.24	1.74
126.0	1.22	1.47	2.36	0.81	0.92	1.26
126.5	0.62	0.71	0.92	0.44	0.49	0.59
127.0	0.34	0.46	0.50	0.26	0.33	0.35
127.5	0.14	0.32	0.33	0.11	0.24	0.25
128.0	0.49	0.59	0.69	0.36	0.41	0.47
128.5	0.40	0.51	0.57	0.30	0.36	0.40
129.0	1.09	1.27	1.97	0.73	0.82	1.11
129.5	1.89	2.41	4.11	1.19	1.40	1.92
130.0	0.95	1.10	1.64	0.64	0.71	0.94
130.5	1.21	1.45	2.33	0.80	0.91	1.24
131.0	0.84	0.96	1.36	0.58	0.64	0.82
132.0	0.99	1.14	1.71	0.67	0.74	0.98
135.0	0.67	0.77	1.00	0.47	0.53	0.64
136.0	0.29	0.42	0.45	0.22	0.31	0.33
137.0	0.62	0.71	0.90	0.44	0.49	0.59
138.0	1.19	1.42	2.26	0.80	0.90	1.23
139.0	1.21	1.44	2.30	0.81	0.92	1.26
140.0	1.57	1.98	3.33	1.02	1.20	1.66
141.0	1.41	1.74	2.88	0.92	1.07	1.48
142.0	1.48	1.85	3.09	0.97	1.13	1.57
142.5	1.79	2.30	3.90	1.13	1.34	1.83

Table SI- 6. PCB Concentrations (ng g^{-1}) in the Lipids of Zooplankton on the Year-day of 2008.

Year-day	lipid (%)	PCB8	PCB 18	PCB 28	PCB 52	PCB 44	PCB 66	PCB 101	PCB 118	PCB 153	Σ_{ICES} PCB
131	4.67%		0.84	0.64	1.32	0.59	0.36	1.79		2.52	6.28
135a	3.09%		0.61	0.67	0.38	0.15	0.19		0.25	0.67	1.98
135b	4.97%	0.12	0.08	0.14	0.28	0.21	0.59	0.50	0.20	0.60	1.73
135c	1.72%	0.28	0.32	0.81			0.44			0.74	1.55
136	4.83%	0.11	0.27	0.24					0.10	0.10	0.45
137a	6.15%	0.16	0.61	0.72	0.40	0.48	0.46	0.29	0.22	0.62	2.26
137b	2.86%	0.64	0.61	1.64	0.63	0.29	0.80	0.64	0.58	0.77	4.26
138a	6.45%	0.86	0.45	0.57	0.26	0.13	0.22	0.21	0.16	0.25	1.44
138b	3.17%	0.58	0.71	1.15	0.84	0.37	1.01	0.71	0.70	1.05	4.45
139	2.24%	0.24	0.72	0.87	0.78	0.31	0.87	0.81	0.59	1.21	4.25
140a	4.83%	0.97	0.57	0.50	0.16	0.18	0.15		0.11	0.48	1.25

Table SI- 7. Physiochemical Properties of Various PCBs and OCPs (Schenker et al 2005)

	PCB 3	PCB 8	PCB 18	PCB 28	PCB 52	PCB 44	PCB 66	PCB 101	PCB 118	PCB 153	PCB 138	PCB 180
Log K_{OW}	4.71	5.29	5.42	5.92	6.26	6.02	6.56	6.76	7.08	7.31	7.7	7.66
ΔU_{OW}	-15	-19.0		-27	-27.5			-19	-25	-27	-22	-26
Log K_{AW}	-2.06	-2.06	-1.89	-1.94	-1.96	-2.15	-1.83	-2.08	-2.36	-2.13	-1.97	-2.51
ΔU_{AW}	52.9	54.9	52.4	51.8	53.8	58.1	55.3	65.2	65.2	68.2	64.7	69.0

	α-HCH	β-HCH	γ-HCH	HCB	HEPX	TC	CC	p,p'-DDE
Log K_{OW}	3.88	3.91	3.76	5.61	5.4	6.27	6.19	6.94
ΔU_{OW}	-5.2	-16	-9.6	-24				
Log K_{OA}	7.48	8.74	7.72	7.12	8.62	8.82	8.84	9.7
ΔU_{OA}	-62	-84	-64	-76				
Log K_{AW}	-3.6	-4.8	-4	-1.5	-3.22	-2.5	-2.7	-2.8
ΔU_{AW}	56.9	67.9	54.3	51.9	31.7	29.2	34.2	39.1
Log S_A	-4	-4.7	-4.5	-4.4	-5.09	-5.4	-5.5	-5.9
Log S_W	-0.5	0.16	-0.6	-2.9	-1.86	-2.82	-2.88	-3.10
Log S_O	3.44	4.07	3.18	2.73	3.54	3.31	3.70	3.84

Table SI- 8. K_{lipid} for different PCB congeners. Regression Slopes, Intercepts, R-Squares for log K_{lipid} vs log K_{ow}.

Year-day	PCB 8	PCB 18	PCB 28	PCB 52	PCB 44	PCB 66	PCB 118	PCB 153	Slope	inter-cept	R square
131		6.09			6.55			6.86	0.38	4.04	0.92
135a		5.39	5.39	5.83	5.77	5.99	6.03	7.21	0.79	0.74	0.74
135b	4.04	4.51	4.72	5.69	5.92	6.49	5.93	7.16	1.29	-2.82	0.82
135c	4.40	5.11	5.47			6.36		7.25	1.26	-2.29	0.97
136	4.21	5.34	5.37				6.05		0.77	0.51	0.70
137a	4.45	5.78	6.06	6.11		7.49	5.87	6.46	0.69	1.54	0.37
137b	5.05	5.79	6.42	6.30		7.73	6.29	6.56	0.64	2.16	0.39
138a	5.31	5.50	6.16						1.22	-1.35	1.00
138b	5.13	5.69	6.47						1.78	-4.52	0.96
139	4.86	6.00					7.06		0.97	0.04	0.80
140a	4.69	6.46	6.60				6.53		0.62	2.28	0.31

Table SI- 9 Summary of Sampling Information for Air and Water Samples Collected

Julian day	Latitude	Longitude	Air volume (m^3)	Water volume (L)	Sample Date	Start Time (GMT)	End Time (GMT)	Air Temp (°C)	Water Temp (°C)
121.5	64.1	-21.9	542		4/30/2008	19:45	8:30	4.02	
122.0	64.1	-21.9	538	N/A	5/1/2008	8:50	20:30	6.46	N/A
122.5	64.2	-22.0	495		5/1/2008	20:50	9:05	4.41	
123.0	62.1	-24.6	520	760	5/2/2008	9:20	21:00	7.06	9.28
123.5	60.9	-25.4	549	709	5/2/2008	21:50	8:30	8.36	9.43
124.0	58.7	-25.8	1294	1189	5/3/~5/4/2008	9:25	17:05	8.97	9.93
125.5	60.9	-26.7	922	759	5/4/~5/5/2008	18:10	13:10	8.97	10.62
126.0	60.8	-27.1	364	726	5/5/2008	13:45	21:49	8.99	9.44
126.5	60.9	-27.2	509	796	5/5/5008	22:40	09:03	8.34	9.31
127.0	60.9	-27.4	512	960	5/6/2008	09:43	20:35	7.93	9.22
127.5	60.8	-27.5	510	567	5/6-5/7/2008	20:59	08:38	8.39	9.42
128.0	61.2	-26.5	541	931	5/7/2008	09:03	20:25	9.12	9.61
128.5	61.1	-26.7	572	518	5/7-5/8/2008	20:44	09:25	8.93	9.55
129.0	61.1	-25.7	505	920	5/8/2008	09:50	21:13	8.90	9.92
129.5	61.1	-26.7	499	639	5/8-5/9/2008	21:31	10:37	7.81	9.22
130.0	60.9	-27.6	447	643	5/9/2008	11:01	21:05	8.79	9.26
130.5	60.6	-27.6	473	539	5/9-5/10/2008	21:45	11:22	7.97	9.30
131.0	61.3	-26.6	462	788	5/10/2008	11:22	21:41	8.62	9.62
132.0	61.5	-26.0	941	1015	5/10-5/11/2008	22:10	19:35	9.39	9.64
135.0	61.2	-26.3	899	871	5/14-5/15/2008	12:52	12:29	8.15	9.84
136.0	61.3	-26.3	815	1029	5/15-5/16/2008	12:53	13:01	8.02	9.78
137.0	61.5	-26.0	623	952	5/16-5/17/2008	16:40	16:50	8.58	9.81
138.0	61.5	-26.1	894	816	5/17-5/18/2008	17:15	15:28	8.88	9.85
139.0	61.2	-25.5	1145	755	5/18-5/19/2008	16:49	20:00	8.81	10.06
140.0	61.2	-25.7	1152	707	5/19-5/20/2008	20:28	20:03	9.16	9.75
141.0	61.5	-25.8	642	770	5/20-5/21/2008	20:25	11:03	9.02	9.70
142.0	61.4	-25.5	467	569	5/21/2008	11:28	22:37	9.31	9.73
142.5	62.8	-24.7	548	237	5/21-5/22/2008	22:58	11:16	8.10	9.05

SI Figures

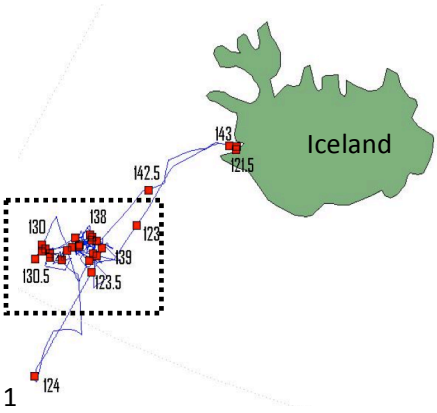

Figure SI- 1. Sampling Location. Blue lines are the ship track of R/V Knorr. Numbers are Year-day of 2008. Dashline denotes a 2°X2° box for the Eulerian model.

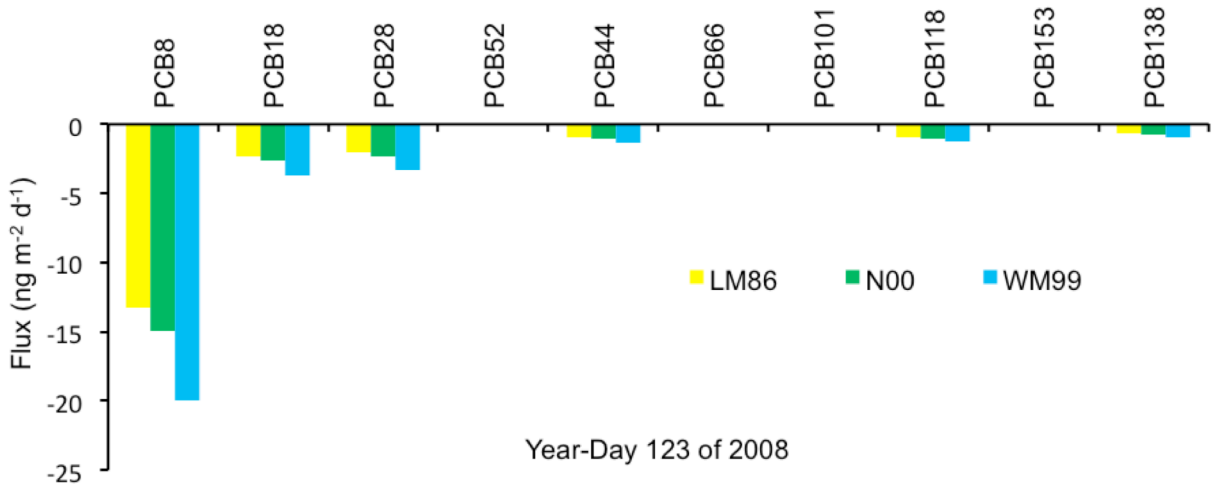

Figure SI-2. Air-Water Exchange Fluxes (ng m^{-2} d^{-1}) of Different PCB Congeners Calculated Using Three Different Relationships on Year-Day 123 of 2008.

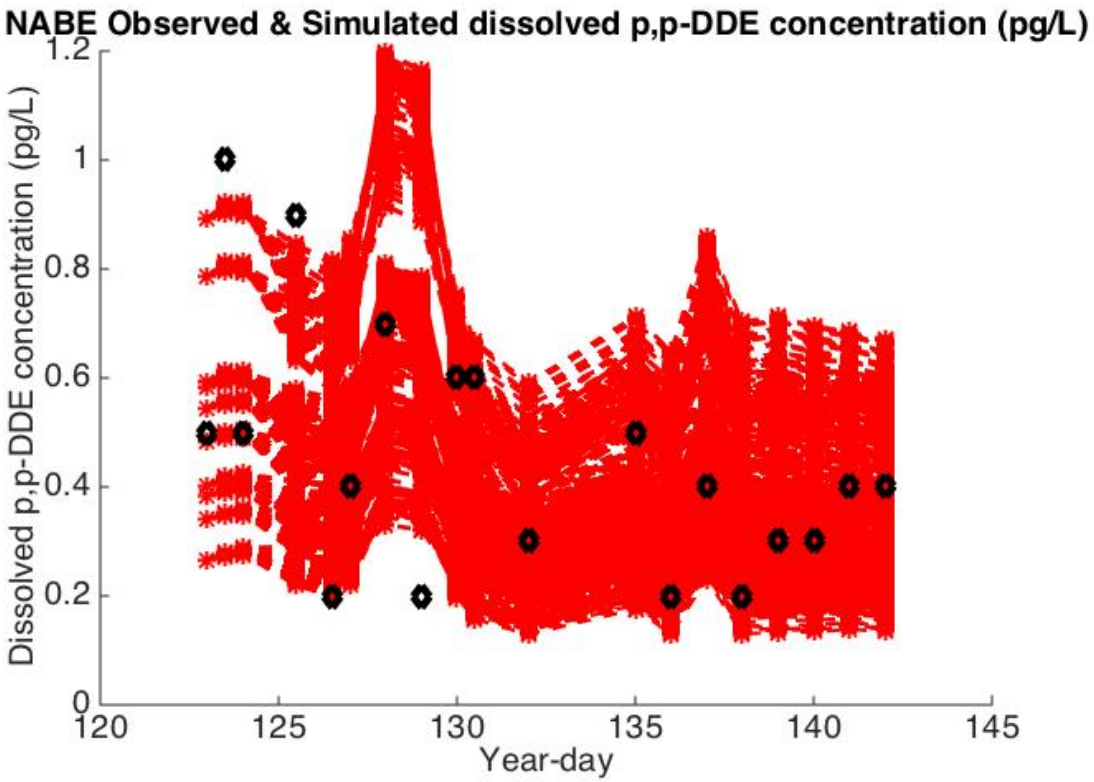

Figure SI-3, 10,000 Monte-Carlo simulation curves (red) by varying initial dissolved p,p'-DDE concentrations, air-water exchange coefficients (K_{AW}), organic carbon-water partitioning coefficients(K_{OA}), chemical degradation constants (k_deg) 10 times each following normal distribution. Observed dissolved concentrations (black) were plotted to compare with simulations.

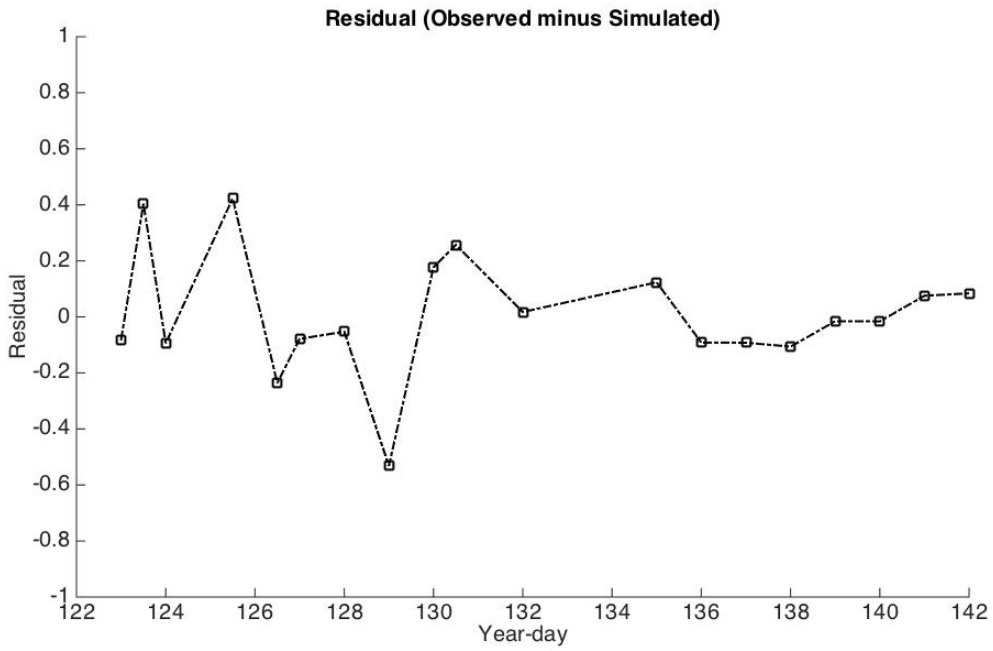

Figure SI-4 Residual (observations minus simulation) plot for dissolved p'p-DDE.

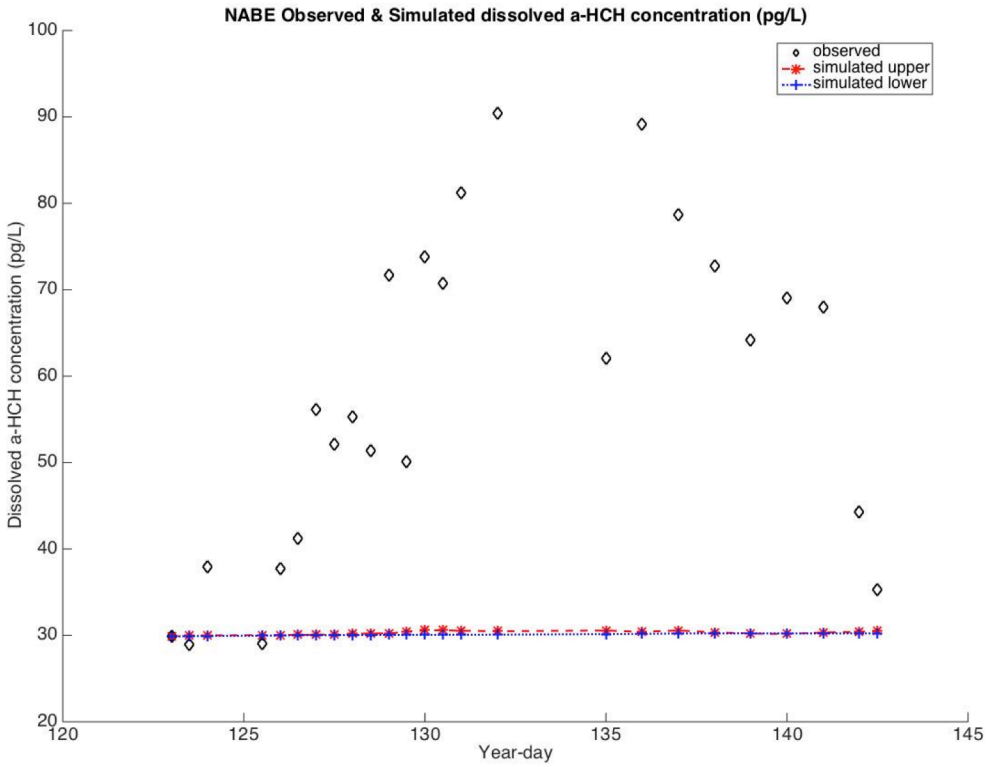

Figure SI- 5. Comparison of Modeled and Observed α-HCH Dissolved Phase Concentrations (pg L^{-1}) as a Function of Year-day 2008.